# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:40 PM UTC

| | | |
|---|---|---|
| PDB ID | : | 6ND5 / pdb_00006nd5 |
| Title | : | Crystal structure of the Thermus thermophilus 70S ribosome in complex with chloramphenicol and bound to mRNA and A-, P-, and E-site tRNAs at 2.60A resolution |
| Authors | : | Svetlov, M.S.; Plessa, E.; Chen, C.-W.; Bougas, A.; Krokidis, M.G.; Dinos, G.P.; Polikanov, Y.S. |
| Deposited on | : | 2018-12-13 |
| Resolution | : | 2.60 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

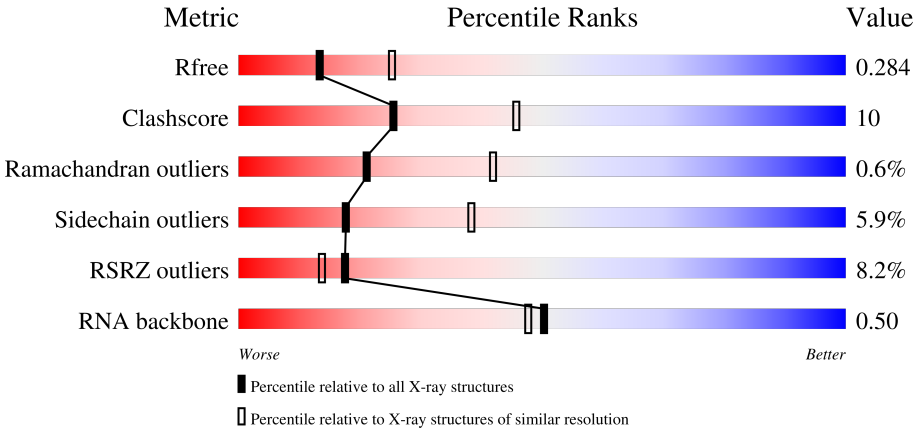
| | | |
|---|---|---|
| MolProbity | : | 4-5-2 with Phenix2.0 |
| Mogul | : | 2022.3.0, CSD as543be (2022) |
| Xtriage (Phenix) | : | 2.0 |
| EDS | : | 3.0 |
| Buster-report | : | wwPDB partial adaption of 1.1.7 (2018) |
| Percentile statistics | : | 20250101.v01 (using entries in the PDB archive January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

# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 Å.

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




| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|---|---|---|
| $R_{free}$ | 180053 | 4008 (2.60-2.60) |
| Clashscore | 190562 | 4347 (2.60-2.60) |
| Ramachandran outliers | 187476 | 4277 (2.60-2.60) |
| Sidechain outliers | 187428 | 4277 (2.60-2.60) |
| RSRZ outliers | 180081 | 4008 (2.60-2.60) |
| RNA backbone | 3983 | 1014 (2.84-2.36) |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | 1A | 2915 | 3% 61% 31% 7% |
| 1 | 2A | 2915 | 3% 54% 35% 7% |
| 2 | 1B | 121 | 71% 24% |
| 2 | 2B | 121 | 7% 44% 44% 12% |

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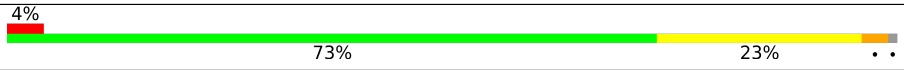
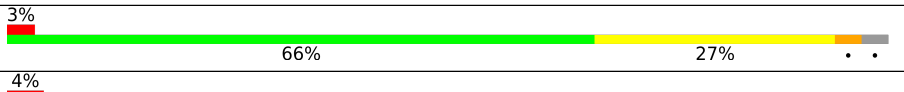
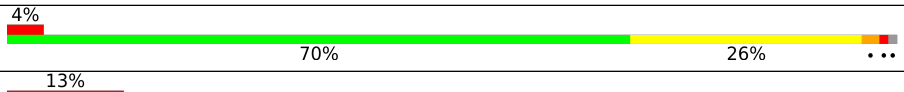
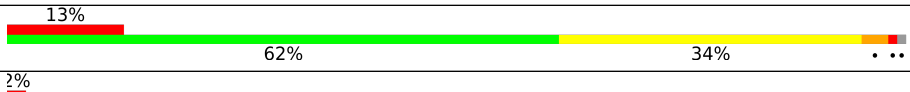
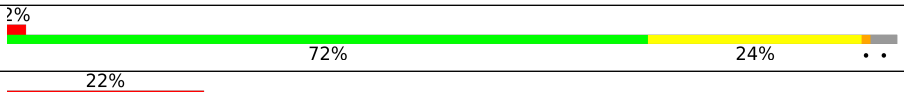
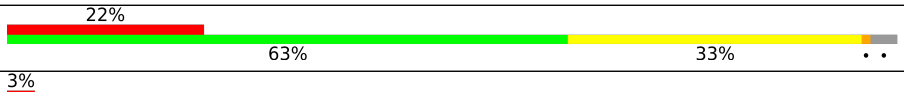
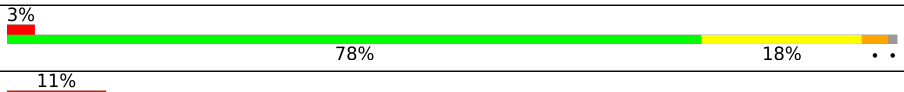
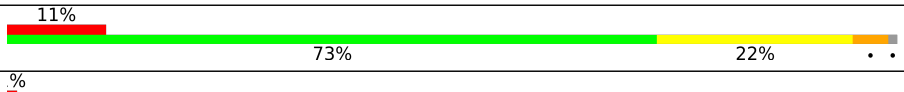
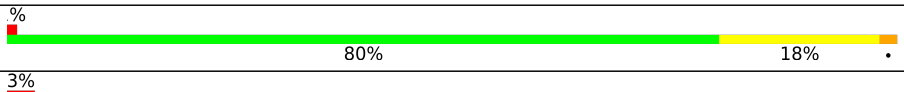
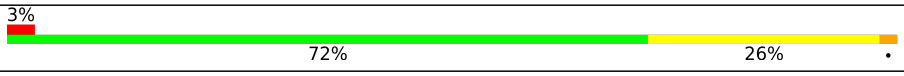
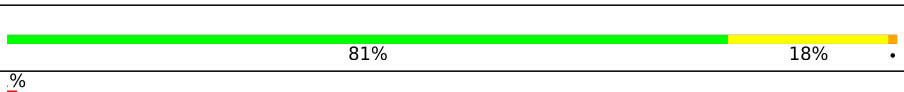
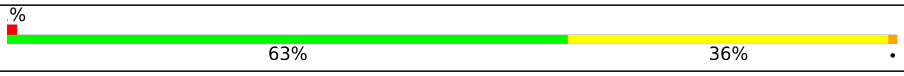
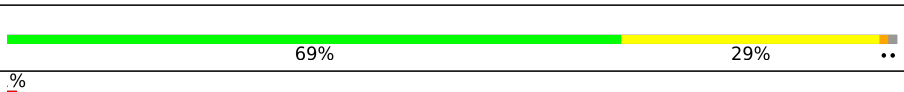
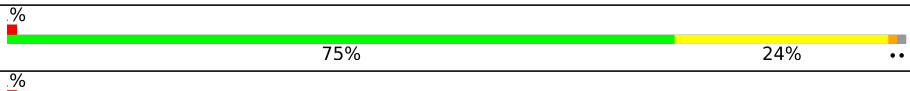
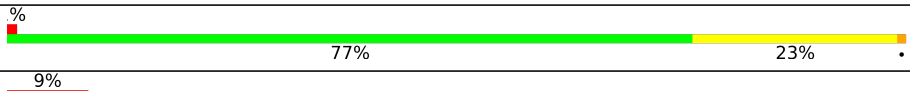
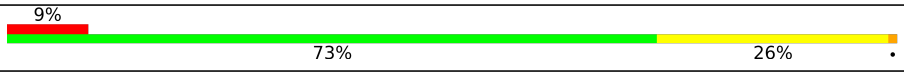
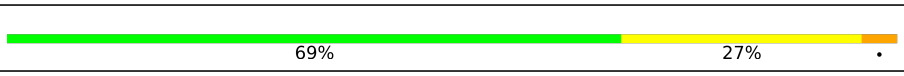
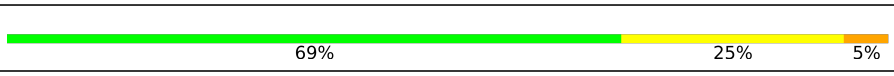
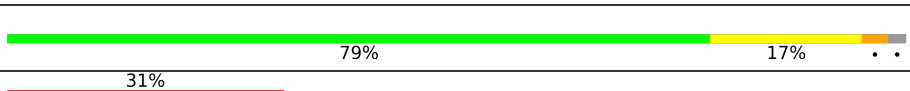
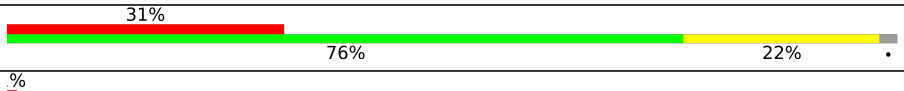
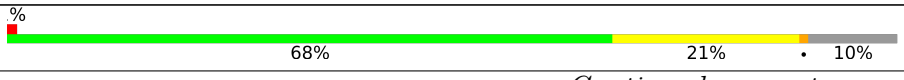
| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 3 | 1D | 276 | |
| 3 | 2D | 276 | |
| 4 | 1E | 206 | |
| 4 | 2E | 206 |   |
| 5 | 1F | 210 | |
| 5 | 2F | 210 |   |
| 6 | 1G | 182 |   |
| 6 | 2G | 182 |   |
| 7 | 1H | 180 |   |
| 7 | 2H | 180 |   |
| 8 | 1I | 148 |   |
| 8 | 2I | 148 |   |
| 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 |   |
| 15 | 1T | 146 |   |

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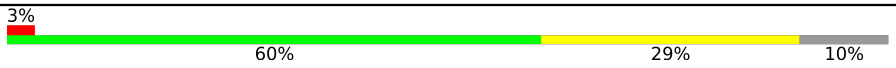
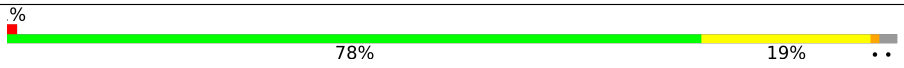
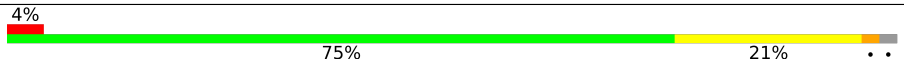
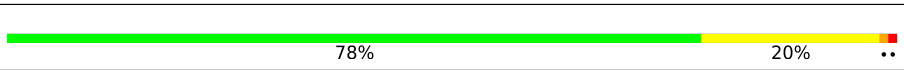
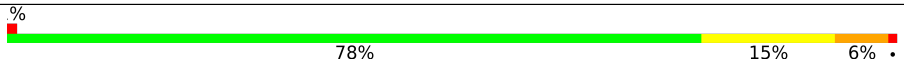
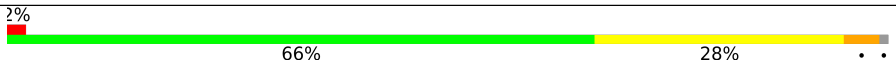
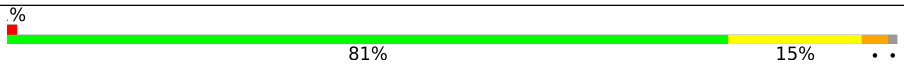
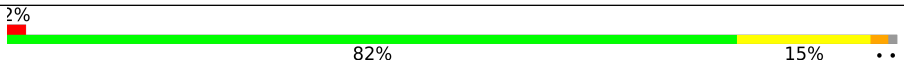
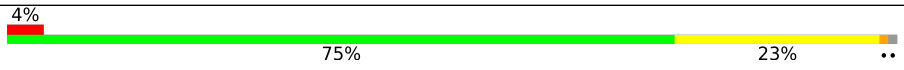
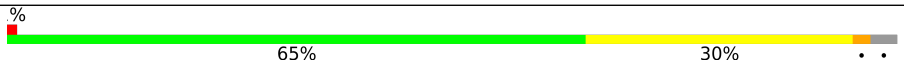
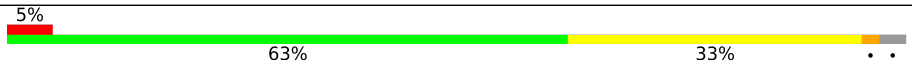
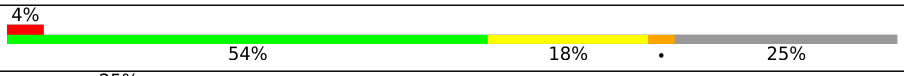
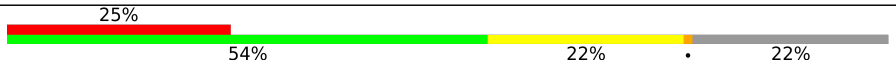
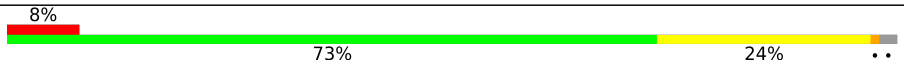
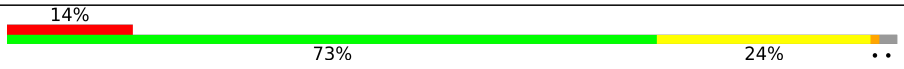
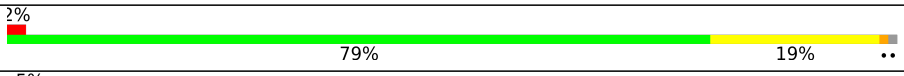
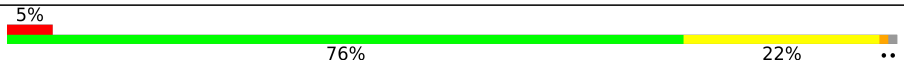
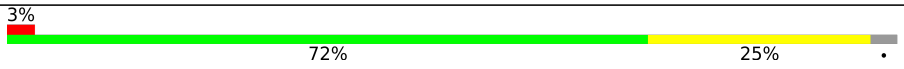
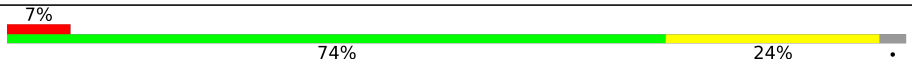
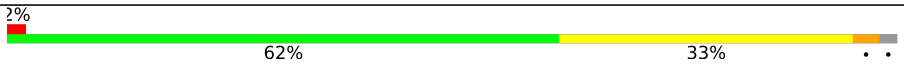
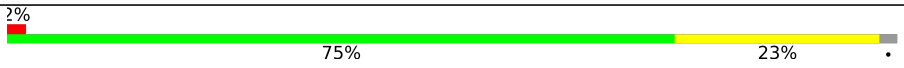
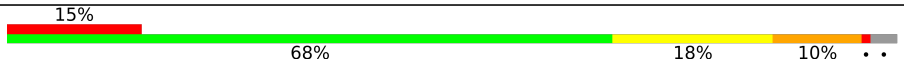
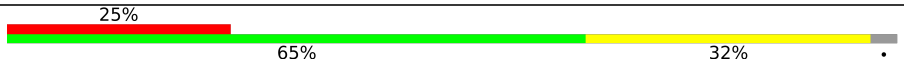
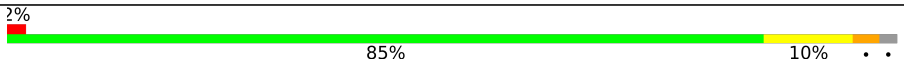
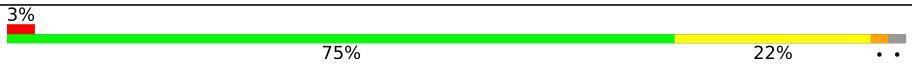
| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 15 | 2T | 146 |   |
| 16 | 1U | 118 |   |
| 16 | 2U | 118 |   |
| 17 | 1V | 101 |   |
| 17 | 2V | 101 |   |
| 18 | 1W | 113 |   |
| 18 | 2W | 113 |   |
| 19 | 1X | 96 |   |
| 19 | 2X | 96 |   |
| 20 | 1Y | 110 |   |
| 20 | 2Y | 110 |   |
| 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 |   |
| 27 | 25 | 60 |   |

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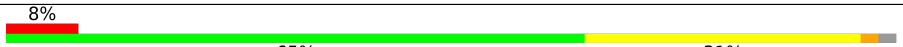
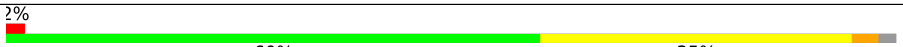
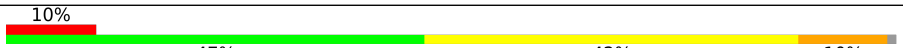
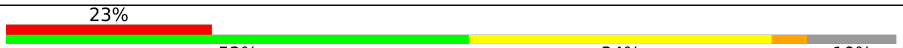
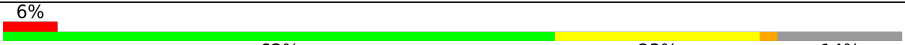
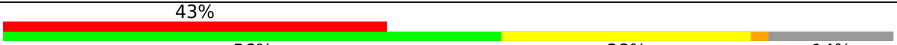
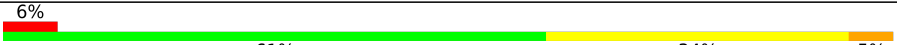
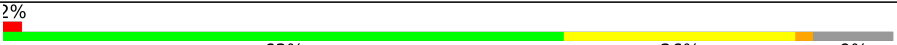
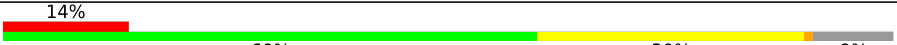
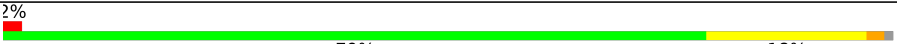
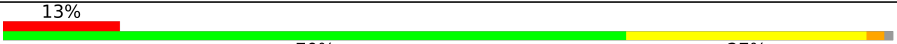
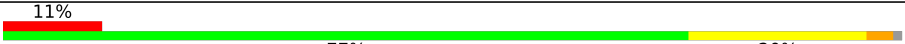
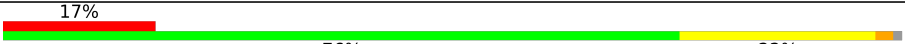
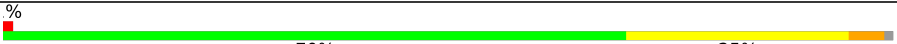
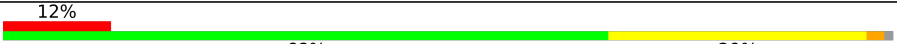
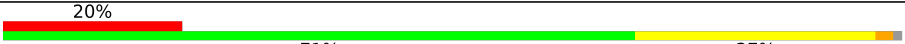
| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 28 | 16 | 54 | |
| 28 | 26 | 54 | |
| 29 | 17 | 49 | |
| 29 | 27 | 49 |   |
| 30 | 18 | 65 |   |
| 30 | 28 | 65 | |
| 31 | 19 | 37 | |
| 31 | 29 | 37 | |
| 32 | 1a | 1521 | |
| 32 | 2a | 1521 |   |
| 33 | 1b | 256 | |
| 33 | 2b | 256 |   |
| 34 | 1c | 239 |   |
| 34 | 2c | 239 |   |
| 35 | 1d | 209 | |
| 35 | 2d | 209 |   |
| 36 | 1e | 162 |   |
| 36 | 2e | 162 |   |
| 37 | 1f | 101 |   |
| 37 | 2f | 101 |   |
| 38 | 1g | 156 |   |
| 38 | 2g | 156 |   |
| 39 | 1h | 138 |   |
| 39 | 2h | 138 |   |
| 40 | 1i | 128 |   |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 40 | 2i | 128 | 52% 58% 38% |
| 41 | 1j | 105 | 21% 57% 32% 8% |
| 41 | 2j | 105 | 70% 51% 35% 5% 9% |
| 42 | 1k | 129 | 3% 74% 13% 12% |
| 42 | 2k | 129 | 15% 69% 18% 12% |
| 43 | 1l | 132 | 8% 68% 23% 8% |
| 43 | 2l | 132 | 18% 67% 22% 8% |
| 44 | 1m | 126 | 8% 74% 23% |
| 44 | 2m | 126 | 37% 60% 35% |
| 45 | 1n | 61 | 13% 61% 34% |
| 45 | 2n | 61 | 72% 52% 41% 5% |
| 46 | 1o | 89 | 6% 70% 29% |
| 46 | 2o | 89 | 17% 71% 27% |
| 47 | 1p | 88 | 14% 66% 26% 7% |
| 47 | 2p | 88 | 7% 61% 32% 7% |
| 48 | 1q | 105 | 15% 68% 25% 6% |
| 48 | 2q | 105 | 8% 68% 26% 6% |
| 49 | 1r | 88 | 7% 55% 23% 23% |
| 49 | 2r | 88 | 3% 43% 31% 23% |
| 50 | 1s | 93 | 10% 55% 34% 11% |
| 50 | 2s | 93 | 62% 55% 33% 11% |
| 51 | 1t | 106 | 8% 71% 17% 9% |
| 51 | 2t | 106 | 16% 58% 30% 9% |
| 52 | 1u | 27 | 15% 63% 22% 15% |
| 52 | 2u | 27 | 44% 48% 37% 15% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 53 | 1v | 24 | 4% 38% 12% 46% |
| 53 | 2v | 24 | 33% 29% 12% 12% 46% |
| 54 | 1w | 76 | 20% 36% 34% 26% |
| 54 | 1y | 76 | 4% 42% 37% 16% |
| 54 | 2w | 76 | 30% 25% 46% 24% 5% |
| 54 | 2y | 76 | 13% 39% 37% 18% |
| 55 | 1x | 77 | 4% 64% 27% 8% |
| 55 | 2x | 77 | 3% 44% 44% 10% |

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 |
|---|---|---|---|---|---|---|---|
| 60 | SF4 | 1d | 302 | - | - | X | - |
| 60 | SF4 | 2d | 302 | - | - | X | - |

# 2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 300833 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 53 is a RNA chain called mRNA.

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

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

| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 54 | 1w | 74 | Total | C | N | O | P | S | 0 | 0 | 0 |
| | | | 1592 | 713 | 285 | 518 | 74 | 2 | | | |
| 54 | 1y | 74 | Total | C | N | O | P | S | 0 | 0 | 0 |
| | | | 1585 | 707 | 285 | 518 | 74 | 1 | | | |
| 54 | 2w | 72 | Total | C | N | O | P | S | 0 | 0 | 0 |
| | | | 1544 | 690 | 278 | 502 | 72 | 2 | | | |
| 54 | 2y | 73 | Total | C | N | O | P | S | 0 | 0 | 0 |
| | | | 1565 | 698 | 283 | 510 | 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 | 0 |
| | | | 1625 | 725 | 294 | 529 | 76 | 1 | | | |
| 55 | 2x | 76 | Total | C | N | O | P | S | 0 | 0 | 0 |
| | | | 1625 | 725 | 294 | 529 | 76 | 1 | | | |

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

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|
| 56 | 1A | 1101 | Total | Mg | 0 | 0 |
| | | | 1101 | 1101 | | |
| 56 | 1B | 39 | Total | Mg | 0 | 0 |
| | | | 39 | 39 | | |
| 56 | 1D | 13 | Total | Mg | 0 | 0 |
| | | | 13 | 13 | | |
| 56 | 1E | 15 | Total | Mg | 0 | 0 |
| | | | 15 | 15 | | |
| 56 | 1F | 10 | Total | Mg | 0 | 0 |
| | | | 10 | 10 | | |
| 56 | 1G | 4 | Total | Mg | 0 | 0 |
| | | | 4 | 4 | | |
| 56 | 1I | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 56 | 1N | 6 | Total | Mg | 0 | 0 |
| | | | 6 | 6 | | |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 56 | 1O | 5 | Total Mg<br>5 5 | 0 | 0 |
| 56 | 1P | 9 | Total Mg<br>9 9 | 0 | 0 |
| 56 | 1Q | 8 | Total Mg<br>8 8 | 0 | 0 |
| 56 | 1R | 3 | Total Mg<br>3 3 | 0 | 0 |
| 56 | 1S | 3 | Total Mg<br>3 3 | 0 | 0 |
| 56 | 1T | 4 | Total Mg<br>4 4 | 0 | 0 |
| 56 | 1U | 12 | Total Mg<br>12 12 | 0 | 0 |
| 56 | 1V | 7 | Total Mg<br>7 7 | 0 | 0 |
| 56 | 1W | 5 | Total Mg<br>5 5 | 0 | 0 |
| 56 | 1X | 5 | Total Mg<br>5 5 | 0 | 0 |
| 56 | 1Y | 3 | Total Mg<br>3 3 | 0 | 0 |
| 56 | 1Z | 3 | Total Mg<br>3 3 | 0 | 0 |
| 56 | 10 | 6 | Total Mg<br>6 6 | 0 | 0 |
| 56 | 11 | 5 | Total Mg<br>5 5 | 0 | 0 |
| 56 | 12 | 2 | Total Mg<br>2 2 | 0 | 0 |
| 56 | 13 | 3 | Total Mg<br>3 3 | 0 | 0 |
| 56 | 14 | 1 | Total Mg<br>1 1 | 0 | 0 |
| 56 | 15 | 5 | Total Mg<br>5 5 | 0 | 0 |
| 56 | 16 | 3 | Total Mg<br>3 3 | 0 | 0 |
| 56 | 17 | 8 | Total Mg<br>8 8 | 0 | 0 |
| 56 | 18 | 7 | Total Mg<br>7 7 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 56 | 19 | 1 | Total Mg<br>1 1 | 0 | 0 |
| 56 | 1a | 233 | Total Mg<br>233 233 | 0 | 0 |
| 56 | 1b | 2 | Total Mg<br>2 2 | 0 | 0 |
| 56 | 1d | 1 | Total Mg<br>1 1 | 0 | 0 |
| 56 | 1e | 2 | Total Mg<br>2 2 | 0 | 0 |
| 56 | 1f | 2 | Total Mg<br>2 2 | 0 | 0 |
| 56 | 1h | 1 | Total Mg<br>1 1 | 0 | 0 |
| 56 | 1l | 2 | Total Mg<br>2 2 | 0 | 0 |
| 56 | 1m | 2 | Total Mg<br>2 2 | 0 | 0 |
| 56 | 1n | 1 | Total Mg<br>1 1 | 0 | 0 |
| 56 | 1s | 1 | Total Mg<br>1 1 | 0 | 0 |
| 56 | 1t | 1 | Total Mg<br>1 1 | 0 | 0 |
| 56 | 1v | 1 | Total Mg<br>1 1 | 0 | 0 |
| 56 | 1w | 12 | Total Mg<br>12 12 | 0 | 0 |
| 56 | 1x | 18 | Total Mg<br>18 18 | 0 | 0 |
| 56 | 2A | 887 | Total Mg<br>887 887 | 0 | 0 |
| 56 | 2B | 20 | Total Mg<br>20 20 | 0 | 0 |
| 56 | 2D | 10 | Total Mg<br>10 10 | 0 | 0 |
| 56 | 2E | 4 | Total Mg<br>4 4 | 0 | 0 |
| 56 | 2F | 6 | Total Mg<br>6 6 | 0 | 0 |
| 56 | 2G | 1 | Total Mg<br>1 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 56 | 2N | 1 | Total Mg<br>1 1 | 0 | 0 |
| 56 | 2O | 1 | Total Mg<br>1 1 | 0 | 0 |
| 56 | 2P | 4 | Total Mg<br>4 4 | 0 | 0 |
| 56 | 2Q | 4 | Total Mg<br>4 4 | 0 | 0 |
| 56 | 2R | 2 | Total Mg<br>2 2 | 0 | 0 |
| 56 | 2T | 4 | Total Mg<br>4 4 | 0 | 0 |
| 56 | 2U | 3 | Total Mg<br>3 3 | 0 | 0 |
| 56 | 2V | 3 | Total Mg<br>3 3 | 0 | 0 |
| 56 | 2W | 3 | Total Mg<br>3 3 | 0 | 0 |
| 56 | 2X | 1 | Total Mg<br>1 1 | 0 | 0 |
| 56 | 2Z | 1 | Total Mg<br>1 1 | 0 | 0 |
| 56 | 20 | 3 | Total Mg<br>3 3 | 0 | 0 |
| 56 | 21 | 1 | Total Mg<br>1 1 | 0 | 0 |
| 56 | 23 | 3 | Total Mg<br>3 3 | 0 | 0 |
| 56 | 25 | 5 | Total Mg<br>5 5 | 0 | 0 |
| 56 | 27 | 2 | Total Mg<br>2 2 | 0 | 0 |
| 56 | 28 | 3 | Total Mg<br>3 3 | 0 | 0 |
| 56 | 2a | 241 | Total Mg<br>241 241 | 0 | 0 |
| 56 | 2d | 1 | Total Mg<br>1 1 | 0 | 0 |
| 56 | 2e | 1 | Total Mg<br>1 1 | 0 | 0 |
| 56 | 2f | 2 | Total Mg<br>2 2 | 0 | 0 |

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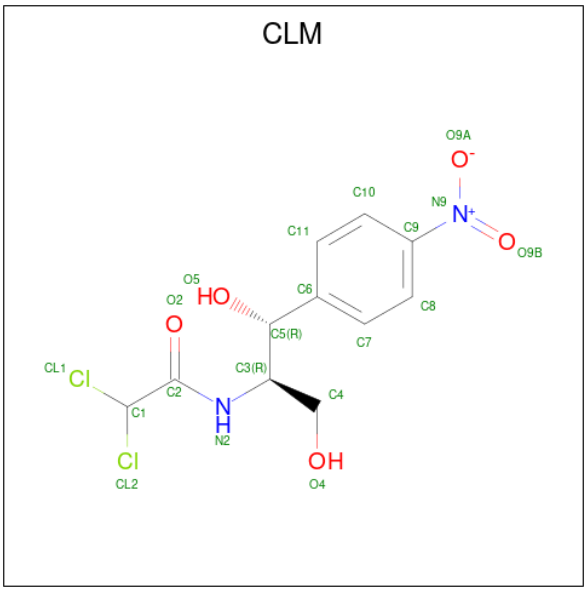
| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 56 | 2g | 1 | Total Mg<br>1 1 | 0 | 0 |
| 56 | 2i | 1 | Total Mg<br>1 1 | 0 | 0 |
| 56 | 2j | 1 | Total Mg<br>1 1 | 0 | 0 |
| 56 | 2k | 1 | Total Mg<br>1 1 | 0 | 0 |
| 56 | 2l | 4 | Total Mg<br>4 4 | 0 | 0 |
| 56 | 2m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

- Molecule 57 is CHLORAMPHENICOL (CCD ID: CLM) (formula: $C_{11}H_{12}Cl_2N_2O_5$).




| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|---|---|
| 57 | 1A | 1 | Total | C | Cl | N | O | 0 | 0 |
| | | | 20 | 11 | 2 | 2 | 5 | | |
| 57 | 2A | 1 | Total | C | Cl | N | O | 0 | 0 |
| | | | 20 | 11 | 2 | 2 | 5 | | |

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

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|
| 59 | 1Y | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 59 | 14 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 59 | 15 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 59 | 16 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 59 | 19 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |

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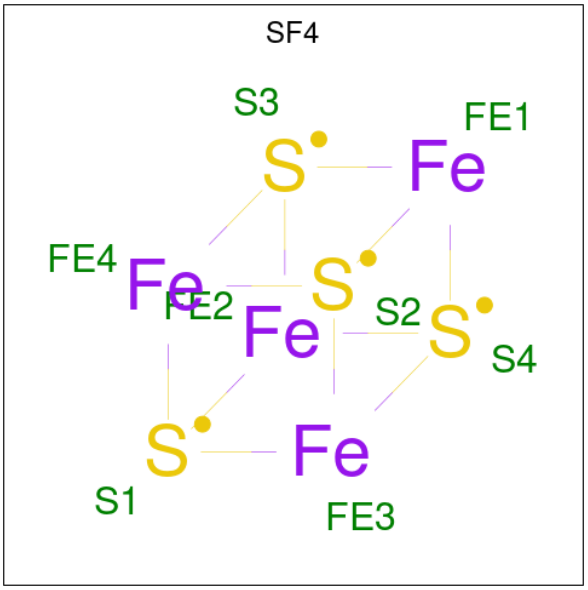
| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 59 | 1n | 1 | Total Zn<br>1 1 | 0 | 0 |
| 59 | 2Y | 1 | Total Zn<br>1 1 | 0 | 0 |
| 59 | 24 | 1 | Total Zn<br>1 1 | 0 | 0 |
| 59 | 25 | 1 | Total Zn<br>1 1 | 0 | 0 |
| 59 | 26 | 1 | Total Zn<br>1 1 | 0 | 0 |
| 59 | 29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

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




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

- Molecule 61 is water.

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 61 | 1A | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 1A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 1A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 1A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 1A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 1A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 1A | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 1A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 1A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 1A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 1A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 1A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 1A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 1A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 1A | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 1A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 1A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1A | 5 | Total O<br>5 5 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 61 | 1A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 1A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 1A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 1A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 1A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 1A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 1A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 1A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 1A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 1A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 1A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 1A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 1A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 1A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 1A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 1A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 1A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 1A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 1A | 2 | Total O<br>2 2 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 61 | 1A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 1A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 1A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1A | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 1A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 1A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 1A | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 1A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 1A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 1A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 1A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 1A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 1A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 1A | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 1A | 4 | Total O<br>4 4 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 61 | 1A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 1A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 1A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 1A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 1A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 1A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 1A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 1A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 1A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 1A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 1A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 1A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 1A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 1A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 1A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 1A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 1A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 1A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 1A | 1 | Total O<br>1 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 61 | 1A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 1A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 1A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 1A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 1A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 1A | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 1A | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 1A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 1A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 1A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 1A | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 1A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 1A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 1A | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 1A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1A | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 1A | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 1A | 1 | Total O<br>1 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 61 | 1A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 1A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 1A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 1A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 1A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 1A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 1A | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 1A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1A | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 1A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 1A | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 1A | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 1A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 1A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 1A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 1A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 1A | 3 | Total O<br>3 3 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 61 | 1A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 1A | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 1A | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 1A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 1A | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 1A | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 1A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 1A | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 1A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 1A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 1A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 1A | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 1A | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 1A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 1A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 1A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 1A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 1A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 1A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 1A | 1 | Total O<br>1 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 61 | 1A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 1A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 1A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 1A | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 1A | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 1A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 1A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 1A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 1A | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 1A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 1A | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 1A | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 1A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 1A | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 1A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 1A | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 1A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 1A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 1A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 1A | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 1A | 5 | Total O<br>5 5 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 61 | 1A | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 1A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 1A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 1A | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 1A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 1A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 1A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 1A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 1A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 1A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 1A | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 1A | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 1A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 1A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 1A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 1A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 1A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 1A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 1A | 2 | Total O<br>2 2 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 61 | 1A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 1A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 1A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 1A | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 1A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 1A | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 1A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 1A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 1A | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 1A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 1A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 1A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 1A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 1A | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 1A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 1A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1A | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 1A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1A | 5 | Total O<br>5 5 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 61 | 1A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1A | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 1A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 1A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 1A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 1A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 1A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1A | 2 | Total O<br>2 2 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 61 | 1A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 1A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 1A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1A | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 1A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 1A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1A | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 1A | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 1A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 1A | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 1A | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 1A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 1A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 1A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 1A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 1A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 1A | 3 | Total O<br>3 3 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 61 | 1A | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 1A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 1A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 1A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 1A | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 1A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 1A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 1A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 1A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 1A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 1A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1A | 1 | Total O<br>1 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 61 | 1A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 1A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 1A | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 1A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1A | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 1A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 1A | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 1A | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 1A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1A | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 1A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 1A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 1A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 1A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 1A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 1A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 1A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 1A | 1 | Total O<br>1 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 61 | 1A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1A | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 1A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 1A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 1A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 1A | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 1A | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 1A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1A | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 1A | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 1A | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 1A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 1A | 1 | Total O<br>1 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 61 | 1A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 1A | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 1A | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 1A | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 1A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 1A | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 1A | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 1A | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 1A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 1A | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 1A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 1A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 1A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 1A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 1A | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 1A | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 1A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 1A | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 1A | 6 | Total O<br>6 6 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 61 | 1A | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 1A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 1A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 1A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 1A | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 1A | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 1A | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 1A | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 1A | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 1A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 1A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 1A | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 1A | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 1A | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 1A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 1A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 1A | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 1A | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 1A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 1A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 1A | 5 | Total O<br>5 5 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 61 | 1A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 1A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 1A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 1A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 1A | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 1A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 1A | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 1A | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 1A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 1A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 1A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 1A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 1A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 1A | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 1A | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 1A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 1A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 1A | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 1A | 6 | Total O<br>6 6 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 61 | 1A | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 1A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 1A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 1A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 1A | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 1A | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 1A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 1A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 1A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 1A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 1A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 1A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 1A | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 1A | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 1A | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 1A | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 1A | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 1A | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 1A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 1A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 1A | 5 | Total O<br>5 5 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 61 | 1A | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 1A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 1A | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 1A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 1A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 1A | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 1A | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 1A | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 1A | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 1A | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 1A | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 1A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 1A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 1A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 1A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 1A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 1A | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 1A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 1A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 1A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 1A | 6 | Total O<br>6 6 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 61 | 1A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 1A | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 1A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 1A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 1A | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 1A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 1A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 1A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 1A | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 1A | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 1A | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 1A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 1A | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 1A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 1A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 1A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 1A | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 1A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 1A | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 1A | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 1A | 6 | Total O<br>6 6 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 61 | 1A | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 1A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 1A | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 1A | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 1A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 1A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 1A | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 1A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 1A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 1A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 1A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 1A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1A | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 1A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 1A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 1A | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 1A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 1A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 1A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 1A | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 1A | 5 | Total O<br>5 5 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 61 | 1A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 1A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 1A | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 1A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 1A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 1A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 1A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 1A | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 1A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 1A | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 1A | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 1A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 1A | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 1A | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 1A | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 1A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 1A | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 1A | 1 | Total O<br>1 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 61 | 1A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1A | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 1A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 1A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1A | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 1A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 1A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 1A | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 1A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 1A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1A | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 1A | 500 | Total O<br>500 500 | 0 | 0 |
| 61 | 1B | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 1B | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1B | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 1B | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 1B | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 1B | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1B | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1B | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1B | 1 | Total O<br>1 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 61 | 1B | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1B | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 1B | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 1B | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1B | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 1B | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1B | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 1B | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1B | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 1B | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1B | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1B | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 1B | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 1B | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1B | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 1B | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1B | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 1B | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 1B | 16 | Total O<br>16 16 | 0 | 0 |
| 61 | 1D | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 1D | 2 | Total O<br>2 2 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 61 | 1D | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1D | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1D | 15 | Total O<br>15 15 | 0 | 0 |
| 61 | 1E | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 1E | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 1E | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 1E | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 1E | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 1E | 13 | Total O<br>13 13 | 0 | 0 |
| 61 | 1F | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1F | 8 | Total O<br>8 8 | 0 | 0 |
| 61 | 1G | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 1G | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 1H | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1I | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 1N | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 1O | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 1O | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1O | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 1P | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 1P | 2 | Total O<br>2 2 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 61 | 1P | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 1P | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1P | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 1P | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 1Q | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 1Q | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1Q | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 1R | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1R | 7 | Total O<br>7 7 | 0 | 0 |
| 61 | 1S | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 1S | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 1T | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1T | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1T | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 1U | 9 | Total O<br>9 9 | 0 | 0 |
| 61 | 1V | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1V | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 1W | 9 | Total O<br>9 9 | 0 | 0 |
| 61 | 1X | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 1X | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 1Y | 3 | Total O<br>3 3 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 61 | 1Z | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 10 | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 10 | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 10 | 7 | Total O<br>7 7 | 0 | 0 |
| 61 | 11 | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 11 | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 11 | 8 | Total O<br>8 8 | 0 | 0 |
| 61 | 12 | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 13 | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 13 | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 14 | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 15 | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 15 | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 16 | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 17 | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 17 | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 18 | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 18 | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 18 | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 18 | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 18 | 6 | Total O<br>6 6 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 61 | 18 | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 1a | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 1a | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 1a | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 1a | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1a | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 1a | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 1a | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1a | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 1a | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 1a | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 1a | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 1a | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 1a | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 1a | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1a | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 1a | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1a | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 1a | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 1a | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 1a | 5 | Total O<br>5 5 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 61 | 1a | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 1a | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 1a | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 1a | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 1a | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 1a | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1a | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 1a | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 1a | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 1a | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1a | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1a | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 1a | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 1a | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 1a | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1a | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 1a | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 1a | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1a | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1a | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1a | 6 | Total O<br>6 6 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 61 | 1a | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 1a | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1a | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 1a | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 1a | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1a | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 1a | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1a | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 1a | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 1a | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 1a | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 1a | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 1a | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 1a | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 1a | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 1a | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 1a | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 1a | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 1a | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 1a | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 1a | 2 | Total O<br>2 2 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 61 | 1a | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 1a | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 1a | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 1a | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 1a | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 1a | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 1a | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 1a | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 1a | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 1a | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 1a | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 1a | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 1a | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 1a | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 1a | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 1a | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 1a | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 1a | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 1a | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 1a | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 1a | 6 | Total O<br>6 6 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 61 | 1a | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 1a | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 1a | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 1a | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 1a | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 1a | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1a | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1a | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1a | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 1a | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1a | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1a | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 1a | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1a | 78 | Total O<br>78 78 | 0 | 0 |
| 61 | 1b | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1d | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1f | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1l | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 1l | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1q | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 1w | 6 | Total O<br>6 6 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 61 | 1w | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1w | 9 | Total O<br>9 9 | 0 | 0 |
| 61 | 1x | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 1x | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 1x | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1x | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 1x | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1x | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1x | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 1y | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2A | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 2A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 2A | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 2A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 2A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 2A | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 2A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2A | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 2A | 1 | Total O<br>1 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 61 | 2A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 2A | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 2A | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 2A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 2A | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 2A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 2A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 2A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 2A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 2A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 2A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 2A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 2A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 2A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 2A | 1 | Total O<br>1 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 61 | 2A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 2A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 2A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 2A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 2A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2A | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 2A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 2A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 2A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 2A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 2A | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 2A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 2A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 2A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 2A | 3 | Total O<br>3 3 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 61 | 2A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 2A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 2A | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 2A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 2A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 2A | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 2A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 2A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 2A | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 2A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 2A | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 2A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 2A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 2A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 2A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 2A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 2A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 2A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 2A | 2 | Total O<br>2 2 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 61 | 2A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 2A | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 2A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 2A | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 2A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 2A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 2A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 2A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 2A | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 2A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 2A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 2A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 2A | 6 | Total O<br>6 6 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 61 | 2A | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 2A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 2A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 2A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 2A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 2A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 2A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 2A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 2A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2A | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 2A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 2A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 2A | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 2A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 2A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 2A | 4 | Total O<br>4 4 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 61 | 2A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 2A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 2A | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 2A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 2A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 2A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2A | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 2A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 2A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 2A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2A | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 2A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2A | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 2A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 2A | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 2A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 2A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 2A | 1 | Total O<br>1 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 61 | 2A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 2A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 2A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 2A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 2A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 2A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 2A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 2A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 2A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 2A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2A | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 2A | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 2A | 2 | Total O<br>2 2 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 61 | 2A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 2A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 2A | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 2A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 2A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 2A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2A | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 2A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 2A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 2A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 2A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 2A | 3 | Total O<br>3 3 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 61 | 2A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 2A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 2A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 2A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 2A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 2A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 2A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 2A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 2A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 2A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 2A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 2A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 2A | 2 | Total O<br>2 2 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 61 | 2A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 2A | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 2A | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 2A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 2A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 2A | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 2A | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 2A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 2A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 2A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 2A | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 2A | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 2A | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 2A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 2A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 2A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 2A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 2A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2A | 2 | Total O<br>2 2 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 61 | 2A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 2A | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 2A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 2A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 2A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 2A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 2A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 2A | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 2A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 2A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2A | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 2A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 2A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 2A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 2A | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 2A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 2A | 4 | Total O<br>4 4 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 61 | 2A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 2A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2A | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 2A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2A | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 2A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 2A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 2A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 2A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 2A | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 2A | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 2A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 2A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2A | 1 | Total O<br>1 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 61 | 2A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 2A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 2A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2A | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 2A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 2A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 2A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 2A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 2A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2A | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 2A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 2A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 2A | 1 | Total O<br>1 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 61 | 2A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 2A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 2A | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 2A | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 2A | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 2A | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 2A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 2A | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 2A | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 2A | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 2A | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 2A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 2A | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 2A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2A | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 2A | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 2A | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 2A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 2A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 2A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 2A | 6 | Total O<br>6 6 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 61 | 2A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 2A | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 2A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 2A | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 2A | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 2A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 2A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 2A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 2A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 2A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 2A | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 2A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 2A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 2A | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 2A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 2A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 2A | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 2A | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 2A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 2A | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 2A | 6 | Total O<br>6 6 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 61 | 2A | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 2A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 2A | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 2A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 2A | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 2A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 2A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 2A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 2A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 2A | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 2A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 2A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 2A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 2A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 2A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 2A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 2A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 2A | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 2A | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 2A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 2A | 6 | Total O<br>6 6 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 61 | 2A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 2A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 2A | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 2A | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 2A | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 2A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 2A | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 2A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 2A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 2A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 2A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 2A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 2A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 2A | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 2A | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 2A | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 2A | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 2A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 2A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 2A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 2A | 6 | Total O<br>6 6 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 61 | 2A | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 2A | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 2A | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 2A | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 2A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 2A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 2A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2A | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 2A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 2A | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 2A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 2A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 2A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 2A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 2A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 2A | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 2A | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 2A | 2 | Total O<br>2 2 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 61 | 2A | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 2A | 222 | Total O<br>222 222 | 0 | 0 |
| 61 | 2B | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 2B | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 2B | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 2B | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2B | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 2B | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2B | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2B | 12 | Total O<br>12 12 | 0 | 0 |
| 61 | 2D | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 2D | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 2D | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 2D | 7 | Total O<br>7 7 | 0 | 0 |
| 61 | 2E | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 2F | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 2I | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 2N | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2O | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2P | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 2P | 2 | Total O<br>2 2 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 61 | 2P | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 2Q | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2Q | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2R | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2R | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 2T | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 2T | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 2U | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 2W | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 2Z | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 20 | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 20 | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 20 | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 21 | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 22 | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 25 | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 27 | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 27 | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 28 | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 28 | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 28 | 1 | Total O<br>1 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 61 | 29 | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2a | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 2a | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 2a | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 2a | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 2a | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 2a | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 2a | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 2a | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 2a | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 2a | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 2a | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 2a | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 2a | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 2a | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 2a | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 2a | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 2a | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 2a | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 2a | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 2a | 2 | Total O<br>2 2 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 61 | 2a | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 2a | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 2a | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 2a | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 2a | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 2a | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 2a | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 2a | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 2a | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 2a | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 2a | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 2a | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 2a | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 2a | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 2a | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 2a | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 2a | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 2a | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 2a | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 2a | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 2a | 4 | Total O<br>4 4 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 61 | 2a | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 2a | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 2a | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 2a | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 2a | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 2a | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 2a | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2a | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 2a | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 2a | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 2a | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 2a | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 2a | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 2a | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 2a | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2a | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 2a | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2a | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 2a | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2a | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 2a | 1 | Total O<br>1 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 61 | 2a | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 2a | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2a | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 2a | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 2a | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2a | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 2a | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2a | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2a | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 2a | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 2a | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2a | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2a | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 2a | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 2a | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 2a | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 2a | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2a | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2a | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 2a | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 2a | 2 | Total O<br>2 2 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 61 | 2a | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 2a | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 2a | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2a | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2a | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2a | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2a | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2a | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2a | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2a | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2a | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2a | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2a | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2a | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2a | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 2a | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 2a | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 2a | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 2a | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2a | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 2a | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2a | 2 | Total O<br>2 2 | 0 | 0 |

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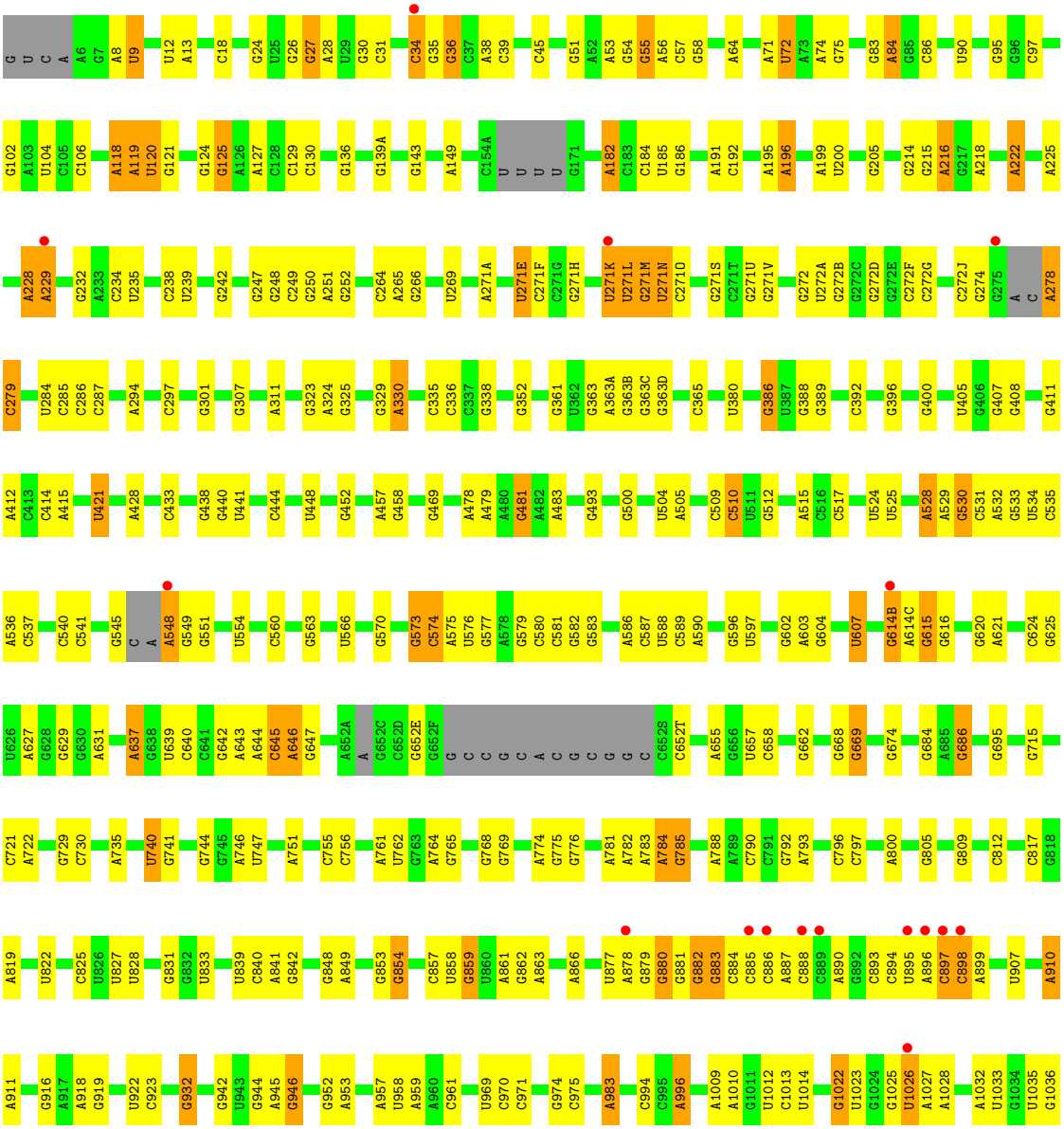
| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 61 | 2a | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 2a | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 2a | 40 | Total O<br>40 40 | 0 | 0 |
| 61 | 2d | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2g | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2i | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2j | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 2j | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2l | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2l | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2p | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2r | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2t | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 2x | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 2x | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 2x | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 2y | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 2y | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2y | 6 | Total O<br>6 6 | 0 | 0 |

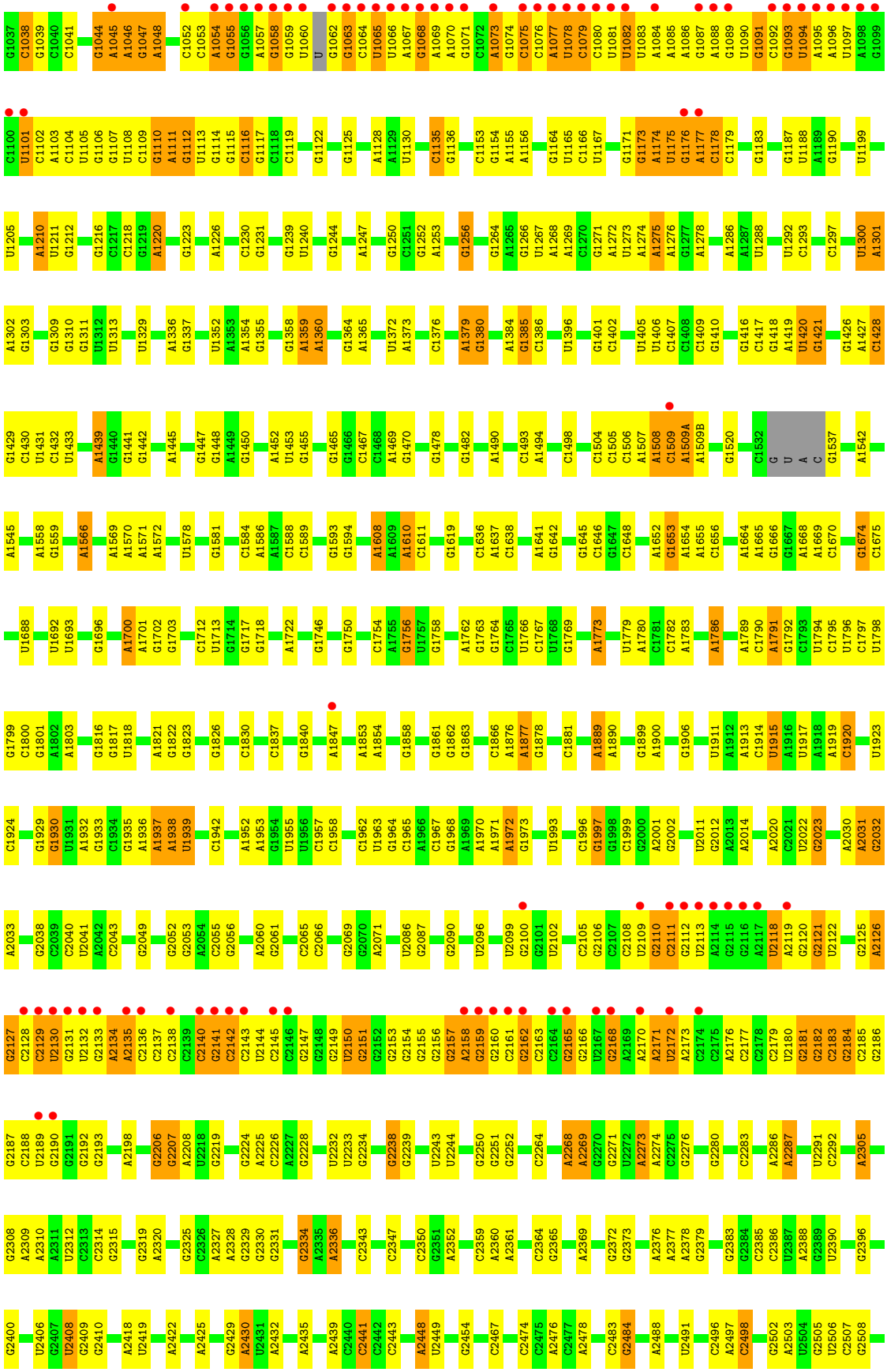
# 3 Residue-property plots (i)

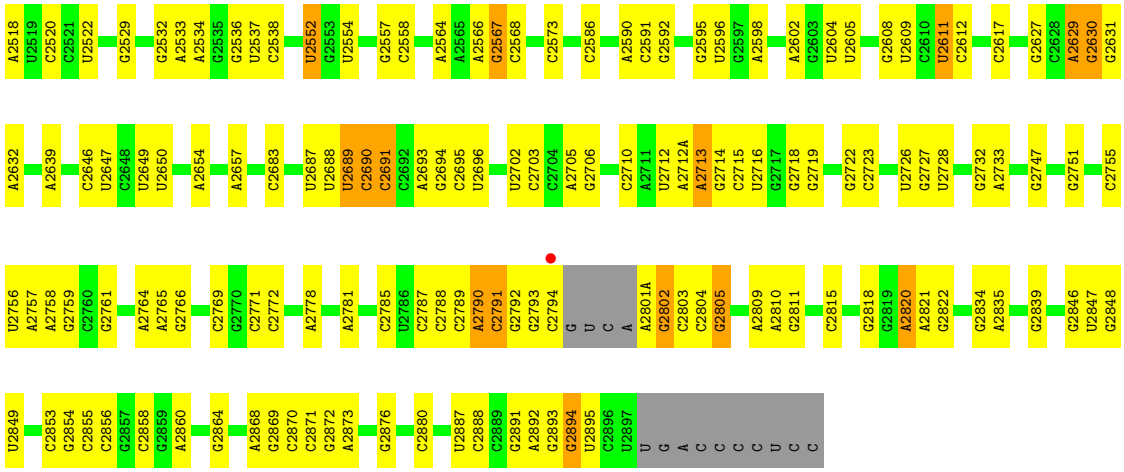
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: 23S Ribosomal RNA

Chain 1A:

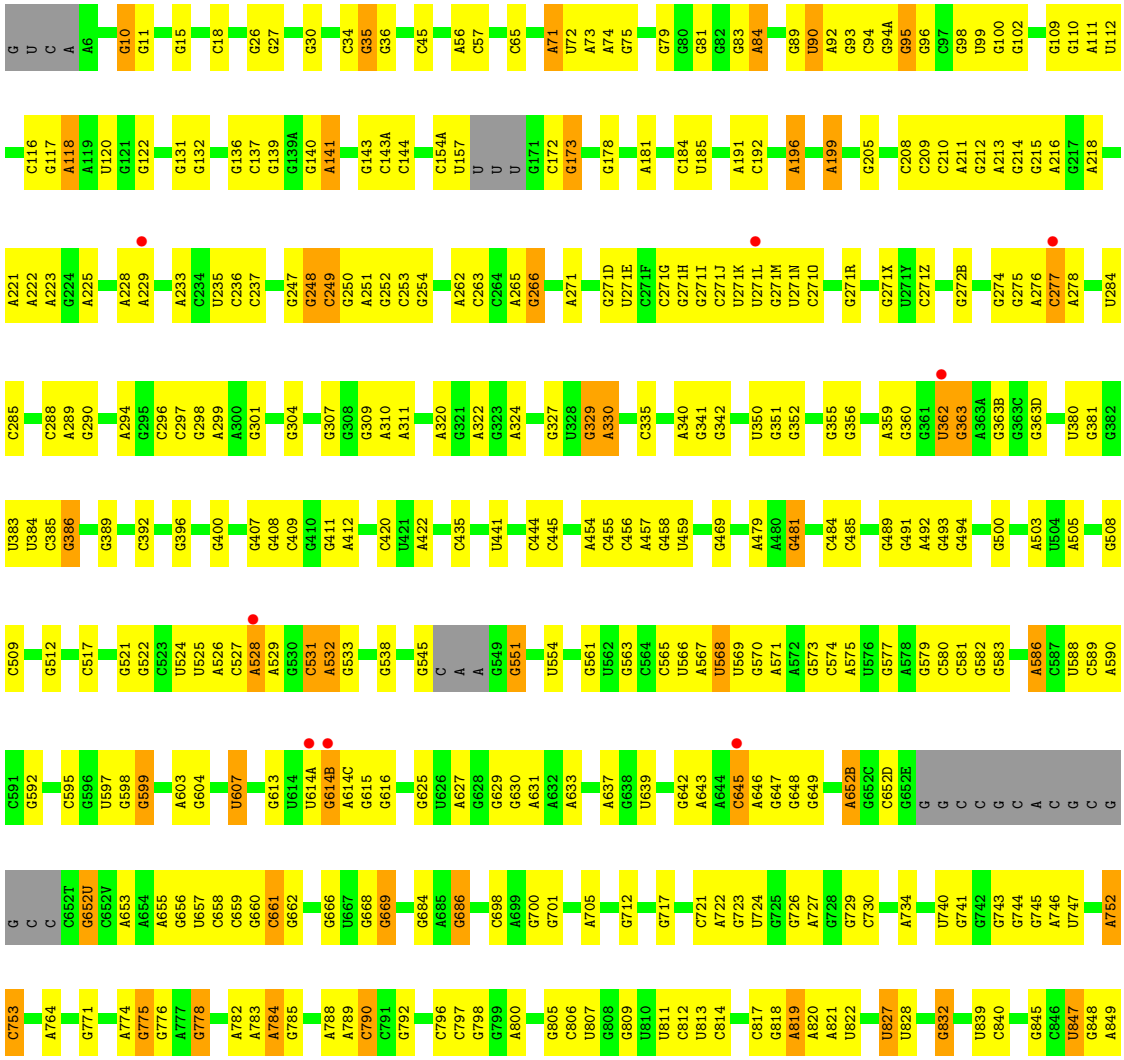


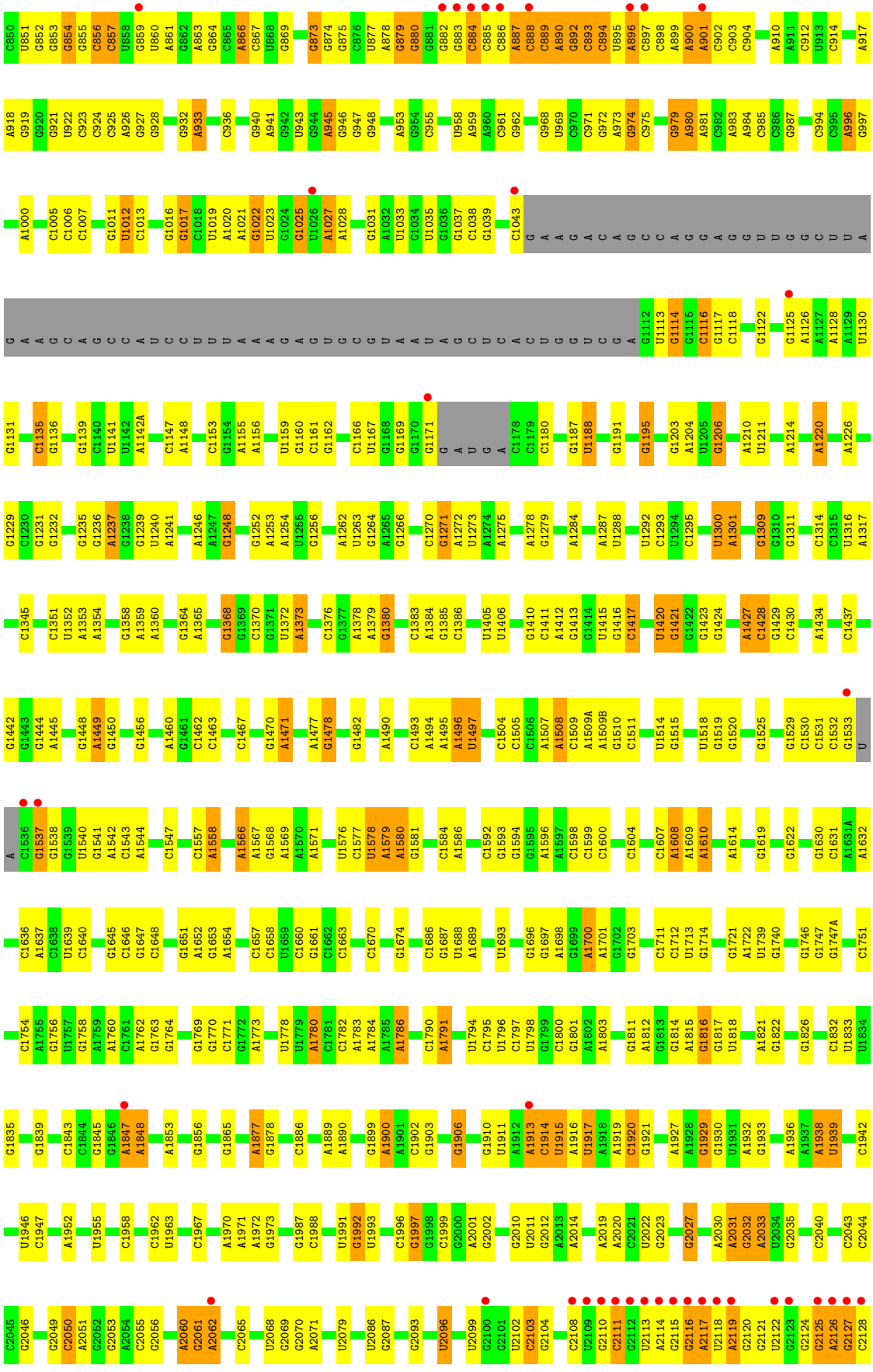

G1037 C1038 G1039 C1040 C1041 G1044 A1045 A1046 G1047 A1048 C1052 C1053 A1054 G1055 G1056 A1057 G1058 G1059 U1060 U G1062 G1063 C1064 U1065 U1066 A1067 G1068 A1069 A1070 G1071 C1072 A1073 G1074 C1075 C1076 A1077 U1078 C1079 C1080 U1081 U1082 U1083 A1084 A1085 A1086 G1087 A1088 G1089 U1090 G1091 C1092 G1093 U1094 A1095 A1096 U1097 A1098 G1099
C1100 U1101 C1102 A1103 C1104 U1105 G1106 G1107 U1108 C1109 G1110 A1111 G1112 U1113 G1114 G1115 C1116 G1117 C1118 C1119 G1122 G1125 A1128 A1129 U1130 C1135 G1136 C1153 G1154 A1155 A1156 G1164 U1165 C1166 U1167 G1171 G1173 A1174 U1175 G1176 A1177 C1178 C1179 G1183 G1187 U1188 A1189 G1190 U1199
U1205 A1210 U1211 G1212 G1216 C1217 C1218 G1219 A1220 G1223 A1226 C1230 G1231 G1239 U1240 G1244 A1247 G1250 C1251 G1252 A1253 G1256 G1264 A1265 C1266 U1267 A1268 A1269 C1270 G1271 A1272 U1273 A1274 A1275 A1276 G1277 A1278 A1286 A1287 U1288 U1292 C1293 C1297 U1300 A1301
A1302 G1303 G1309 G1310 G1311 U1312 U1313 U1329 A1336 G1337 U1352 A1353 A1354 G1355 G1358 A1359 A1360 G1364 A1365 U1372 A1373 C1376 A1379 G1380 A1384 G1385 C1386 U1396 G1401 C1402 U1405 U1406 C1407 C1408 C1409 G1410 G1416 C1417 G1418 A1419 U1420 G1421 G1426 A1427 C1428
G1429 C1430 U1431 C1432 U1433 A1439 G1440 G1441 G1442 A1445 G1447 G1448 A1449 G1450 A1452 U1453 G1455 G1465 G1466 C1467 C1468 A1469 G1470 G1478 G1482 A1490 C1493 A1494 C1498 C1504 C1505 C1506 A1507 A1508 C1509 A1509A A1509B G1520 C1532 G U A C G1537 A1542
A1545 A1558 G1559 A1566 A1569 A1570 A1571 A1572 U1578 G1581 C1584 A1586 A1587 C1588 C1589 G1593 G1594 A1608 A1609 A1610 C1611 G1619 C1636 A1637 C1638 A1641 G1642 G1645 C1646 G1647 C1648 A1652 G1653 A1654 A1655 C1656 A1664 A1665 G1666 G1667 A1668 A1669 C1670 G1674 C1675
U1688 U1692 U1693 G1696 A1700 A1701 G1702 G1703 C1712 U1713 G1714 G1717 G1718 A1722 G1746 G1750 C1754 A1755 G1756 U1757 G1758 A1762 G1763 G1764 C1765 U1766 C1767 U1768 G1769 A1773 U1779 A1780 C1781 C1782 A1783 A1786 A1789 C1790 A1791 G1792 C1793 U1794 C1795 U1796 C1797 U1798
G1799 C1800 G1801 A1802 A1803 G1816 G1817 U1818 A1821 G1822 G1823 G1826 C1830 C1837 G1840 A1847 A1853 A1854 G1858 G1861 G1862 G1863 C1866 A1876 A1877 G1878 C1881 A1889 A1890 G1899 A1900 G1906 U1911 A1912 A1913 C1914 U1915 A1916 U1917 A1918 A1919 C1920 U1923
C1924 G1929 G1930 U1931 A1932 G1933 C1934 G1935 A1936 A1937 A1938 U1939 C1942 A1952 A1953 G1954 U1955 U1956 C1957 C1958 C1962 U1963 G1964 C1965 A1966 A1969 A1970 A1971 A1972 G1973 U1993 C1996 G1997 G1998 C1999 G2000 A2001 G2002 U2011 G2012 A2013 A2014 A2020 C2021 U2022 G2023 A2030 A2031 G2032
A2033 G2038 C2039 C2040 U2041 A2042 C2043 G2049 G2052 G2053 A2054 C2055 G2056 A2060 G2061 C2065 C2066 G2069 G2070 A2071 U2086 G2087 G2090 U2096 U2099 G2100 G2101 U2102 C2105 G2106 C2107 C2108 U2109 G2110 C2111 G2112 U2113 A2114 G2115 G2116 A2117 U2118 A2119 G2120 G2121 U2122 G2125 A2126
G2127 C2128 C2129 U2130 G2131 U2132 G2133 A2134 A2135 C2136 C2137 C2138 C2139 C2140 G2141 C2142 C2143 U2144 C2145 C2146 C2147 G2148 G2149 U2150 G2151 G2152 G2153 G2154 G2155 G2156 G2157 A2158 G2159 G2160 C2161 G2162 C2163 C2164 G2165 G2166 U2167 G2168 A2169 A2170 A2171 U2172 A2173 C2174 C2175 A2176 C2177 C2178 C2179 U2180 G2181 G2182 C2183 G2184 C2185 C2186
G2187 C2188 U2189 G2190 G2191 G2192 G2193 A2198 G2206 G2207 A2208 U2218 G2219 G2224 A2225 C2226 A2227 G2228 U2232 U2233 G2234 G2238 G2239 U2243 U2244 G2250 G2251 G2252 C2264 A2268 A2269 G2270 G2271 U2272 A2273 A2274 C2275 G2276 G2280 C2283 A2286 A2287 U2291 C2292 A2305
G2308 A2309 A2310 A2311 U2312 C2313 C2314 G2315 G2319 A2320 G2326 C2326 A2327 A2328 G2329 G2330 G2331 G2334 A2335 A2336 C2343 C2347 C2350 G2351 A2352 C2359 A2360 A2361 C2364 G2365 A2369 G2372 G2373 A2376 A2377 A2378 G2379 G2383 G2384 C2385 C2386 U2387 A2388 G2389 U2390 G2396
G2400 U2406 G2407 U2408 G2409 G2410 A2418 U2419 A2422 A2425 G2429 A2430 U2431 A2432 A2435 A2439 C2440 C2441 C2442 C2443 A2448 U2449 G2454 C2467 C2474 C2475 A2476 C2477 A2478 C2483 G2484 A2488 U2491 C2496 A2497 C2498 G2502 A2503 U2504 G2505 U2506 C2507 G2508



• Molecule 1: 23S Ribosomal RNA

Chain 2A:

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A1000 C1005 C1006 C1007 G1011 U1012 C1013 G1016 G1017 C1018 U1019 A1020 A1021 G1022 U1023 G1024 G1025 U1026 A1027 A1028 G1031 A1032 U1033 G1034 U1035 G1036 G1037 C1038 G1039 C1043 G A A A G A C A G C C A G C C U U U U A A A G U C C U U U U C C G U A A C C U G G U U C G A G C C A G1112 U1113 G1114 G1115 C1116 G1117 C1118 G1122 G1125 A1126 A1127 A1128 A1129 U1130
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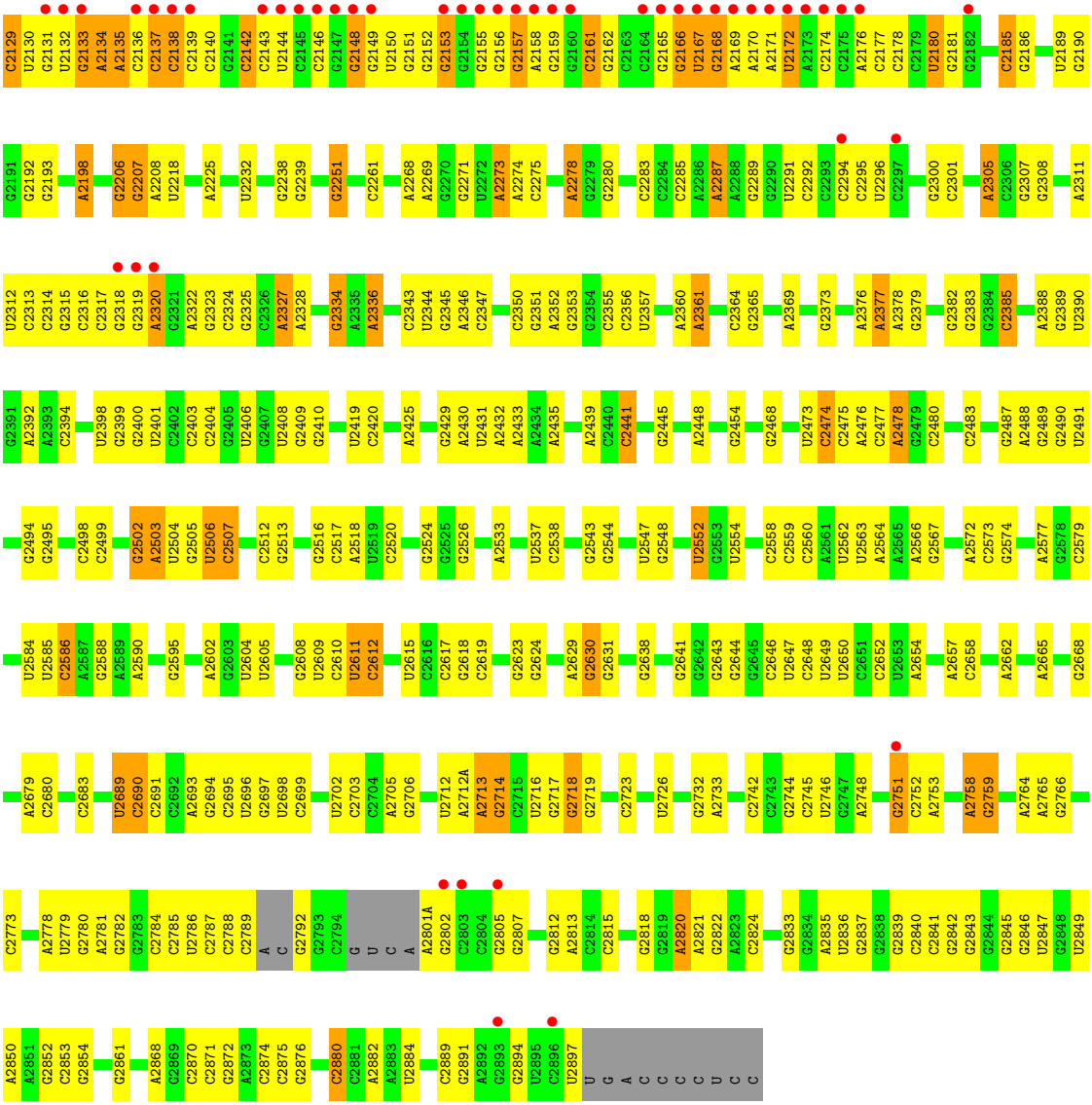
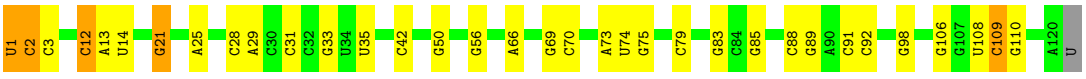


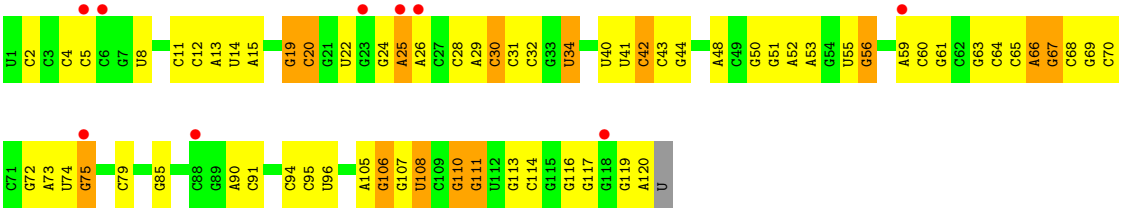
• Molecule 2: 5S Ribosomal RNA

Chain 1B:



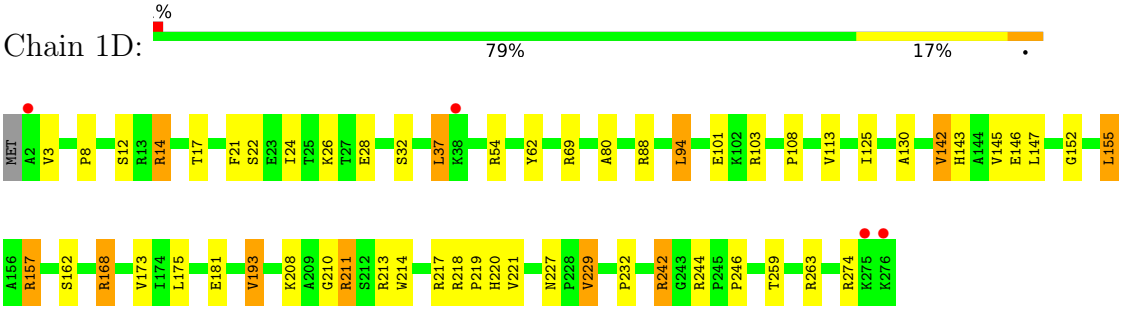
• Molecule 2: 5S Ribosomal RNA

Chain 2B:



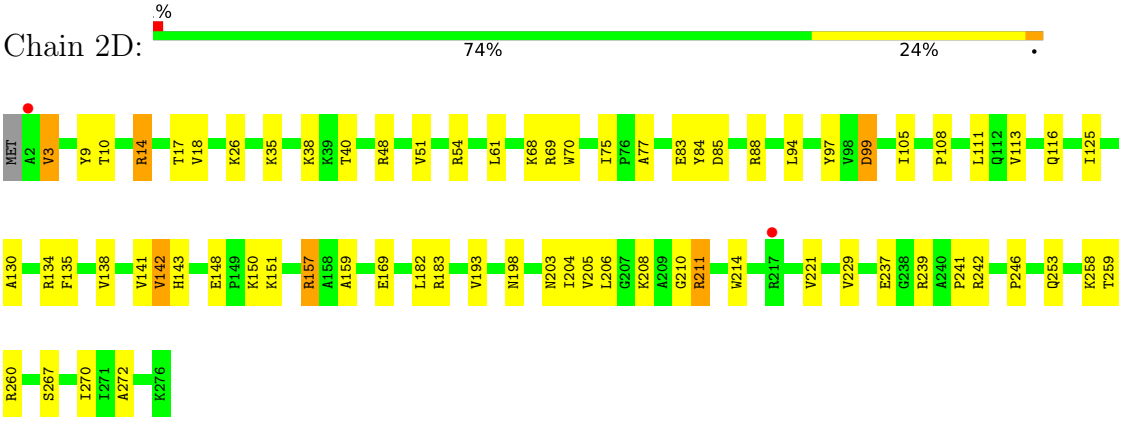
• Molecule 3: 50S ribosomal protein L2

Chain 1D:



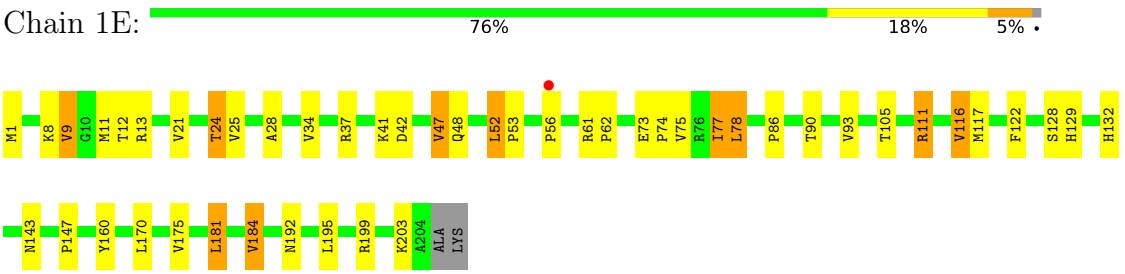

• Molecule 3: 50S ribosomal protein L2

Chain 2D:



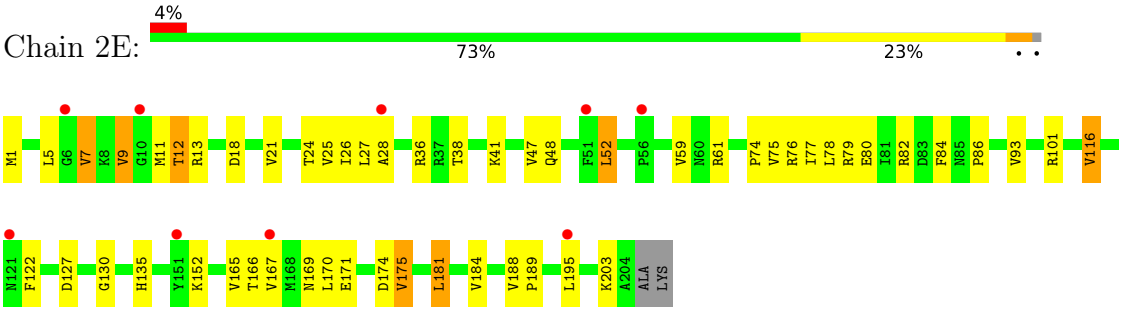

• Molecule 4: 50S ribosomal protein L3

Chain 1E:



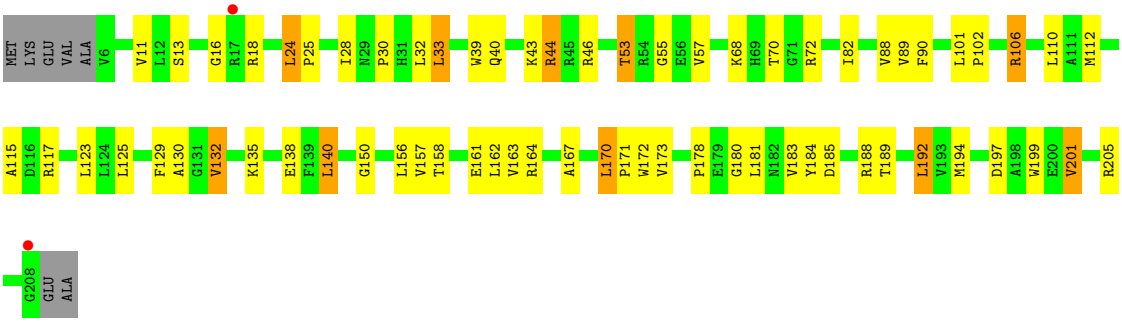

• Molecule 4: 50S ribosomal protein L3

Chain 2E:




• Molecule 5: 50S ribosomal protein L4

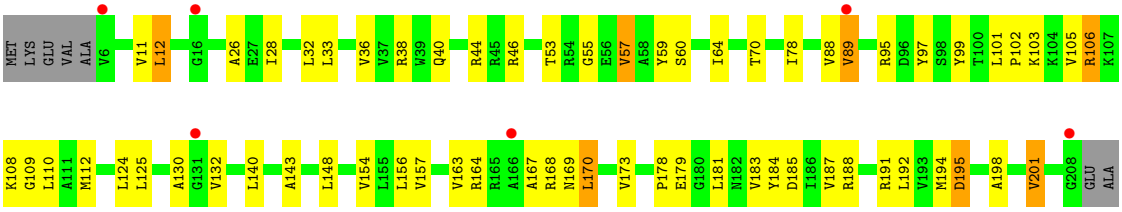
Chain 1F:





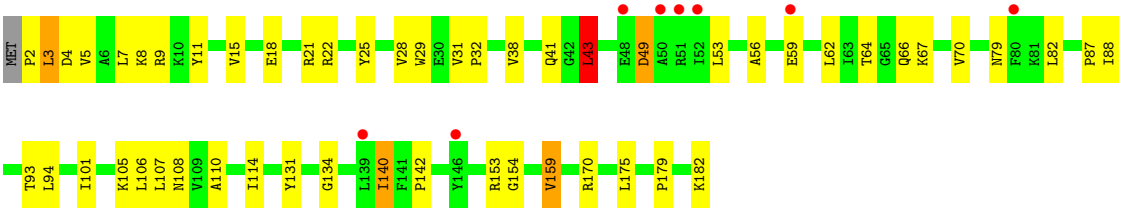
• Molecule 5: 50S ribosomal protein L4

Chain 2F:



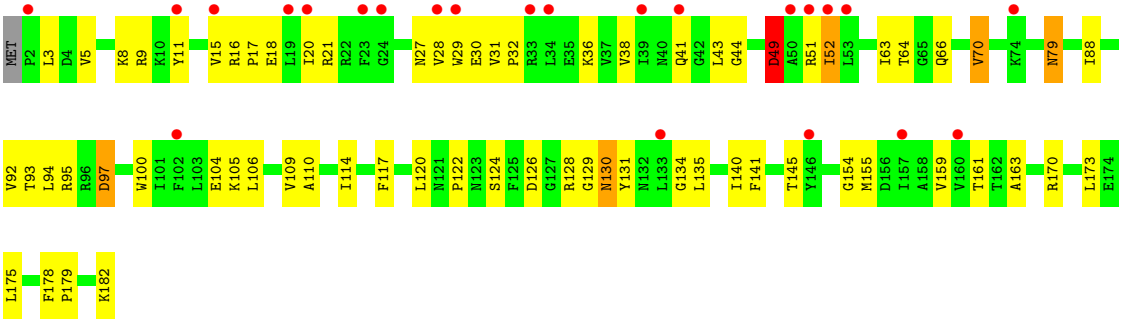
• Molecule 6: 50S ribosomal protein L5

Chain 1G:



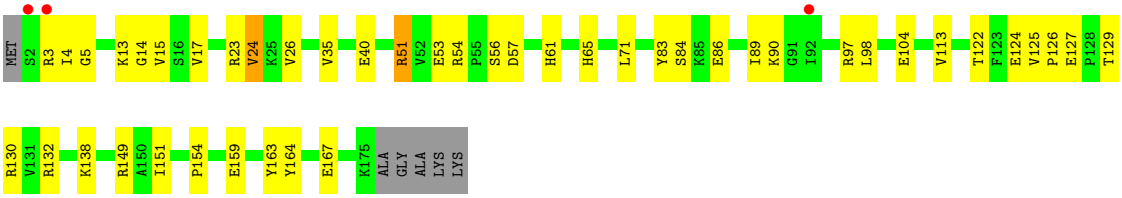
• Molecule 6: 50S ribosomal protein L5

Chain 2G:



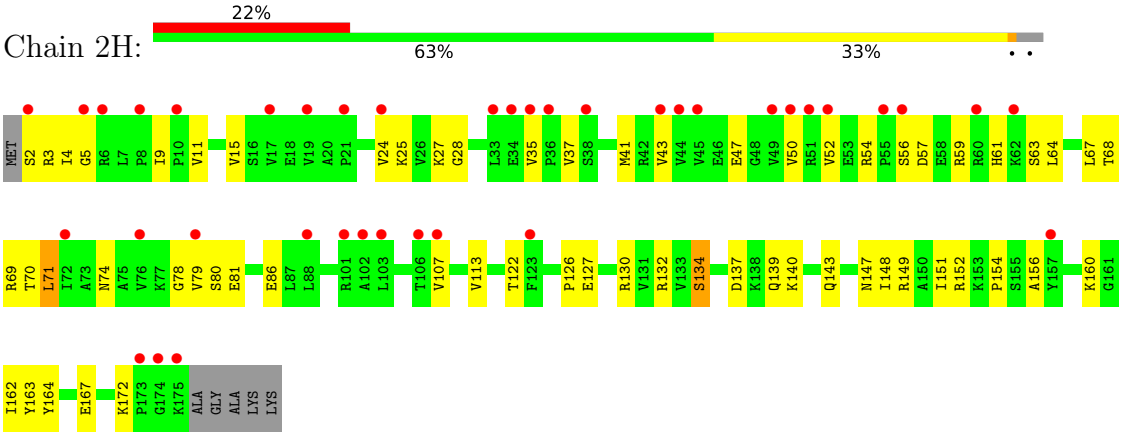
• Molecule 7: 50S ribosomal protein L6

Chain 1H:



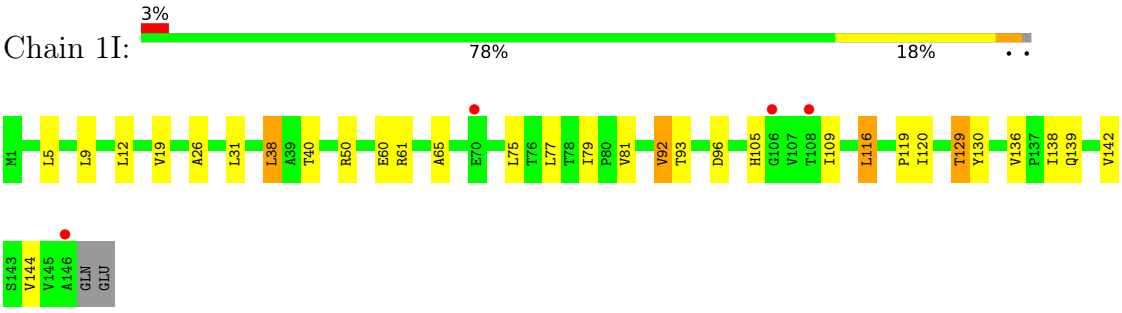

• Molecule 7: 50S ribosomal protein L6

Chain 2H:



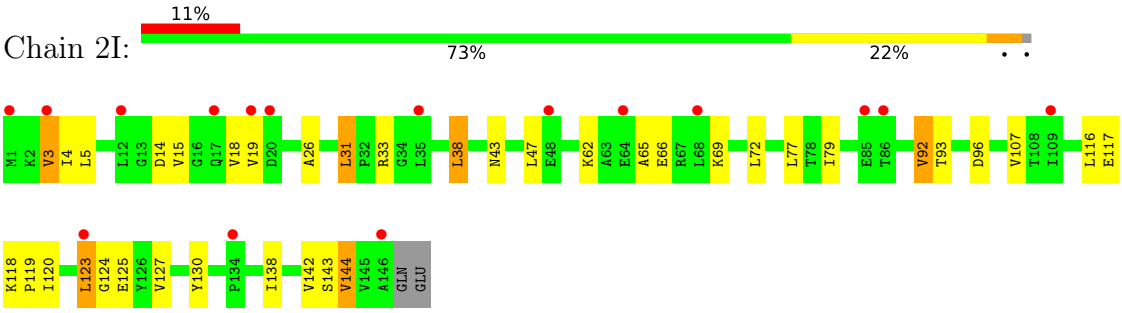

• Molecule 8: 50S ribosomal protein L9

Chain 1I:



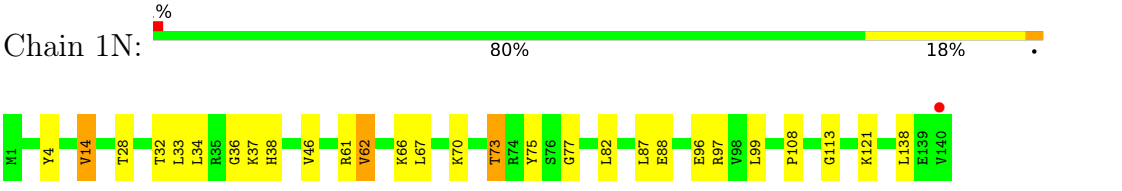

• Molecule 8: 50S ribosomal protein L9

Chain 2I:



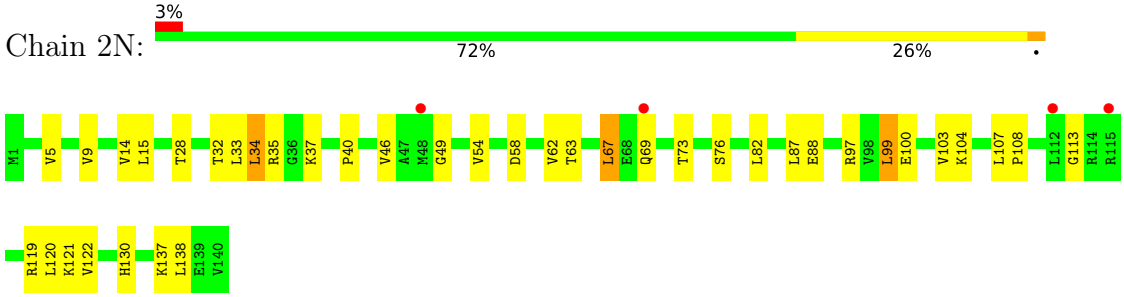

• Molecule 9: 50S ribosomal protein L13

Chain 1N:



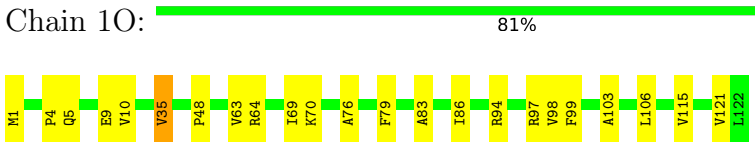
• Molecule 9: 50S ribosomal protein L13

Chain 2N:



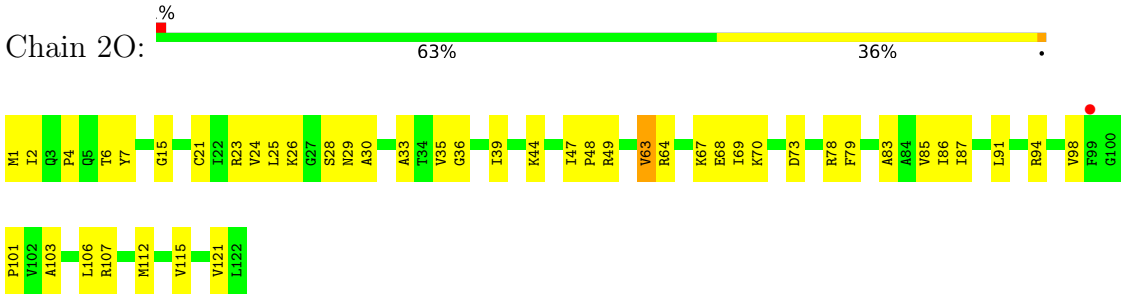

• Molecule 10: 50S ribosomal protein L14

Chain 1O:



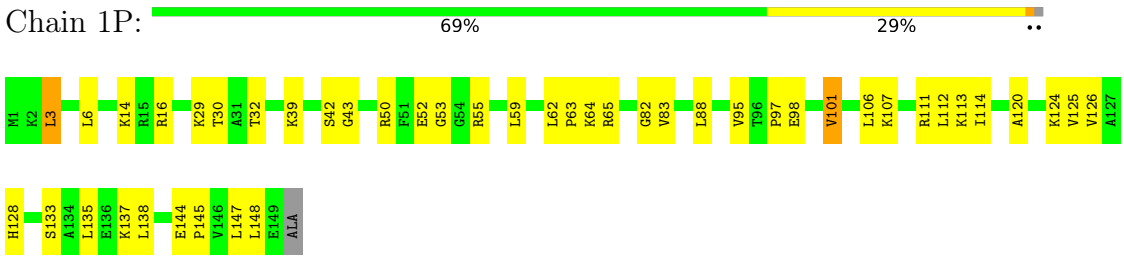

• Molecule 10: 50S ribosomal protein L14

Chain 2O:



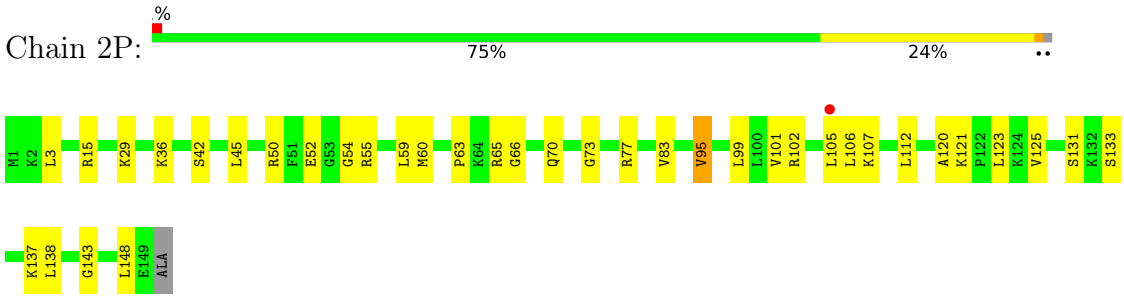

• Molecule 11: 50S ribosomal protein L15

Chain 1P:



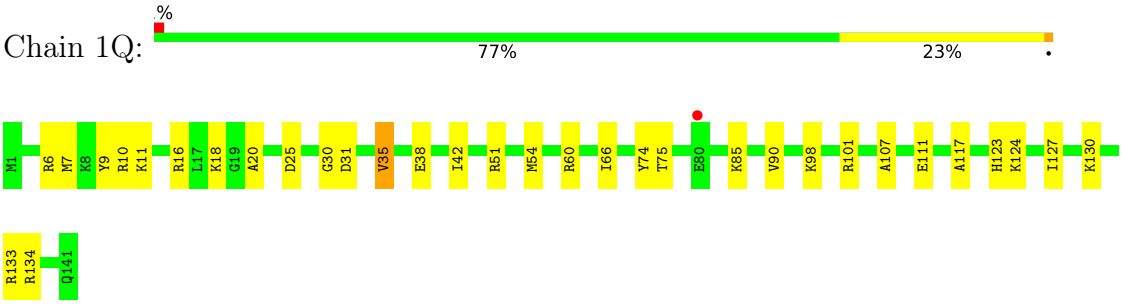

• Molecule 11: 50S ribosomal protein L15

Chain 2P:



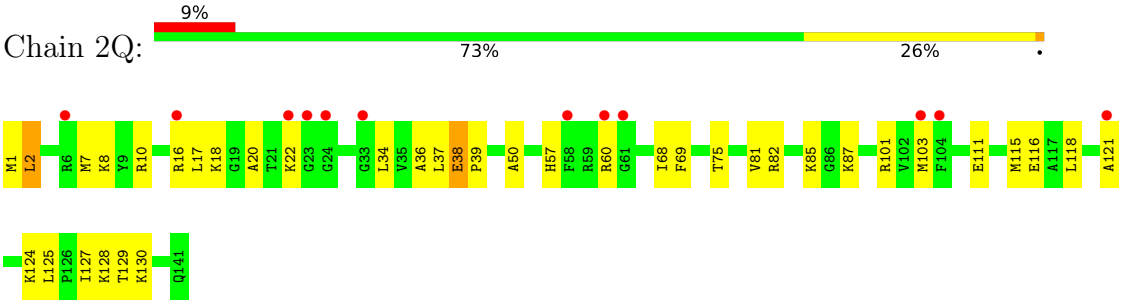

• Molecule 12: 50S ribosomal protein L16

Chain 1Q:



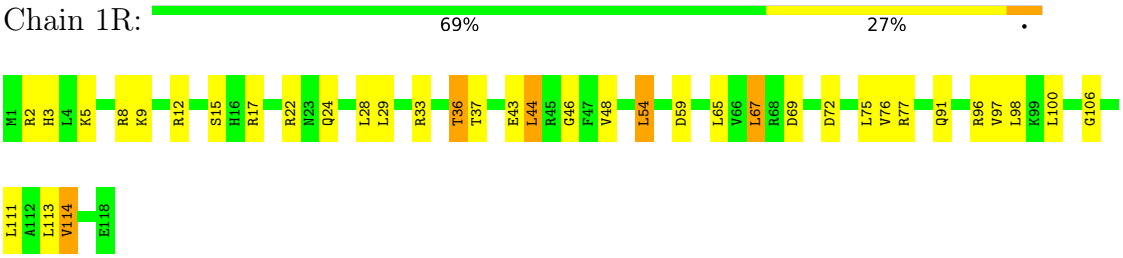

• Molecule 12: 50S ribosomal protein L16

Chain 2Q:



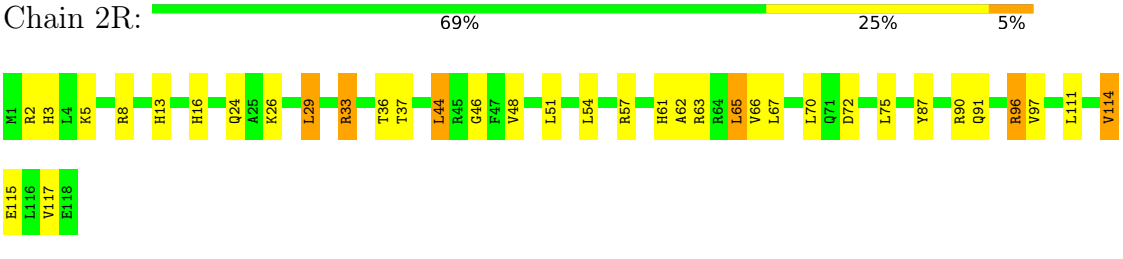

• Molecule 13: 50S ribosomal protein L17

Chain 1R:



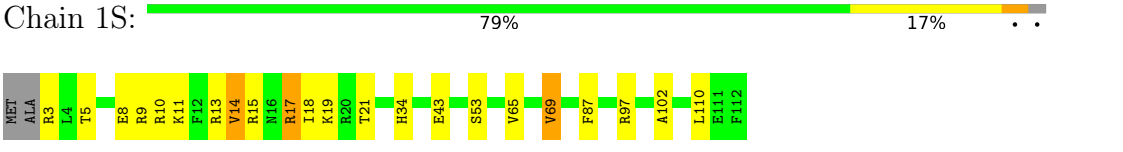

• Molecule 13: 50S ribosomal protein L17

Chain 2R:



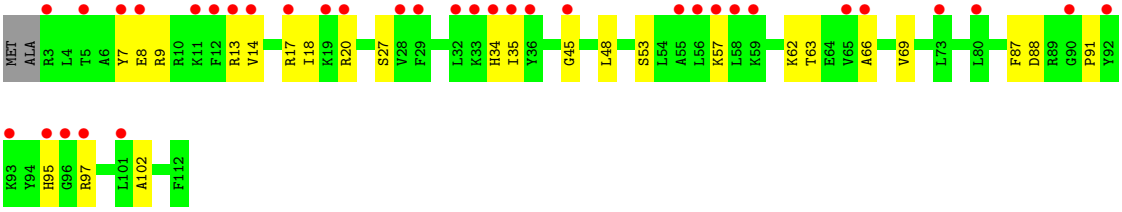

• Molecule 14: 50S ribosomal protein L18

Chain 1S:



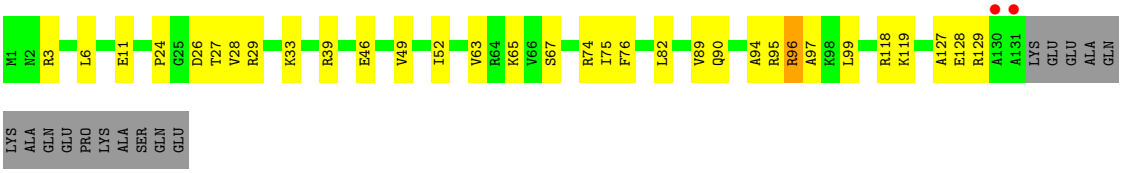

• Molecule 14: 50S ribosomal protein L18

Chain 2S:



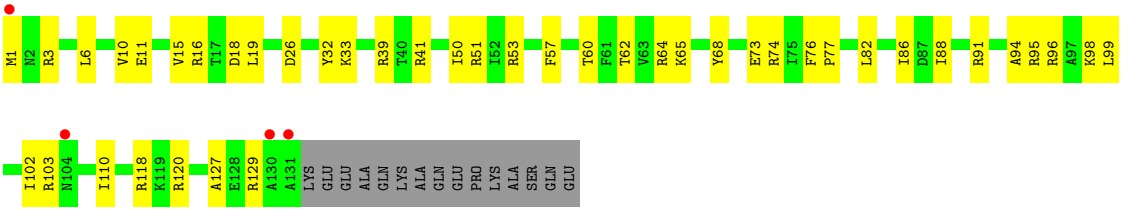

• Molecule 15: 50S ribosomal protein L19

Chain 1T:



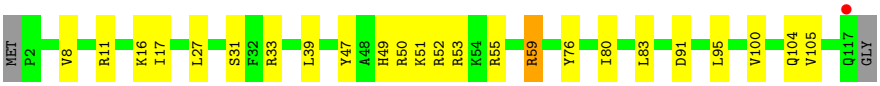

• Molecule 15: 50S ribosomal protein L19

Chain 2T:



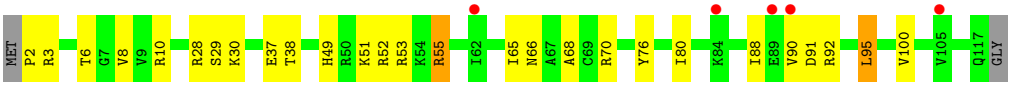

• Molecule 16: 50S ribosomal protein L20

Chain 1U:



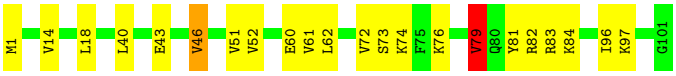

• Molecule 16: 50S ribosomal protein L20

Chain 2U:



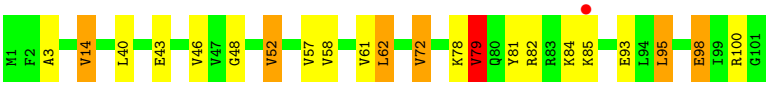

• Molecule 17: 50S ribosomal protein L21

Chain 1V:



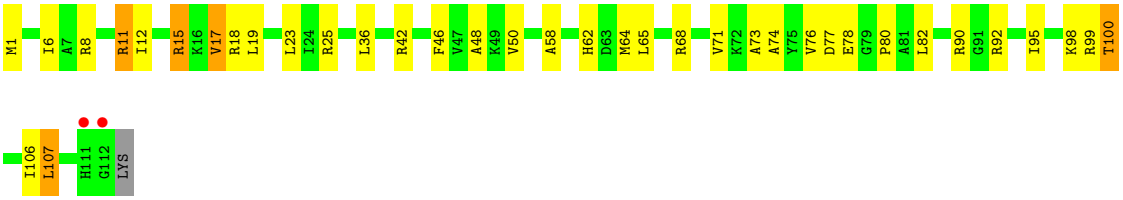
• Molecule 17: 50S ribosomal protein L21

Chain 2V:




• Molecule 18: 50S ribosomal protein L22

Chain 1W:




• Molecule 18: 50S ribosomal protein L22

Chain 2W:

• Molecule 19: 50S ribosomal protein L23

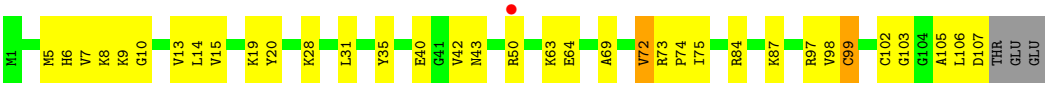
Chain 1X:

• Molecule 19: 50S ribosomal protein L23

Chain 2X:

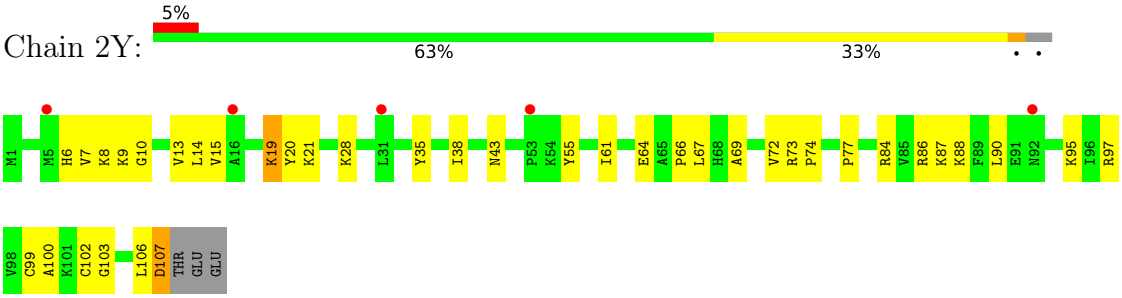
• Molecule 20: 50S ribosomal protein L24

Chain 1Y:



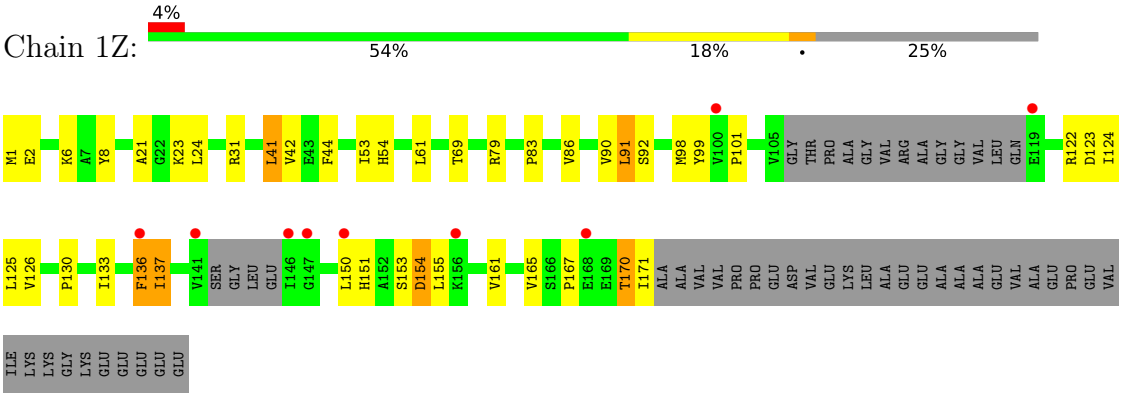

• Molecule 20: 50S ribosomal protein L24

Chain 2Y:



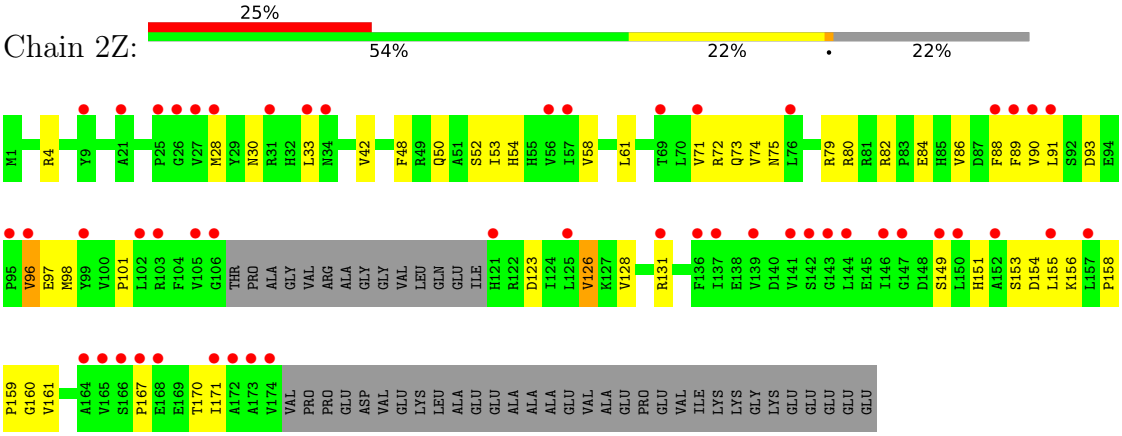

• Molecule 21: 50S ribosomal protein L25

Chain 1Z:



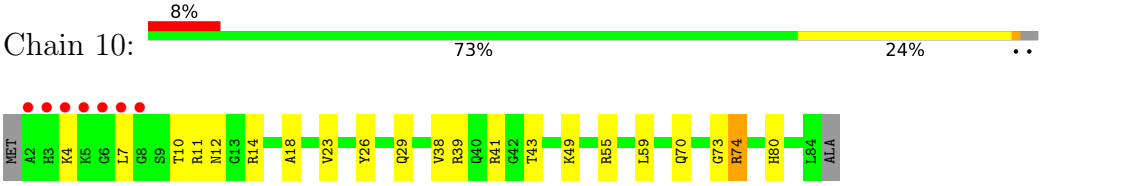

• Molecule 21: 50S ribosomal protein L25

Chain 2Z:



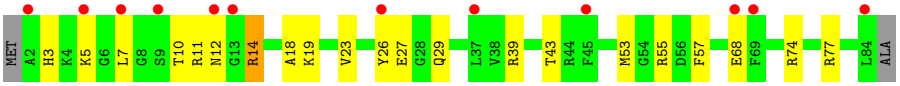

• Molecule 22: 50S ribosomal protein L27

Chain 10:

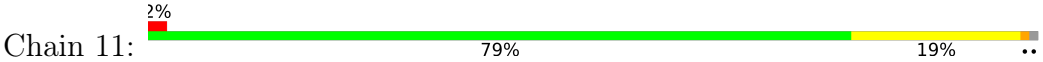


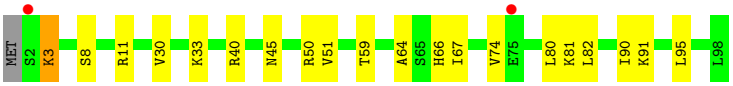

• Molecule 22: 50S ribosomal protein L27

Chain 20:

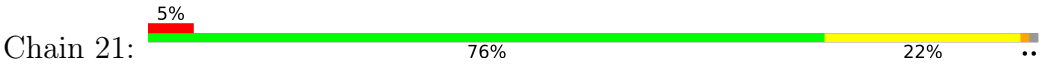



• Molecule 23: 50S ribosomal protein L28

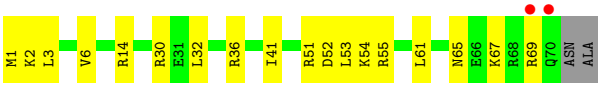


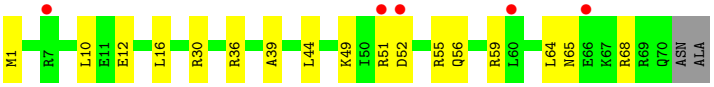

• Molecule 23: 50S ribosomal protein L28



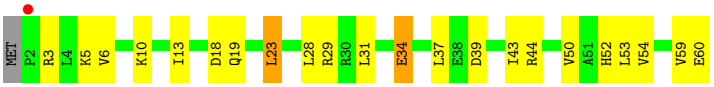
• Molecule 24: 50S ribosomal protein L29



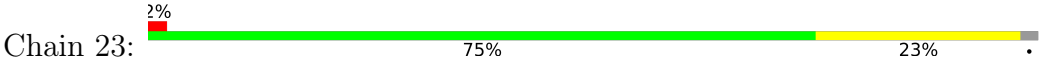

• Molecule 24: 50S ribosomal protein L29

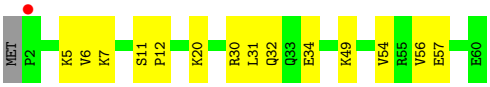



• Molecule 25: 50S ribosomal protein L30



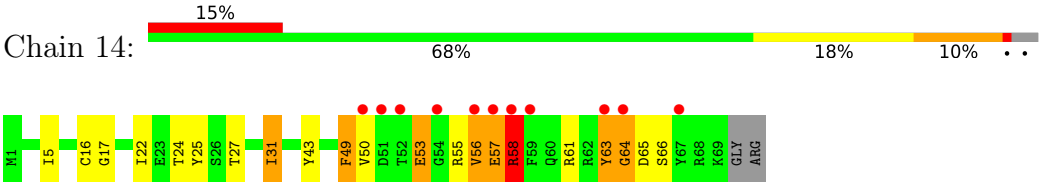

• Molecule 25: 50S ribosomal protein L30



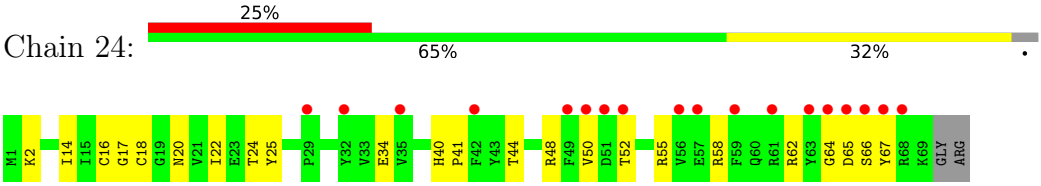

• Molecule 26: 50S ribosomal protein L31

Chain 14:



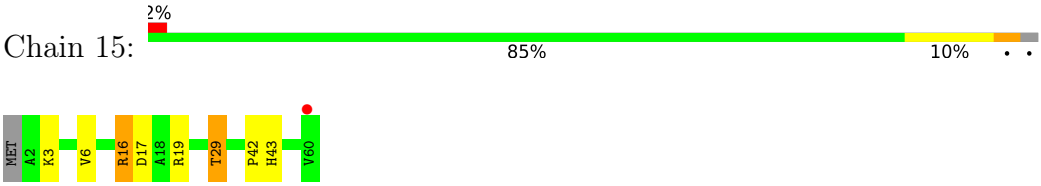

• Molecule 26: 50S ribosomal protein L31

Chain 24:



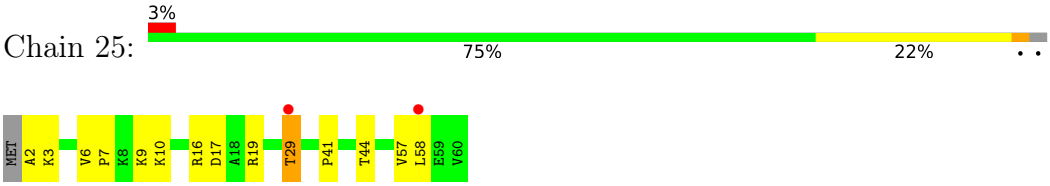

• Molecule 27: 50S ribosomal protein L32

Chain 15:



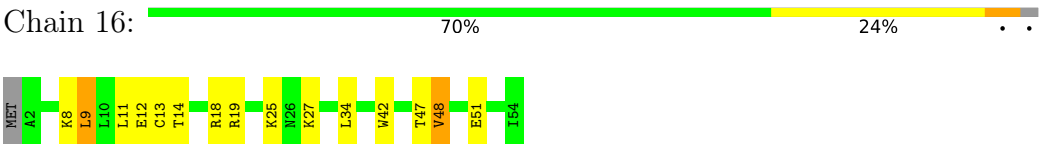

• Molecule 27: 50S ribosomal protein L32

Chain 25:



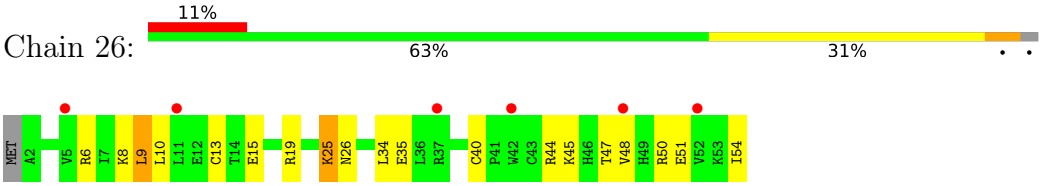

• Molecule 28: 50S ribosomal protein L33

Chain 16:



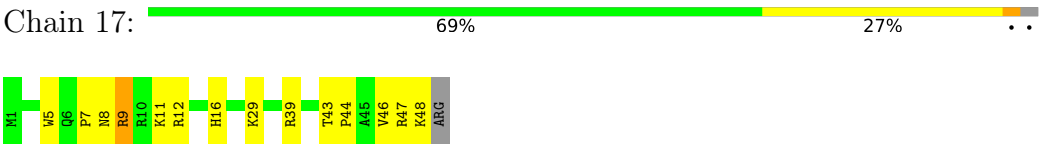

• Molecule 28: 50S ribosomal protein L33

Chain 26:



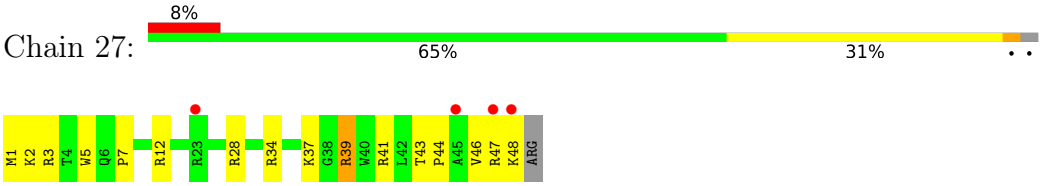

• Molecule 29: 50S ribosomal protein L34

Chain 17:



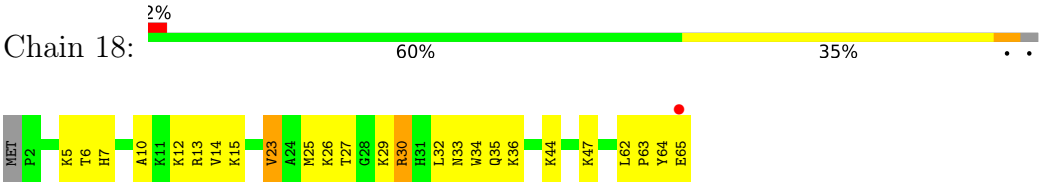

• Molecule 29: 50S ribosomal protein L34

Chain 27:



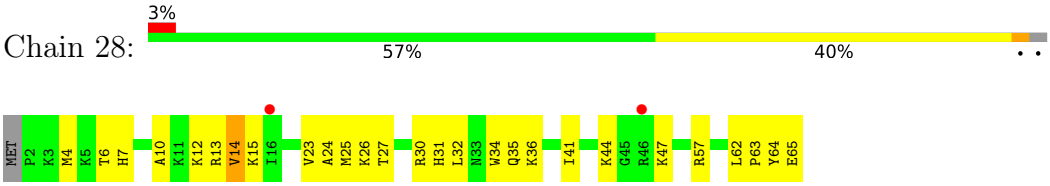

• Molecule 30: 50S ribosomal protein L35

Chain 18:



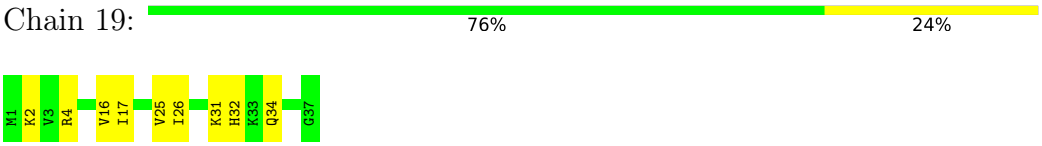

• Molecule 30: 50S ribosomal protein L35

Chain 28:



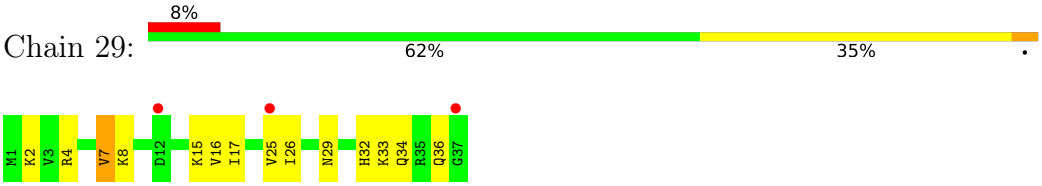

• Molecule 31: 50S ribosomal protein L36

Chain 19:



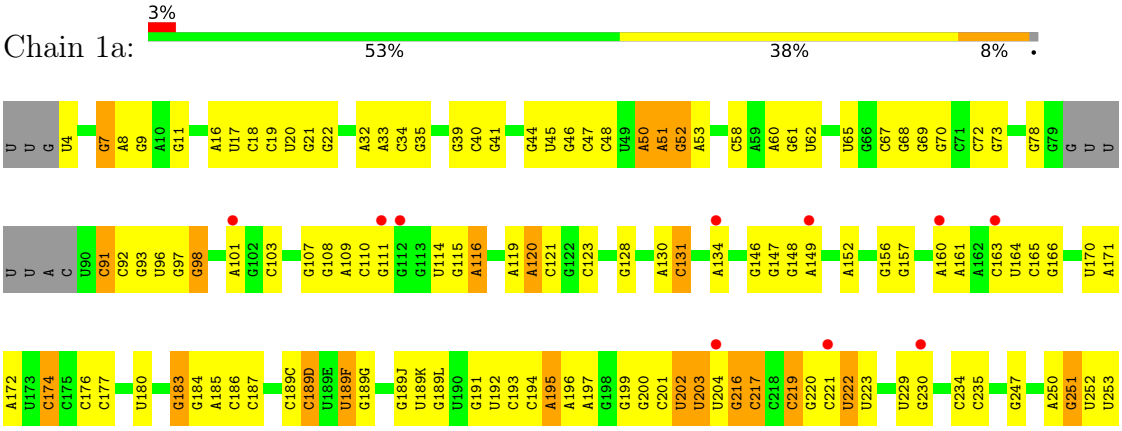

• Molecule 31: 50S ribosomal protein L36

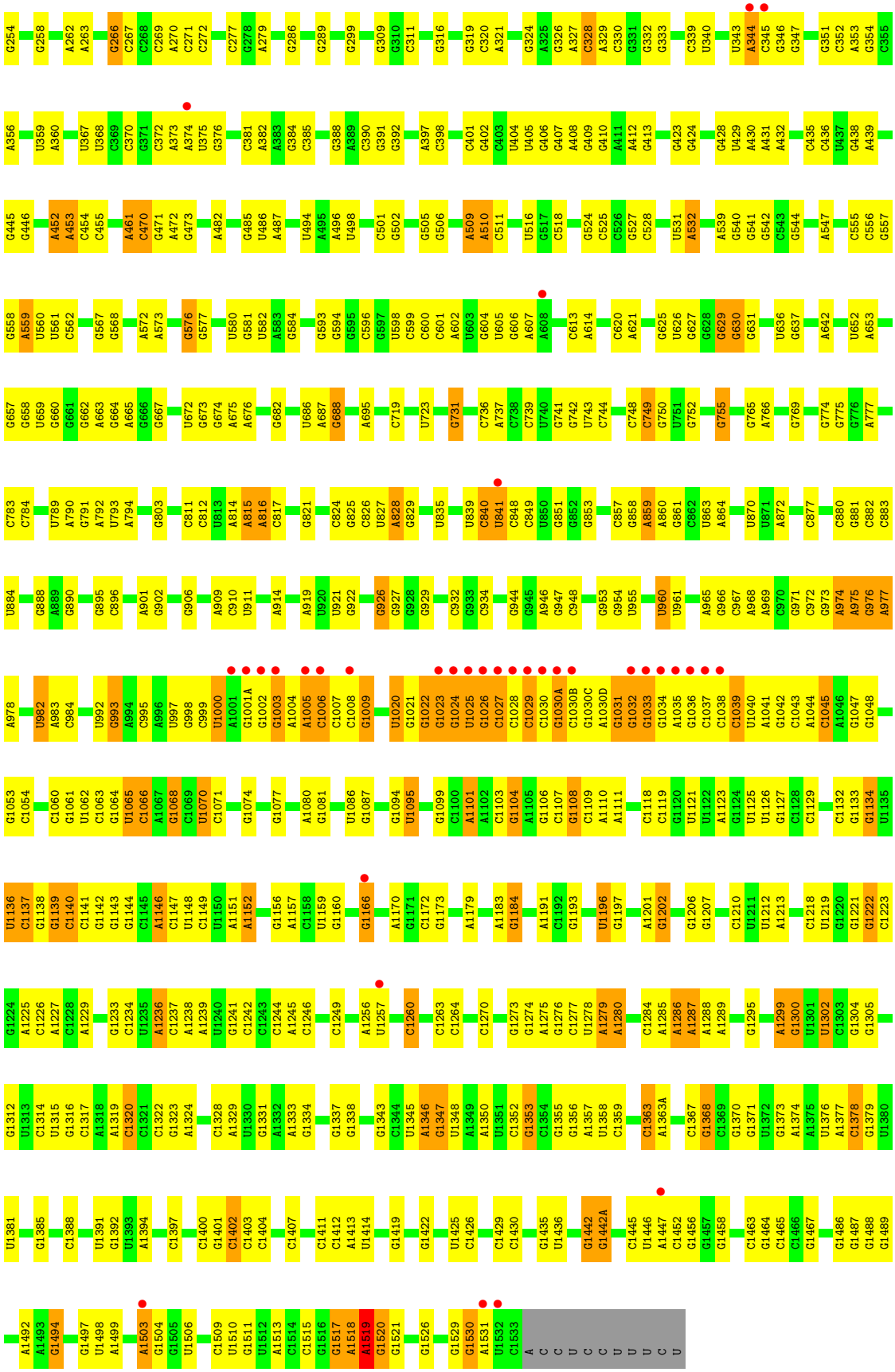
Chain 29:




• Molecule 32: 16S Ribosomal RNA

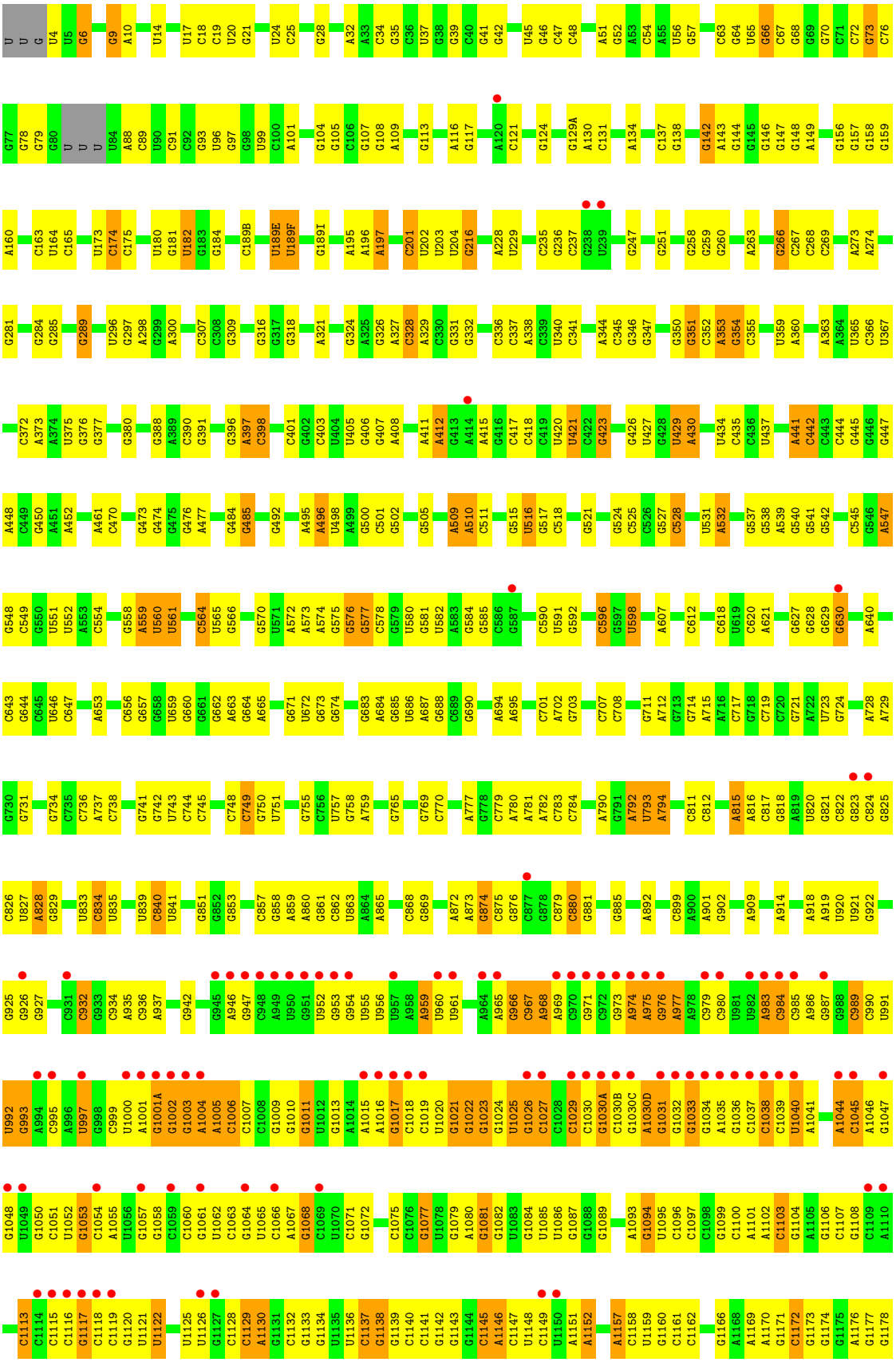
Chain 1a:

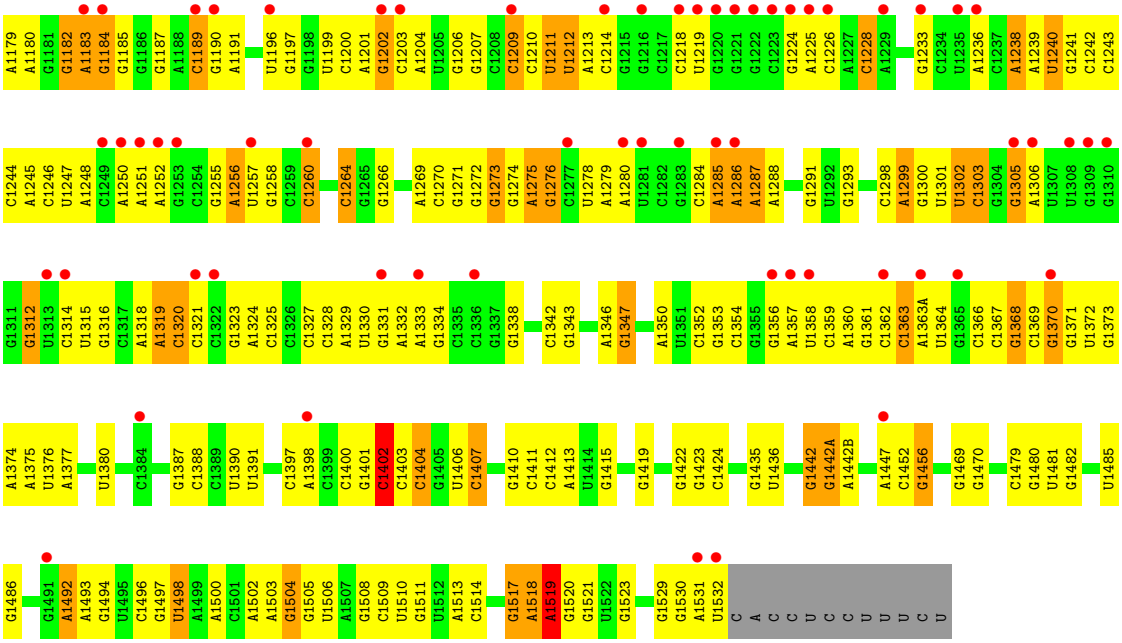




• Molecule 32: 16S Ribosomal RNA

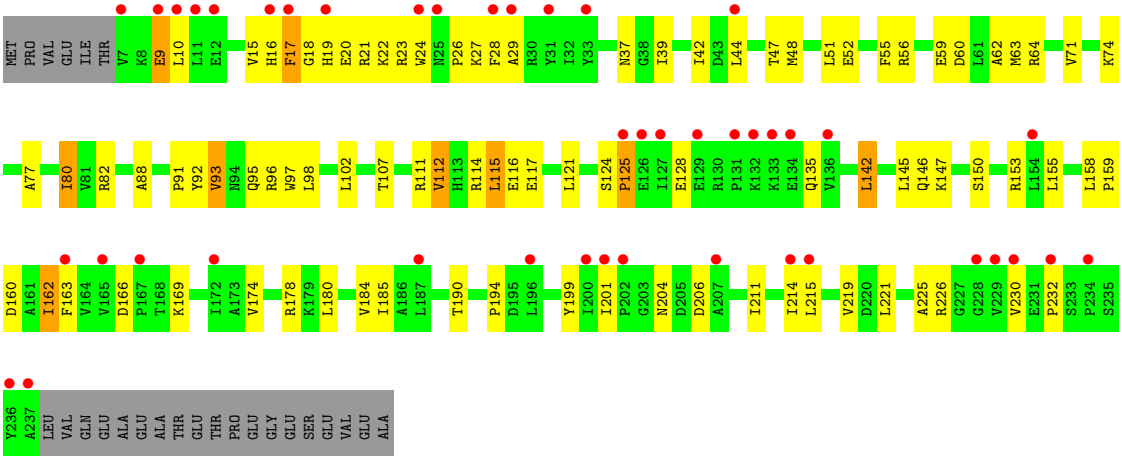
Chain 2a:





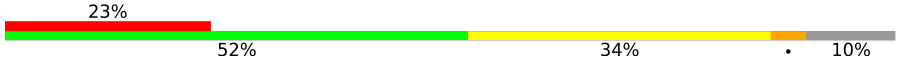
• Molecule 33: 30S ribosomal protein S2

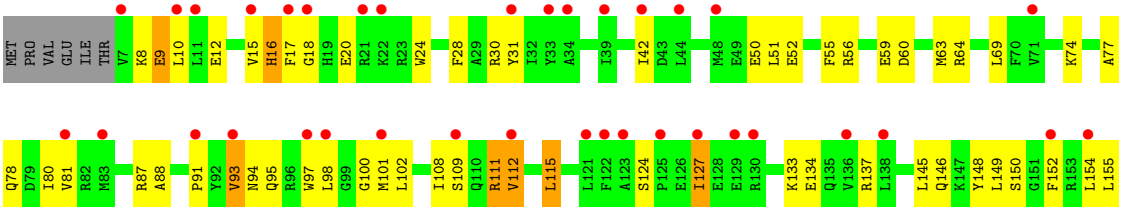
Chain 1b:

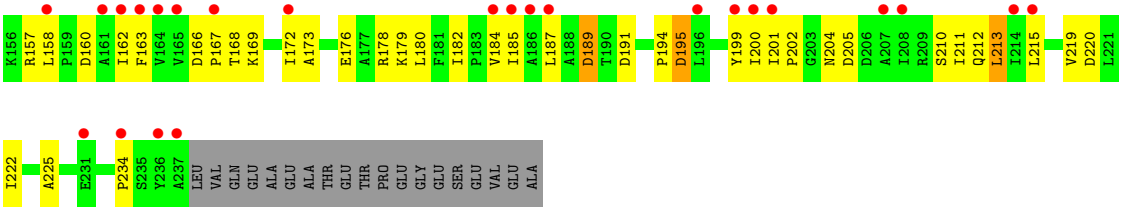


• Molecule 33: 30S ribosomal protein S2

Chain 2b:



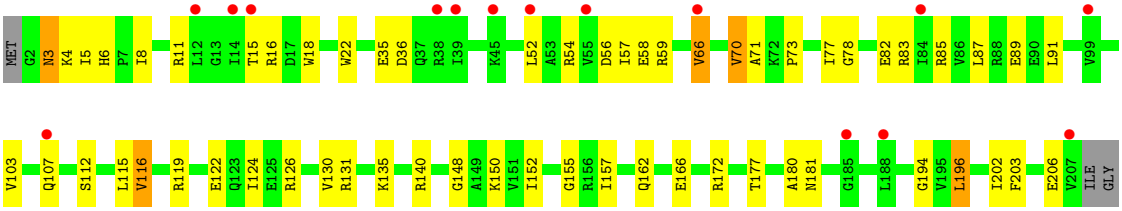



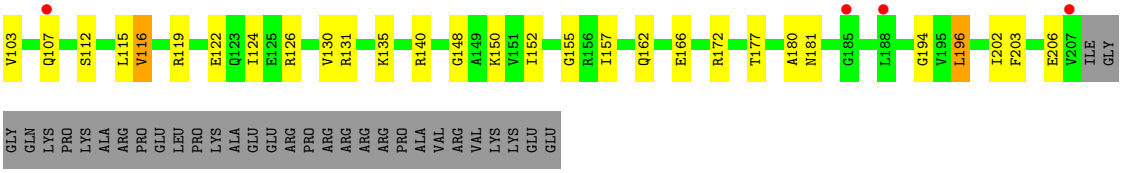




• Molecule 34: 30S ribosomal protein S3

Chain 1c:

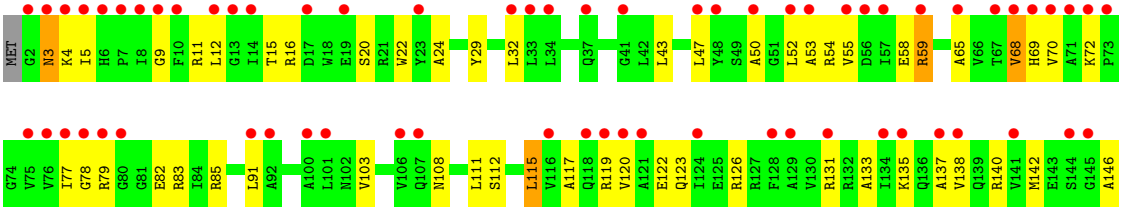


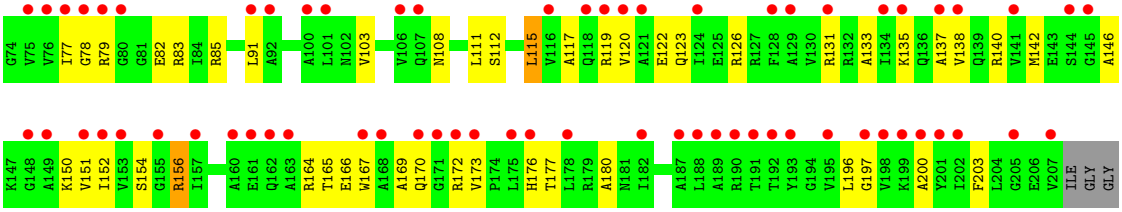


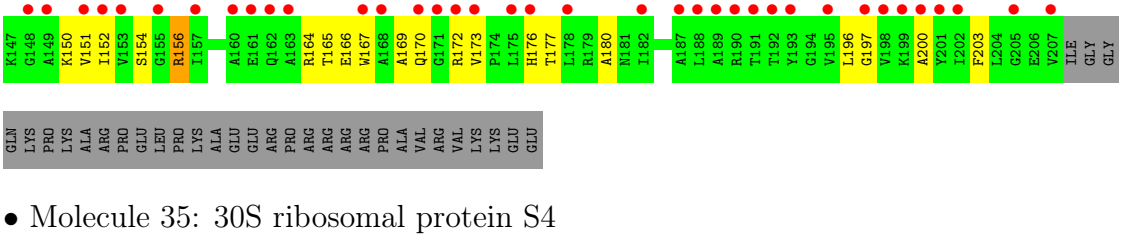


• Molecule 34: 30S ribosomal protein S3

Chain 2c:



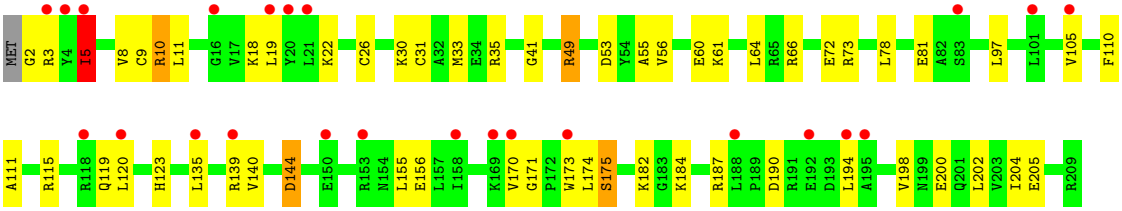






• Molecule 35: 30S ribosomal protein S4

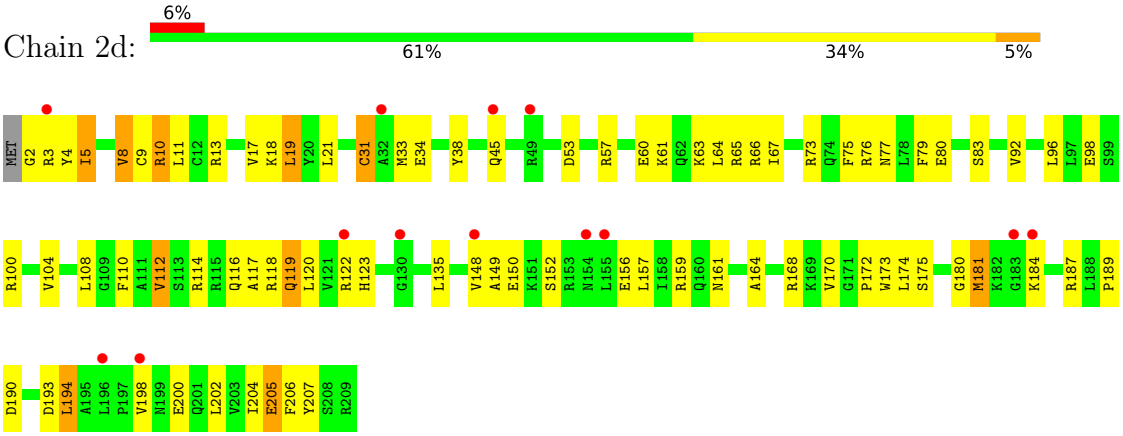
Chain 1d:





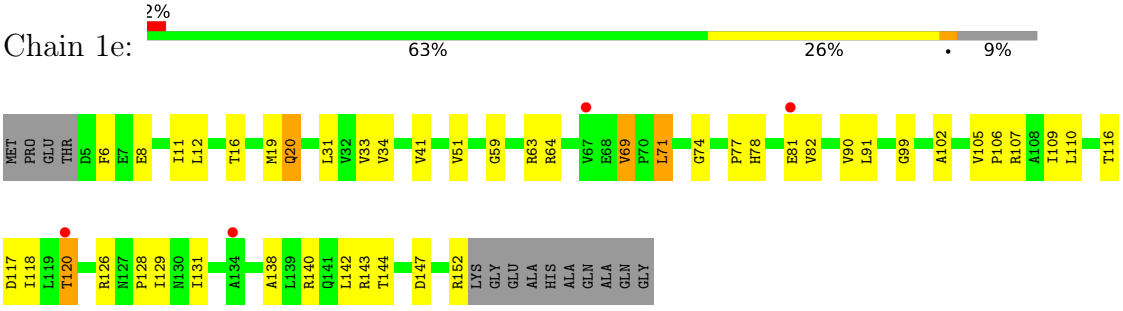
• Molecule 35: 30S ribosomal protein S4

Chain 2d:



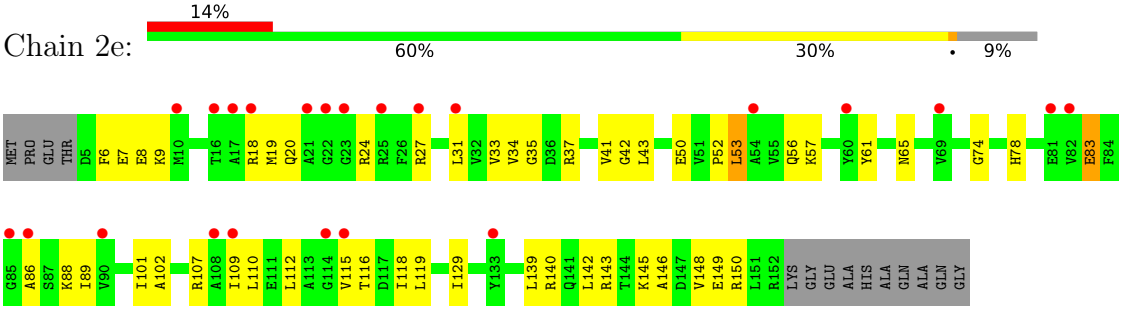

• Molecule 36: 30S ribosomal protein S5

Chain 1e:



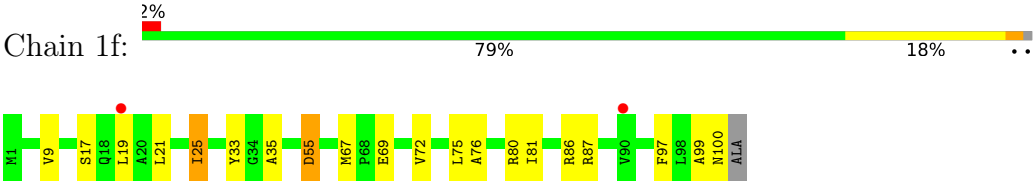

• Molecule 36: 30S ribosomal protein S5

Chain 2e:



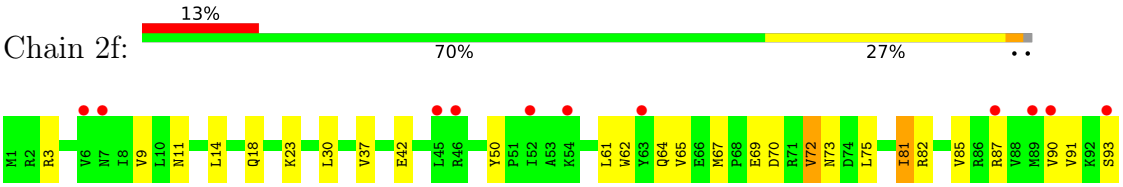

• Molecule 37: 30S ribosomal protein S6

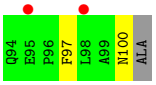
Chain 1f:




• Molecule 37: 30S ribosomal protein S6

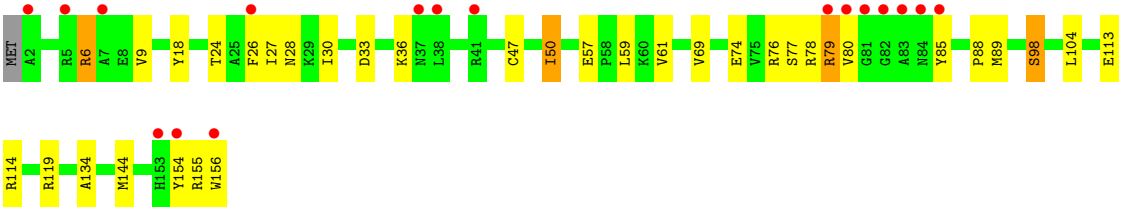
Chain 2f:





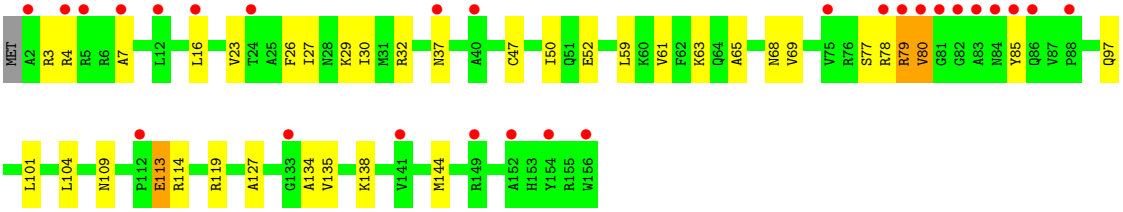

• Molecule 38: 30S ribosomal protein S7

Chain 1g:



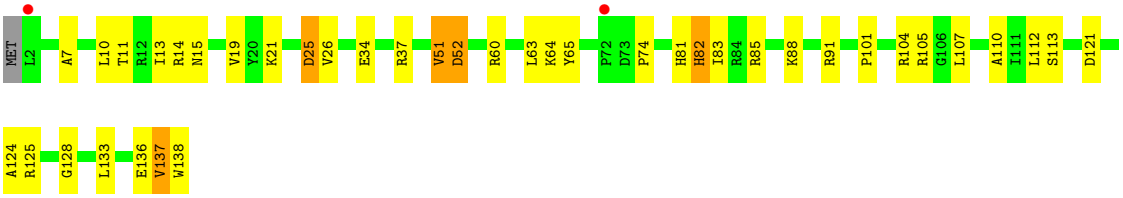

• Molecule 38: 30S ribosomal protein S7

Chain 2g:



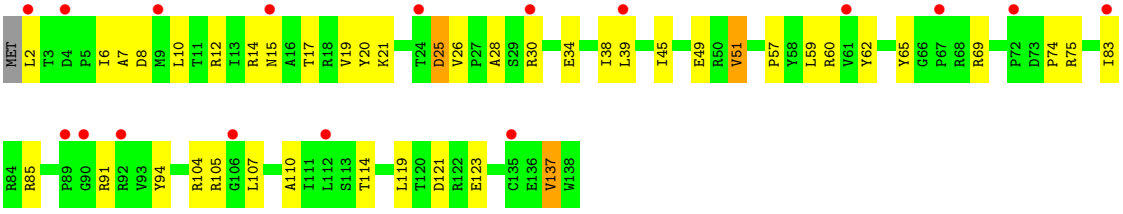

• Molecule 39: 30S ribosomal protein S8

Chain 1h:



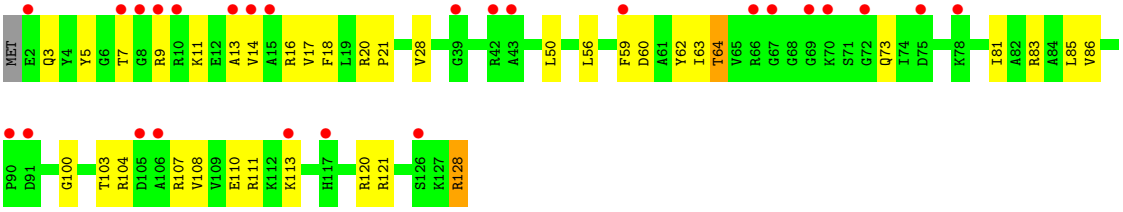

• Molecule 39: 30S ribosomal protein S8

Chain 2h:

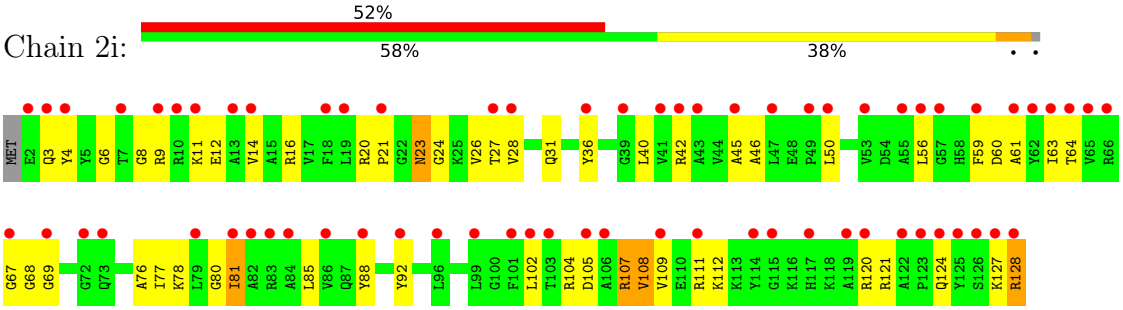



• Molecule 40: 30S ribosomal protein S9

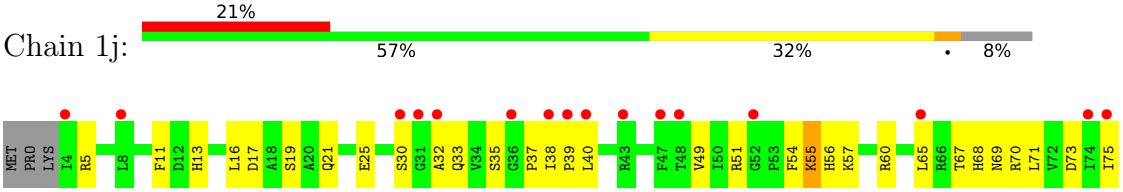
Chain 1i:



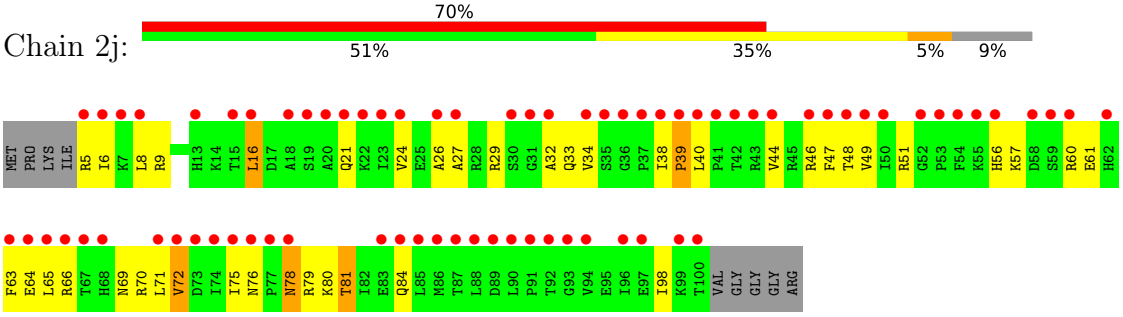

• Molecule 40: 30S ribosomal protein S9



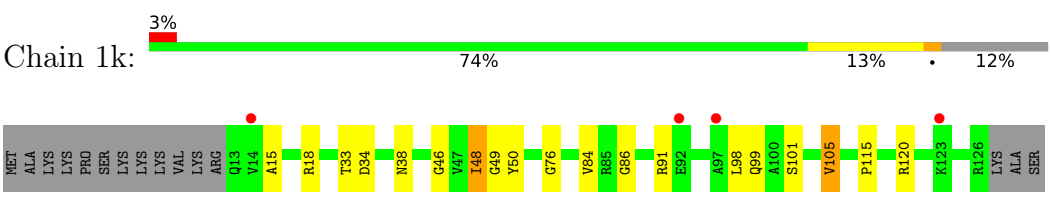

• Molecule 41: 30S ribosomal protein S10




• Molecule 41: 30S ribosomal protein S10

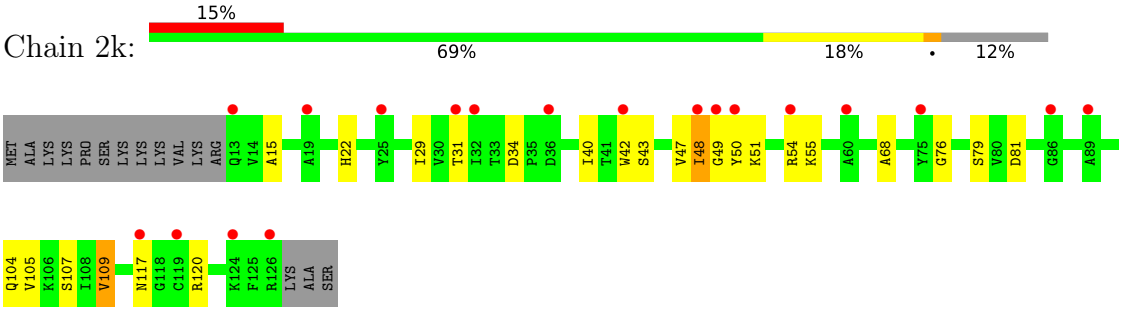



• Molecule 42: 30S ribosomal protein S11



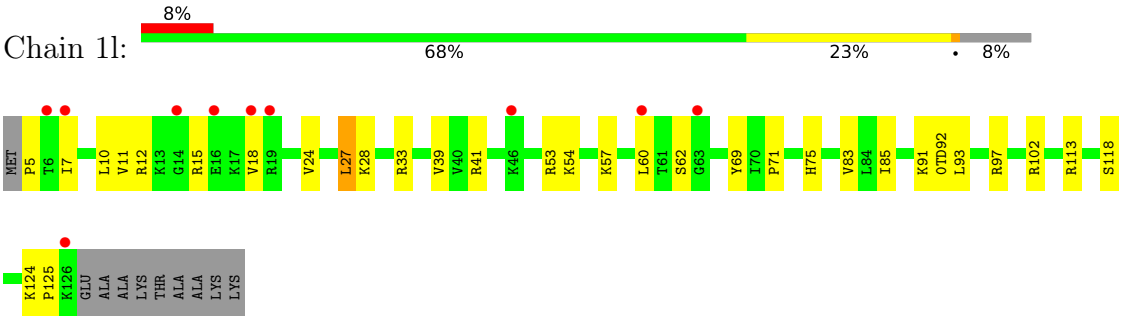

• Molecule 42: 30S ribosomal protein S11

Chain 2k:



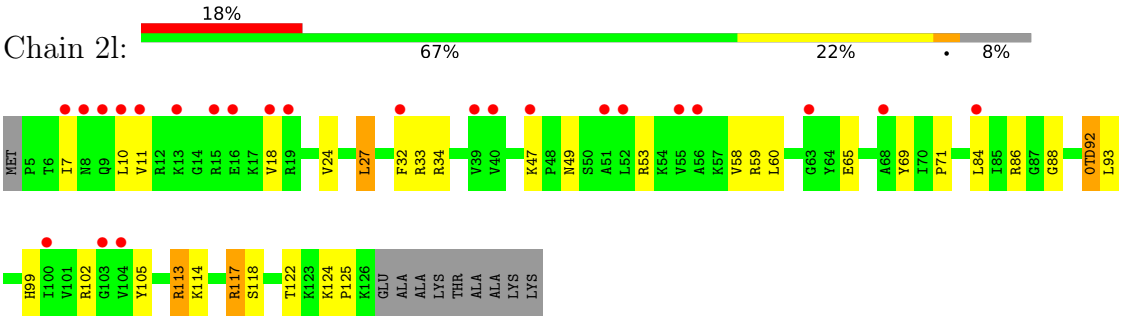

• Molecule 43: 30S ribosomal protein S12

Chain 1l:



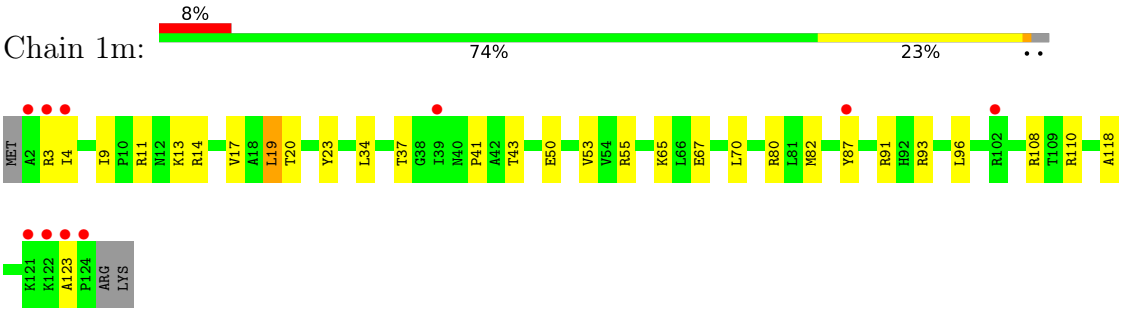

• Molecule 43: 30S ribosomal protein S12

Chain 2l:



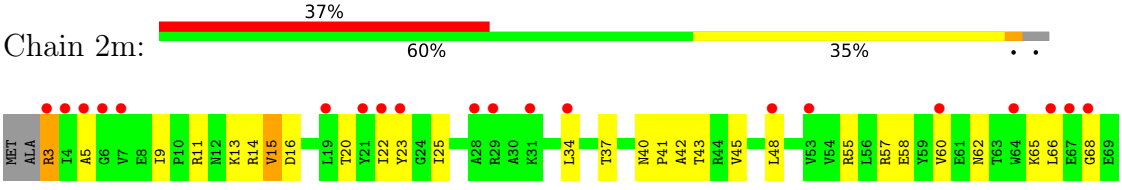

• Molecule 44: 30S ribosomal protein S13

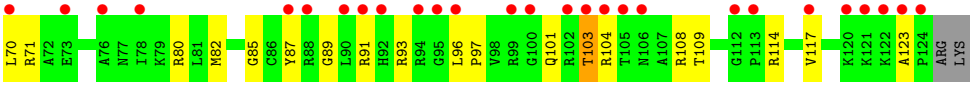
Chain 1m:




• Molecule 44: 30S ribosomal protein S13

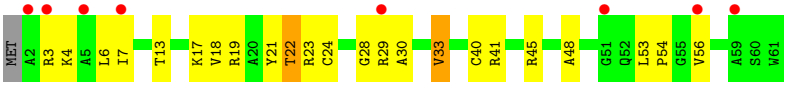
Chain 2m:





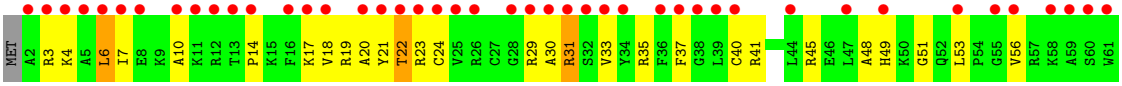

• Molecule 45: 30S ribosomal protein S14 type Z

Chain 1n:



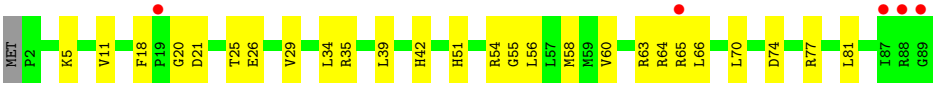

• Molecule 45: 30S ribosomal protein S14 type Z

Chain 2n:



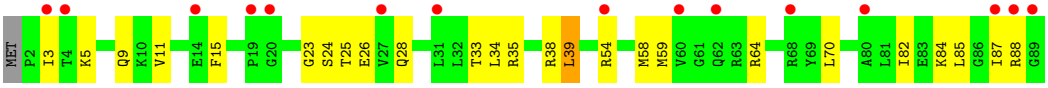

• Molecule 46: 30S ribosomal protein S15

Chain 1o:




• Molecule 46: 30S ribosomal protein S15

Chain 2o:

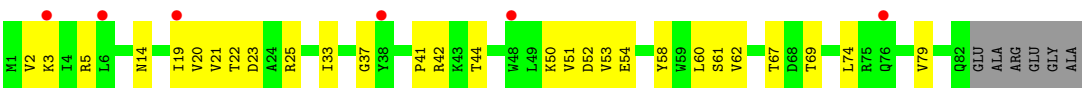



• Molecule 47: 30S ribosomal protein S16

Chain 1p:

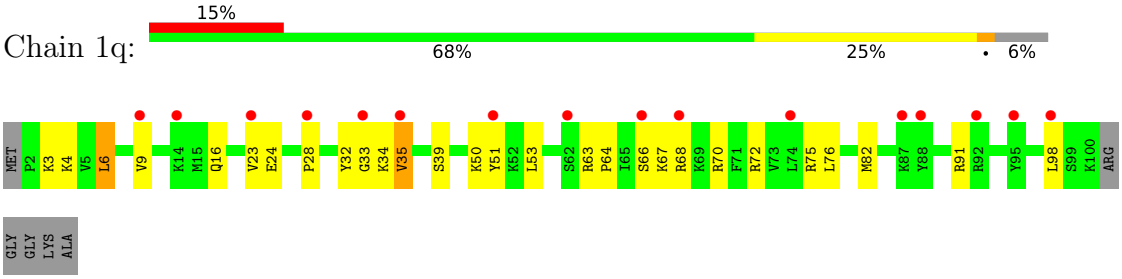
• Molecule 47: 30S ribosomal protein S16

Chain 2p:



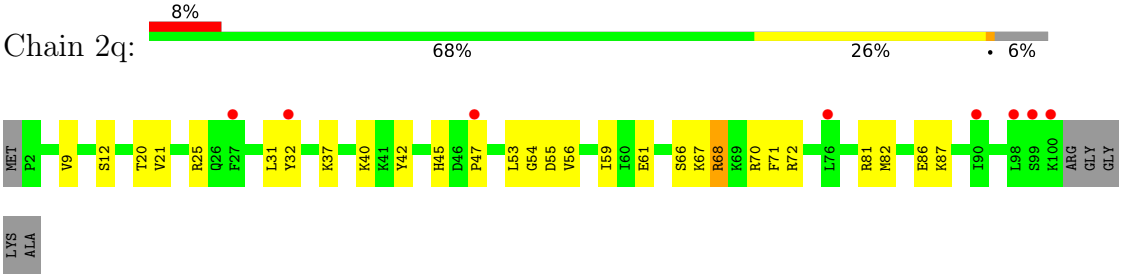

• Molecule 48: 30S ribosomal protein S17

Chain 1q:



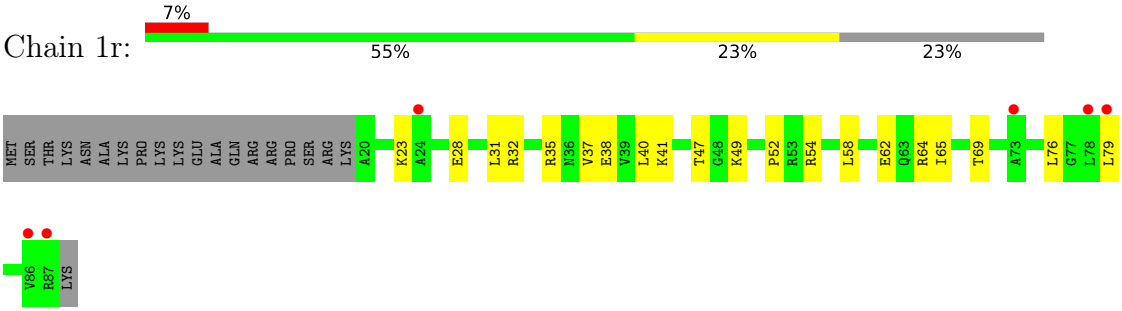

• Molecule 48: 30S ribosomal protein S17

Chain 2q:



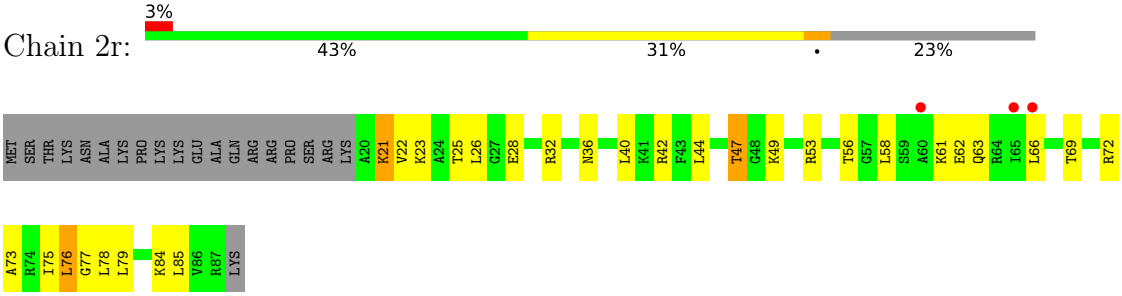

• Molecule 49: 30S ribosomal protein S18

Chain 1r:



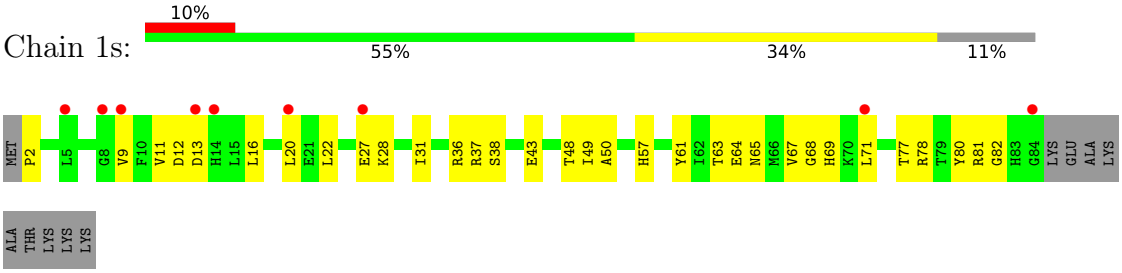

• Molecule 49: 30S ribosomal protein S18

Chain 2r:



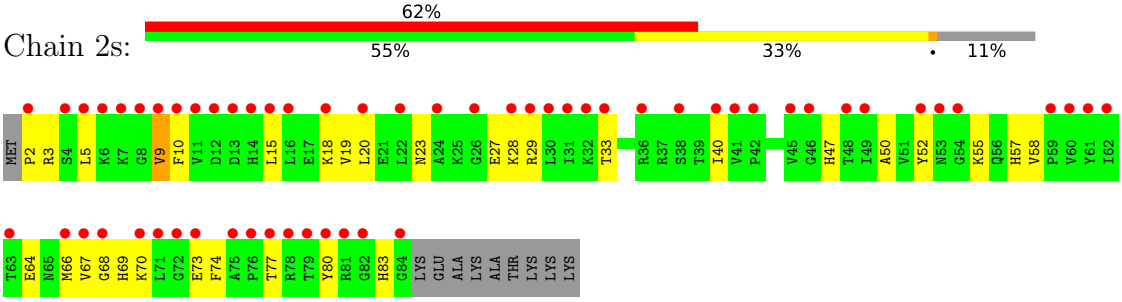

• Molecule 50: 30S ribosomal protein S19

Chain 1s:



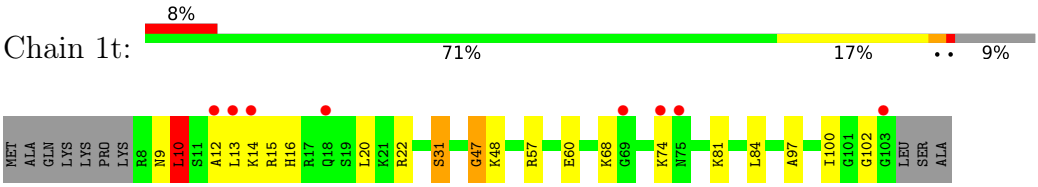
• Molecule 50: 30S ribosomal protein S19

Chain 2s:



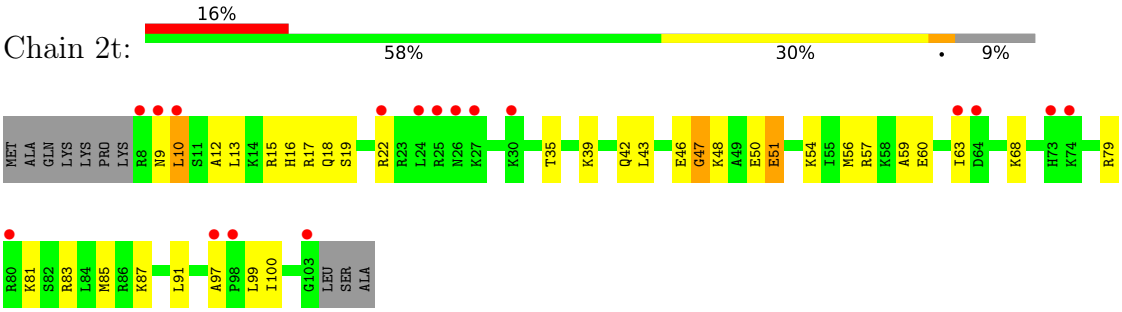

• Molecule 51: 30S ribosomal protein S20

Chain 1t:



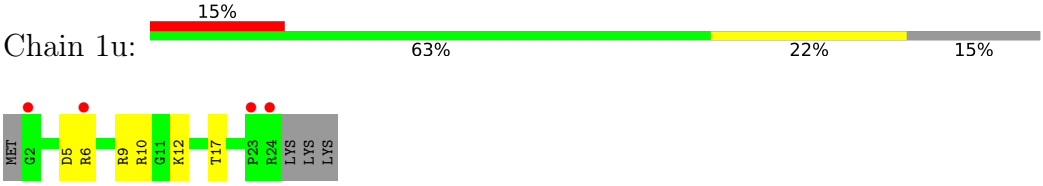

• Molecule 51: 30S ribosomal protein S20

Chain 2t:



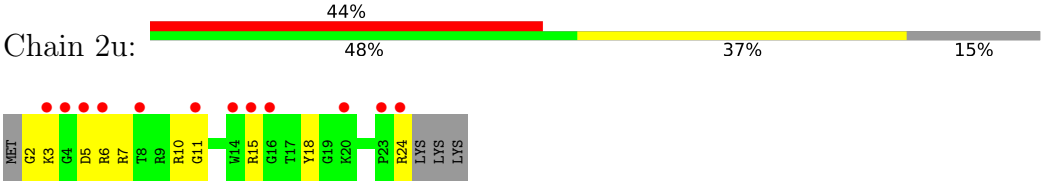

• Molecule 52: 30S ribosomal protein Thx

Chain 1u:



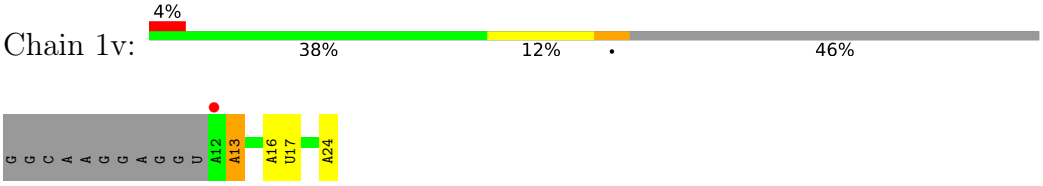

• Molecule 52: 30S ribosomal protein Thx

Chain 2u:



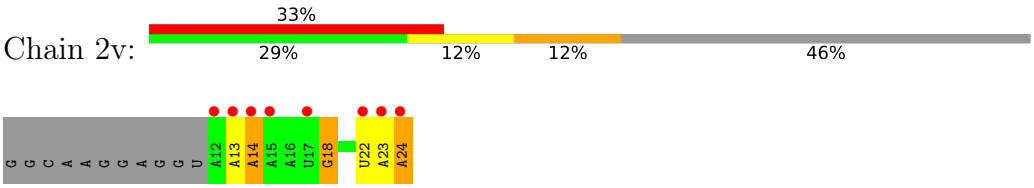

• Molecule 53: mRNA

Chain 1v:



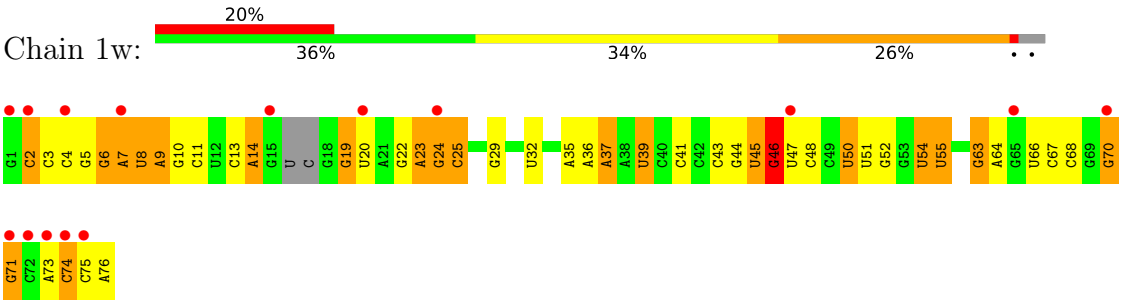
• Molecule 53: mRNA

Chain 2v:



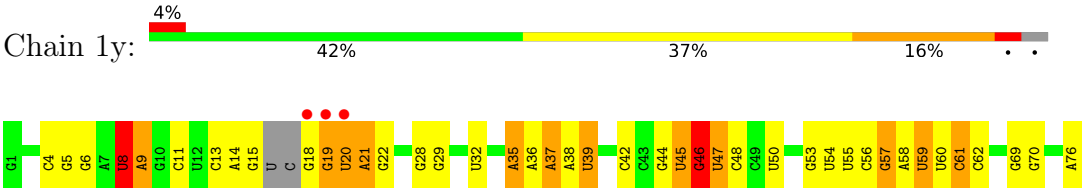

• Molecule 54: A-site and E-site tRNAs

Chain 1w:



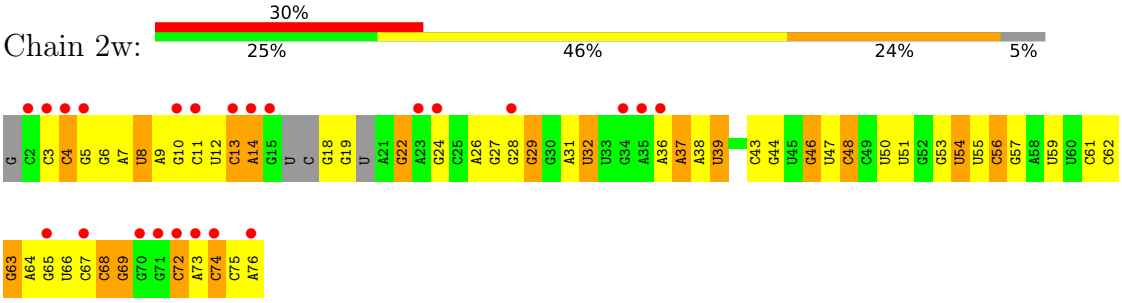

• Molecule 54: A-site and E-site tRNAs

Chain 1y:



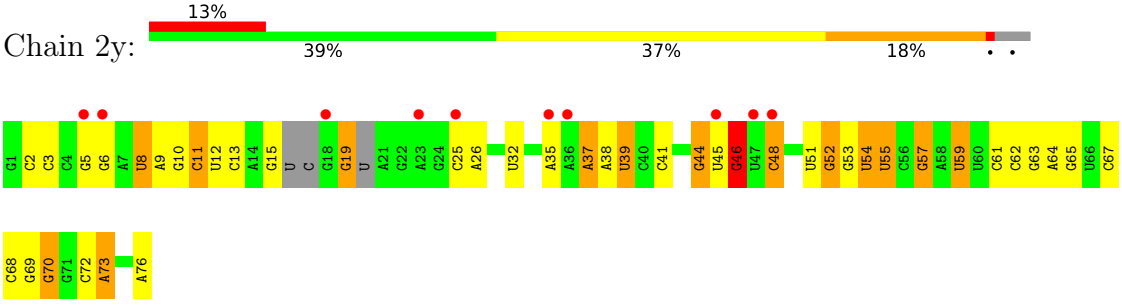

• Molecule 54: A-site and E-site tRNAs

Chain 2w:



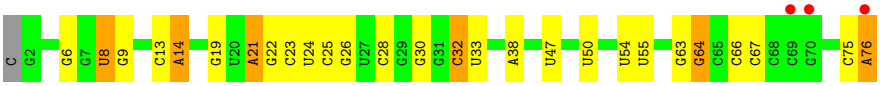

• Molecule 54: A-site and E-site tRNAs

Chain 2y:



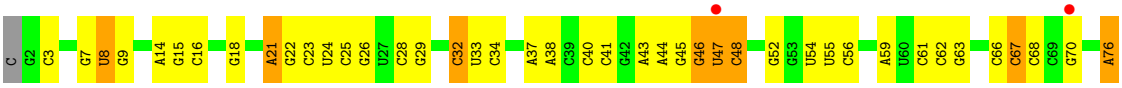

• Molecule 55: P-site tRNA

Chain 1x:




• Molecule 55: P-site tRNA

Chain 2x:



# 4 Data and refinement statistics (i)

| Property | Value | Source |
|---|---|---|
| Space group | P 21 21 21 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 208.99Å 448.29Å 618.52Å<br>90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 127.28 – 2.60<br>127.28 – 2.60 | Depositor<br>EDS |
| % Data completeness<br>(in resolution range) | 98.7 (127.28-2.60)<br>98.7 (127.28-2.60) | Depositor<br>EDS |
| $R_{merge}$ | 0.20 | Depositor |
| $R_{sym}$ | (Not available) | Depositor |
| $< I/\sigma(I) >$ [1] | 1.19 (at 2.62Å) | Xtriage |
| Refinement program | PHENIX 1.8.2 | Depositor |
| R, $R_{free}$ | 0.229 , 0.276<br>0.240 , 0.284 | Depositor<br>DCC |
| $R_{free}$ test set | 86986 reflections (4.96%) | wwPDB-VP |
| Wilson B-factor (Å$^2$) | 52.3 | Xtriage |
| Anisotropy | 0.172 | Xtriage |
| Bulk solvent $k_{sol}$(e/Å$^3$), $B_{sol}$(Å$^2$) | 0.30 , 50.4 | EDS |
| L-test for twinning[2] | $< \|L\| > = 0.38$, $< L^2 > = 0.21$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| $F_o$,$F_c$ correlation | 0.91 | EDS |
| Total number of atoms | 300833 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 58.0 | wwPDB-VP |

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

[1] Intensities estimated from amplitudes.

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

# 5 Model quality (i)

## 5.1 Standard geometry (i)

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

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

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #$\|Z\|$ >5 | RMSZ | #$\|Z\|$ >5 |
| 1 | 1A | 0.19 | 0/69009 | 0.37 | 0/107712 |
| 1 | 2A | 0.14 | 0/67293 | 0.32 | 0/105034 |
| 2 | 1B | 0.14 | 0/2882 | 0.31 | 0/4494 |
| 2 | 2B | 0.13 | 0/2879 | 0.32 | 0/4487 |
| 3 | 1D | 0.25 | 0/2186 | 0.46 | 0/2944 |
| 3 | 2D | 0.17 | 0/2186 | 0.41 | 0/2944 |
| 4 | 1E | 0.18 | 0/1592 | 0.43 | 0/2149 |
| 4 | 2E | 0.15 | 0/1592 | 0.39 | 0/2149 |
| 5 | 1F | 0.17 | 0/1619 | 0.42 | 0/2193 |
| 5 | 2F | 0.14 | 0/1615 | 0.35 | 0/2188 |
| 6 | 1G | 0.16 | 0/1448 | 0.37 | 0/1957 |
| 6 | 2G | 0.13 | 0/1453 | 0.39 | 0/1963 |
| 7 | 1H | 0.16 | 0/1356 | 0.35 | 0/1834 |
| 7 | 2H | 0.13 | 0/1356 | 0.33 | 0/1834 |
| 8 | 1I | 0.13 | 0/1112 | 0.33 | 0/1514 |
| 8 | 2I | 0.14 | 0/1079 | 0.36 | 0/1475 |
| 9 | 1N | 0.18 | 0/1144 | 0.39 | 0/1543 |
| 9 | 2N | 0.13 | 0/1144 | 0.36 | 0/1543 |
| 10 | 1O | 0.19 | 0/943 | 0.38 | 0/1269 |
| 10 | 2O | 0.15 | 0/943 | 0.35 | 0/1269 |
| 11 | 1P | 0.19 | 0/1152 | 0.41 | 0/1533 |
| 11 | 2P | 0.15 | 0/1152 | 0.39 | 0/1533 |
| 12 | 1Q | 0.18 | 0/1143 | 0.38 | 0/1527 |
| 12 | 2Q | 0.14 | 0/1143 | 0.37 | 0/1527 |
| 13 | 1R | 0.18 | 0/982 | 0.41 | 0/1312 |
| 13 | 2R | 0.14 | 0/982 | 0.37 | 0/1312 |
| 14 | 1S | 0.15 | 0/883 | 0.41 | 0/1176 |
| 14 | 2S | 0.13 | 0/880 | 0.37 | 0/1172 |
| 15 | 1T | 0.17 | 0/1105 | 0.39 | 0/1477 |
| 15 | 2T | 0.14 | 0/1097 | 0.37 | 0/1468 |
| 16 | 1U | 0.19 | 0/977 | 0.38 | 0/1301 |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 16 | 2U | 0.14 | 0/977 | 0.34 | 0/1301 |
| 17 | 1V | 0.19 | 0/782 | 0.39 | 0/1049 |
| 17 | 2V | 0.15 | 0/782 | 0.37 | 0/1049 |
| 18 | 1W | 0.19 | 0/897 | 0.40 | 0/1205 |
| 18 | 2W | 0.14 | 0/897 | 0.34 | 0/1205 |
| 19 | 1X | 0.18 | 0/764 | 0.44 | 0/1025 |
| 19 | 2X | 0.13 | 0/764 | 0.35 | 0/1025 |
| 20 | 1Y | 0.17 | 0/819 | 0.41 | 0/1095 |
| 20 | 2Y | 0.14 | 0/819 | 0.38 | 0/1095 |
| 21 | 1Z | 0.16 | 0/1267 | 0.39 | 0/1717 |
| 21 | 2Z | 0.15 | 0/1299 | 0.39 | 0/1763 |
| 22 | 10 | 0.18 | 0/662 | 0.43 | 0/881 |
| 22 | 20 | 0.15 | 0/662 | 0.43 | 0/881 |
| 23 | 11 | 0.16 | 0/762 | 0.36 | 0/1014 |
| 23 | 21 | 0.15 | 0/762 | 0.34 | 0/1014 |
| 24 | 12 | 0.16 | 0/590 | 0.36 | 0/781 |
| 24 | 22 | 0.14 | 0/590 | 0.31 | 0/781 |
| 25 | 13 | 0.18 | 0/474 | 0.38 | 0/635 |
| 25 | 23 | 0.15 | 0/469 | 0.36 | 0/630 |
| 26 | 14 | 0.20 | 0/565 | 0.53 | 0/761 |
| 26 | 24 | 0.19 | 0/545 | 0.46 | 0/737 |
| 27 | 15 | 0.20 | 0/469 | 0.48 | 0/635 |
| 27 | 25 | 0.16 | 0/469 | 0.38 | 0/635 |
| 28 | 16 | 0.18 | 0/460 | 0.42 | 0/613 |
| 28 | 26 | 0.15 | 0/456 | 0.41 | 0/608 |
| 29 | 17 | 0.19 | 0/426 | 0.42 | 0/561 |
| 29 | 27 | 0.17 | 0/426 | 0.42 | 0/561 |
| 30 | 18 | 0.18 | 0/525 | 0.38 | 0/691 |
| 30 | 28 | 0.14 | 0/525 | 0.32 | 0/691 |
| 31 | 19 | 0.18 | 0/310 | 0.38 | 0/407 |
| 31 | 29 | 0.15 | 0/310 | 0.40 | 0/407 |
| 32 | 1a | 0.14 | 1/35795 (0.0%) | 0.32 | 0/55864 |
| 32 | 2a | 0.14 | 0/35886 | 0.32 | 0/56005 |
| 33 | 1b | 0.15 | 0/1881 | 0.42 | 0/2542 |
| 33 | 2b | 0.17 | 0/1860 | 0.42 | 0/2518 |
| 34 | 1c | 0.14 | 0/1572 | 0.34 | 0/2126 |
| 34 | 2c | 0.14 | 0/1566 | 0.37 | 0/2119 |
| 35 | 1d | 0.15 | 0/1685 | 0.37 | 0/2262 |
| 35 | 2d | 0.14 | 0/1704 | 0.38 | 0/2284 |
| 36 | 1e | 0.14 | 0/1145 | 0.40 | 0/1543 |
| 36 | 2e | 0.15 | 0/1149 | 0.43 | 0/1548 |
| 37 | 1f | 0.14 | 0/823 | 0.35 | 0/1115 |
| 37 | 2f | 0.14 | 0/829 | 0.34 | 0/1123 |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 38 | 1g | 0.14 | 0/1250 | 0.35 | 0/1679 |
| 38 | 2g | 0.14 | 0/1254 | 0.38 | 0/1683 |
| 39 | 1h | 0.13 | 0/1108 | 0.34 | 0/1494 |
| 39 | 2h | 0.12 | 0/1108 | 0.36 | 0/1494 |
| 40 | 1i | 0.16 | 0/1002 | 0.42 | 0/1346 |
| 40 | 2i | 0.15 | 0/997 | 0.42 | 0/1343 |
| 41 | 1j | 0.14 | 0/722 | 0.41 | 0/982 |
| 41 | 2j | 0.15 | 0/727 | 0.43 | 0/988 |
| 42 | 1k | 0.12 | 0/844 | 0.32 | 0/1145 |
| 42 | 2k | 0.12 | 0/848 | 0.31 | 0/1149 |
| 43 | 1l | 0.14 | 0/937 | 0.38 | 0/1260 |
| 43 | 2l | 0.14 | 0/937 | 0.37 | 0/1260 |
| 44 | 1m | 0.16 | 0/969 | 0.37 | 0/1302 |
| 44 | 2m | 0.16 | 0/961 | 0.39 | 0/1291 |
| 45 | 1n | 0.13 | 0/501 | 0.36 | 0/664 |
| 45 | 2n | 0.14 | 0/501 | 0.35 | 0/664 |
| 46 | 1o | 0.13 | 0/739 | 0.33 | 0/985 |
| 46 | 2o | 0.12 | 0/739 | 0.33 | 0/985 |
| 47 | 1p | 0.14 | 0/697 | 0.39 | 0/939 |
| 47 | 2p | 0.18 | 0/693 | 0.43 | 0/935 |
| 48 | 1q | 0.14 | 0/836 | 0.34 | 0/1117 |
| 48 | 2q | 0.14 | 0/836 | 0.36 | 0/1117 |
| 49 | 1r | 0.13 | 0/560 | 0.33 | 0/746 |
| 49 | 2r | 0.12 | 0/560 | 0.33 | 0/746 |
| 50 | 1s | 0.17 | 0/667 | 0.46 | 0/900 |
| 50 | 2s | 0.20 | 0/661 | 0.55 | 0/893 |
| 51 | 1t | 0.14 | 0/730 | 0.41 | 0/965 |
| 51 | 2t | 0.16 | 0/729 | 0.43 | 0/965 |
| 52 | 1u | 0.15 | 0/203 | 0.42 | 0/266 |
| 52 | 2u | 0.17 | 0/203 | 0.43 | 0/266 |
| 53 | 1v | 0.16 | 0/310 | 0.29 | 0/480 |
| 53 | 2v | 0.19 | 0/310 | 0.34 | 0/480 |
| 54 | 1w | 0.21 | 1/1606 (0.1%) | 0.37 | 0/2497 |
| 54 | 1y | 0.20 | 1/1606 (0.1%) | 0.35 | 0/2497 |
| 54 | 2w | 0.21 | 0/1556 | 0.35 | 0/2418 |
| 54 | 2y | 0.20 | 0/1583 | 0.35 | 0/2459 |
| 55 | 1x | 0.21 | 0/1725 | 0.36 | 0/2689 |
| 55 | 2x | 0.19 | 0/1725 | 0.31 | 0/2689 |
| All | All | 0.16 | 3/316686 (0.0%) | 0.35 | 0/474113 |

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 |

All (3) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 54 | 1w | 8 | 4SU | O3'-P | 5.09 | 1.61 | 1.56 |
| 54 | 1y | 8 | 4SU | O3'-P | 5.07 | 1.61 | 1.56 |
| 32 | 1a | 1498 | UR3 | O3'-P | 5.03 | 1.61 | 1.56 |

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 26 | 14 | 57 | GLU | Peptide |

## 5.2 Too-close contacts (i)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 1 | 1A | 61852 | 0 | 31191 | 679 | 0 |
| 1 | 2A | 60322 | 0 | 30425 | 778 | 0 |
| 2 | 1B | 2577 | 0 | 1305 | 23 | 0 |
| 2 | 2B | 2575 | 0 | 1303 | 45 | 0 |
| 3 | 1D | 2136 | 0 | 2218 | 45 | 0 |
| 3 | 2D | 2136 | 0 | 2218 | 61 | 0 |
| 4 | 1E | 1559 | 0 | 1618 | 31 | 0 |
| 4 | 2E | 1559 | 0 | 1618 | 38 | 0 |
| 5 | 1F | 1584 | 0 | 1625 | 44 | 0 |
| 5 | 2F | 1580 | 0 | 1619 | 40 | 0 |
| 6 | 1G | 1423 | 0 | 1436 | 34 | 0 |
| 6 | 2G | 1428 | 0 | 1438 | 46 | 0 |
| 7 | 1H | 1330 | 0 | 1407 | 24 | 0 |
| 7 | 2H | 1330 | 0 | 1407 | 41 | 0 |
| 8 | 1I | 1097 | 0 | 1140 | 17 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 8 | 2I | 1064 | 0 | 1082 | 20 | 0 |
| 9 | 1N | 1117 | 0 | 1184 | 18 | 0 |
| 9 | 2N | 1117 | 0 | 1184 | 26 | 0 |
| 10 | 1O | 933 | 0 | 996 | 18 | 0 |
| 10 | 2O | 933 | 0 | 996 | 31 | 0 |
| 11 | 1P | 1135 | 0 | 1212 | 38 | 0 |
| 11 | 2P | 1135 | 0 | 1212 | 28 | 0 |
| 12 | 1Q | 1122 | 0 | 1179 | 27 | 0 |
| 12 | 2Q | 1122 | 0 | 1179 | 28 | 0 |
| 13 | 1R | 968 | 0 | 1033 | 27 | 0 |
| 13 | 2R | 968 | 0 | 1033 | 26 | 0 |
| 14 | 1S | 873 | 0 | 927 | 18 | 0 |
| 14 | 2S | 870 | 0 | 923 | 18 | 0 |
| 15 | 1T | 1091 | 0 | 1151 | 26 | 0 |
| 15 | 2T | 1083 | 0 | 1136 | 34 | 0 |
| 16 | 1U | 959 | 0 | 1019 | 22 | 0 |
| 16 | 2U | 959 | 0 | 1018 | 20 | 0 |
| 17 | 1V | 771 | 0 | 829 | 10 | 0 |
| 17 | 2V | 771 | 0 | 830 | 15 | 0 |
| 18 | 1W | 886 | 0 | 940 | 24 | 0 |
| 18 | 2W | 886 | 0 | 940 | 11 | 0 |
| 19 | 1X | 750 | 0 | 814 | 9 | 0 |
| 19 | 2X | 750 | 0 | 814 | 16 | 0 |
| 20 | 1Y | 806 | 0 | 881 | 22 | 0 |
| 20 | 2Y | 806 | 0 | 881 | 24 | 0 |
| 21 | 1Z | 1240 | 0 | 1240 | 27 | 0 |
| 21 | 2Z | 1271 | 0 | 1273 | 30 | 0 |
| 22 | 10 | 653 | 0 | 674 | 18 | 0 |
| 22 | 20 | 653 | 0 | 674 | 20 | 0 |
| 23 | 11 | 755 | 0 | 826 | 13 | 0 |
| 23 | 21 | 755 | 0 | 826 | 19 | 0 |
| 24 | 12 | 588 | 0 | 643 | 12 | 0 |
| 24 | 22 | 588 | 0 | 643 | 13 | 0 |
| 25 | 13 | 469 | 0 | 518 | 15 | 0 |
| 25 | 23 | 464 | 0 | 514 | 9 | 0 |
| 26 | 14 | 552 | 0 | 533 | 24 | 0 |
| 26 | 24 | 532 | 0 | 503 | 16 | 0 |
| 27 | 15 | 455 | 0 | 465 | 6 | 0 |
| 27 | 25 | 455 | 0 | 465 | 13 | 0 |
| 28 | 16 | 453 | 0 | 473 | 10 | 0 |
| 28 | 26 | 449 | 0 | 469 | 13 | 0 |
| 29 | 17 | 418 | 0 | 467 | 9 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 29 | 27 | 418 | 0 | 467 | 14 | 0 |
| 30 | 18 | 517 | 0 | 582 | 22 | 0 |
| 30 | 28 | 517 | 0 | 582 | 23 | 0 |
| 31 | 19 | 307 | 0 | 335 | 5 | 0 |
| 31 | 29 | 307 | 0 | 335 | 10 | 0 |
| 32 | 1a | 32246 | 0 | 16295 | 479 | 0 |
| 32 | 2a | 32327 | 0 | 16340 | 586 | 0 |
| 33 | 1b | 1846 | 0 | 1867 | 67 | 0 |
| 33 | 2b | 1825 | 0 | 1828 | 76 | 0 |
| 34 | 1c | 1548 | 0 | 1535 | 39 | 0 |
| 34 | 2c | 1542 | 0 | 1517 | 57 | 0 |
| 35 | 1d | 1655 | 0 | 1675 | 50 | 0 |
| 35 | 2d | 1674 | 0 | 1714 | 61 | 0 |
| 36 | 1e | 1129 | 0 | 1184 | 31 | 0 |
| 36 | 2e | 1133 | 0 | 1191 | 39 | 0 |
| 37 | 1f | 810 | 0 | 804 | 13 | 0 |
| 37 | 2f | 816 | 0 | 808 | 24 | 0 |
| 38 | 1g | 1231 | 0 | 1238 | 21 | 0 |
| 38 | 2g | 1235 | 0 | 1249 | 28 | 0 |
| 39 | 1h | 1088 | 0 | 1126 | 29 | 0 |
| 39 | 2h | 1088 | 0 | 1126 | 33 | 0 |
| 40 | 1i | 983 | 0 | 986 | 24 | 0 |
| 40 | 2i | 978 | 0 | 966 | 44 | 0 |
| 41 | 1j | 709 | 0 | 650 | 24 | 0 |
| 41 | 2j | 714 | 0 | 672 | 31 | 0 |
| 42 | 1k | 829 | 0 | 825 | 10 | 0 |
| 42 | 2k | 833 | 0 | 836 | 16 | 0 |
| 43 | 1l | 932 | 0 | 981 | 19 | 0 |
| 43 | 2l | 932 | 0 | 981 | 25 | 0 |
| 44 | 1m | 958 | 0 | 1002 | 22 | 0 |
| 44 | 2m | 950 | 0 | 988 | 35 | 0 |
| 45 | 1n | 492 | 0 | 529 | 20 | 0 |
| 45 | 2n | 492 | 0 | 529 | 24 | 0 |
| 46 | 1o | 728 | 0 | 760 | 20 | 0 |
| 46 | 2o | 728 | 0 | 760 | 19 | 0 |
| 47 | 1p | 681 | 0 | 697 | 19 | 0 |
| 47 | 2p | 677 | 0 | 686 | 16 | 0 |
| 48 | 1q | 823 | 0 | 891 | 19 | 0 |
| 48 | 2q | 823 | 0 | 891 | 22 | 0 |
| 49 | 1r | 555 | 0 | 618 | 12 | 0 |
| 49 | 2r | 555 | 0 | 618 | 21 | 0 |
| 50 | 1s | 652 | 0 | 662 | 31 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 50 | 2s | 646 | 0 | 644 | 27 | 0 |
| 51 | 1t | 728 | 0 | 798 | 17 | 0 |
| 51 | 2t | 727 | 0 | 796 | 25 | 0 |
| 52 | 1u | 199 | 0 | 208 | 4 | 0 |
| 52 | 2u | 199 | 0 | 208 | 9 | 0 |
| 53 | 1v | 277 | 0 | 140 | 3 | 0 |
| 53 | 2v | 277 | 0 | 140 | 5 | 0 |
| 54 | 1w | 1592 | 0 | 819 | 42 | 0 |
| 54 | 1y | 1585 | 0 | 804 | 30 | 0 |
| 54 | 2w | 1544 | 0 | 788 | 45 | 0 |
| 54 | 2y | 1565 | 0 | 795 | 26 | 0 |
| 55 | 1x | 1625 | 0 | 829 | 14 | 0 |
| 55 | 2x | 1625 | 0 | 829 | 28 | 0 |
| 56 | 10 | 6 | 0 | 0 | 0 | 0 |
| 56 | 11 | 5 | 0 | 0 | 0 | 0 |
| 56 | 12 | 2 | 0 | 0 | 0 | 0 |
| 56 | 13 | 3 | 0 | 0 | 0 | 0 |
| 56 | 14 | 1 | 0 | 0 | 0 | 0 |
| 56 | 15 | 5 | 0 | 0 | 0 | 0 |
| 56 | 16 | 3 | 0 | 0 | 0 | 0 |
| 56 | 17 | 8 | 0 | 0 | 0 | 0 |
| 56 | 18 | 7 | 0 | 0 | 0 | 0 |
| 56 | 19 | 1 | 0 | 0 | 0 | 0 |
| 56 | 1A | 1101 | 0 | 0 | 0 | 0 |
| 56 | 1B | 39 | 0 | 0 | 0 | 0 |
| 56 | 1D | 13 | 0 | 0 | 0 | 0 |
| 56 | 1E | 15 | 0 | 0 | 0 | 0 |
| 56 | 1F | 10 | 0 | 0 | 0 | 0 |
| 56 | 1G | 4 | 0 | 0 | 0 | 0 |
| 56 | 1I | 1 | 0 | 0 | 0 | 0 |
| 56 | 1N | 6 | 0 | 0 | 0 | 0 |
| 56 | 1O | 5 | 0 | 0 | 0 | 0 |
| 56 | 1P | 9 | 0 | 0 | 0 | 0 |
| 56 | 1Q | 8 | 0 | 0 | 0 | 0 |
| 56 | 1R | 3 | 0 | 0 | 0 | 0 |
| 56 | 1S | 3 | 0 | 0 | 0 | 0 |
| 56 | 1T | 4 | 0 | 0 | 0 | 0 |
| 56 | 1U | 12 | 0 | 0 | 0 | 0 |
| 56 | 1V | 7 | 0 | 0 | 0 | 0 |
| 56 | 1W | 5 | 0 | 0 | 0 | 0 |
| 56 | 1X | 5 | 0 | 0 | 0 | 0 |
| 56 | 1Y | 3 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 56 | 1Z | 3 | 0 | 0 | 0 | 0 |
| 56 | 1a | 233 | 0 | 0 | 0 | 0 |
| 56 | 1b | 2 | 0 | 0 | 0 | 0 |
| 56 | 1d | 1 | 0 | 0 | 0 | 0 |
| 56 | 1e | 2 | 0 | 0 | 0 | 0 |
| 56 | 1f | 2 | 0 | 0 | 0 | 0 |
| 56 | 1h | 1 | 0 | 0 | 0 | 0 |
| 56 | 1l | 2 | 0 | 0 | 0 | 0 |
| 56 | 1m | 2 | 0 | 0 | 0 | 0 |
| 56 | 1n | 1 | 0 | 0 | 0 | 0 |
| 56 | 1s | 1 | 0 | 0 | 0 | 0 |
| 56 | 1t | 1 | 0 | 0 | 0 | 0 |
| 56 | 1v | 1 | 0 | 0 | 0 | 0 |
| 56 | 1w | 12 | 0 | 0 | 0 | 0 |
| 56 | 1x | 18 | 0 | 0 | 0 | 0 |
| 56 | 20 | 3 | 0 | 0 | 0 | 0 |
| 56 | 21 | 1 | 0 | 0 | 0 | 0 |
| 56 | 23 | 3 | 0 | 0 | 0 | 0 |
| 56 | 25 | 5 | 0 | 0 | 0 | 0 |
| 56 | 27 | 2 | 0 | 0 | 0 | 0 |
| 56 | 28 | 3 | 0 | 0 | 0 | 0 |
| 56 | 2A | 887 | 0 | 0 | 0 | 0 |
| 56 | 2B | 20 | 0 | 0 | 0 | 0 |
| 56 | 2D | 10 | 0 | 0 | 0 | 0 |
| 56 | 2E | 4 | 0 | 0 | 0 | 0 |
| 56 | 2F | 6 | 0 | 0 | 0 | 0 |
| 56 | 2G | 1 | 0 | 0 | 0 | 0 |
| 56 | 2N | 1 | 0 | 0 | 0 | 0 |
| 56 | 2O | 1 | 0 | 0 | 0 | 0 |
| 56 | 2P | 4 | 0 | 0 | 0 | 0 |
| 56 | 2Q | 4 | 0 | 0 | 0 | 0 |
| 56 | 2R | 2 | 0 | 0 | 0 | 0 |
| 56 | 2T | 4 | 0 | 0 | 0 | 0 |
| 56 | 2U | 3 | 0 | 0 | 0 | 0 |
| 56 | 2V | 3 | 0 | 0 | 0 | 0 |
| 56 | 2W | 3 | 0 | 0 | 0 | 0 |
| 56 | 2X | 1 | 0 | 0 | 0 | 0 |
| 56 | 2Z | 1 | 0 | 0 | 0 | 0 |
| 56 | 2a | 241 | 0 | 0 | 0 | 0 |
| 56 | 2d | 1 | 0 | 0 | 0 | 0 |
| 56 | 2e | 1 | 0 | 0 | 0 | 0 |
| 56 | 2f | 2 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 56 | 2g | 1 | 0 | 0 | 0 | 0 |
| 56 | 2i | 1 | 0 | 0 | 0 | 0 |
| 56 | 2j | 1 | 0 | 0 | 0 | 0 |
| 56 | 2k | 1 | 0 | 0 | 0 | 0 |
| 56 | 2l | 4 | 0 | 0 | 0 | 0 |
| 56 | 2m | 1 | 0 | 0 | 0 | 0 |
| 56 | 2q | 2 | 0 | 0 | 0 | 0 |
| 56 | 2r | 1 | 0 | 0 | 0 | 0 |
| 56 | 2t | 1 | 0 | 0 | 0 | 0 |
| 56 | 2v | 1 | 0 | 0 | 0 | 0 |
| 56 | 2w | 4 | 0 | 0 | 0 | 0 |
| 56 | 2x | 5 | 0 | 0 | 0 | 0 |
| 56 | 2y | 6 | 0 | 0 | 0 | 0 |
| 57 | 1A | 20 | 0 | 11 | 0 | 0 |
| 57 | 2A | 20 | 0 | 11 | 1 | 0 |
| 58 | 1A | 1 | 0 | 0 | 0 | 0 |
| 58 | 2A | 1 | 0 | 0 | 0 | 0 |
| 59 | 14 | 1 | 0 | 0 | 0 | 0 |
| 59 | 15 | 1 | 0 | 0 | 0 | 0 |
| 59 | 16 | 1 | 0 | 0 | 0 | 0 |
| 59 | 19 | 1 | 0 | 0 | 0 | 0 |
| 59 | 1Y | 1 | 0 | 0 | 0 | 0 |
| 59 | 1n | 1 | 0 | 0 | 0 | 0 |
| 59 | 24 | 1 | 0 | 0 | 0 | 0 |
| 59 | 25 | 1 | 0 | 0 | 0 | 0 |
| 59 | 26 | 1 | 0 | 0 | 0 | 0 |
| 59 | 29 | 1 | 0 | 0 | 0 | 0 |
| 59 | 2Y | 1 | 0 | 0 | 0 | 0 |
| 59 | 2n | 1 | 0 | 0 | 0 | 0 |
| 60 | 1d | 8 | 0 | 0 | 11 | 0 |
| 60 | 2d | 8 | 0 | 0 | 3 | 0 |
| 61 | 10 | 12 | 0 | 0 | 1 | 0 |
| 61 | 11 | 10 | 0 | 0 | 0 | 0 |
| 61 | 12 | 4 | 0 | 0 | 0 | 0 |
| 61 | 13 | 4 | 0 | 0 | 0 | 0 |
| 61 | 14 | 2 | 0 | 0 | 0 | 0 |
| 61 | 15 | 7 | 0 | 0 | 0 | 0 |
| 61 | 16 | 1 | 0 | 0 | 1 | 0 |
| 61 | 17 | 7 | 0 | 0 | 0 | 0 |
| 61 | 18 | 19 | 0 | 0 | 2 | 0 |
| 61 | 1A | 2246 | 0 | 0 | 71 | 0 |
| 61 | 1B | 73 | 0 | 0 | 1 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 61 | 1D | 24 | 0 | 0 | 1 | 0 |
| 61 | 1E | 27 | 0 | 0 | 0 | 0 |
| 61 | 1F | 9 | 0 | 0 | 0 | 0 |
| 61 | 1G | 5 | 0 | 0 | 0 | 0 |
| 61 | 1H | 1 | 0 | 0 | 0 | 0 |
| 61 | 1I | 2 | 0 | 0 | 0 | 0 |
| 61 | 1N | 4 | 0 | 0 | 0 | 0 |
| 61 | 1O | 7 | 0 | 0 | 0 | 0 |
| 61 | 1P | 21 | 0 | 0 | 0 | 0 |
| 61 | 1Q | 11 | 0 | 0 | 0 | 0 |
| 61 | 1R | 8 | 0 | 0 | 1 | 0 |
| 61 | 1S | 4 | 0 | 0 | 0 | 0 |
| 61 | 1T | 6 | 0 | 0 | 0 | 0 |
| 61 | 1U | 9 | 0 | 0 | 0 | 0 |
| 61 | 1V | 7 | 0 | 0 | 0 | 0 |
| 61 | 1W | 9 | 0 | 0 | 2 | 0 |
| 61 | 1X | 7 | 0 | 0 | 0 | 0 |
| 61 | 1Y | 3 | 0 | 0 | 0 | 0 |
| 61 | 1Z | 1 | 0 | 0 | 0 | 0 |
| 61 | 1a | 430 | 0 | 0 | 26 | 0 |
| 61 | 1b | 1 | 0 | 0 | 0 | 0 |
| 61 | 1d | 1 | 0 | 0 | 0 | 0 |
| 61 | 1f | 1 | 0 | 0 | 0 | 0 |
| 61 | 1l | 7 | 0 | 0 | 0 | 0 |
| 61 | 1q | 4 | 0 | 0 | 0 | 0 |
| 61 | 1w | 16 | 0 | 0 | 0 | 0 |
| 61 | 1x | 15 | 0 | 0 | 0 | 0 |
| 61 | 1y | 1 | 0 | 0 | 0 | 0 |
| 61 | 20 | 10 | 0 | 0 | 1 | 0 |
| 61 | 21 | 6 | 0 | 0 | 0 | 0 |
| 61 | 22 | 1 | 0 | 0 | 0 | 0 |
| 61 | 25 | 4 | 0 | 0 | 0 | 0 |
| 61 | 27 | 2 | 0 | 0 | 1 | 0 |
| 61 | 28 | 6 | 0 | 0 | 0 | 0 |
| 61 | 29 | 1 | 0 | 0 | 0 | 0 |
| 61 | 2A | 1405 | 0 | 0 | 57 | 0 |
| 61 | 2B | 25 | 0 | 0 | 1 | 0 |
| 61 | 2D | 17 | 0 | 0 | 0 | 0 |
| 61 | 2E | 3 | 0 | 0 | 0 | 0 |
| 61 | 2F | 6 | 0 | 0 | 0 | 0 |
| 61 | 2I | 3 | 0 | 0 | 0 | 0 |
| 61 | 2N | 1 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 61 | 2O | 1 | 0 | 0 | 0 | 0 |
| 61 | 2P | 11 | 0 | 0 | 1 | 0 |
| 61 | 2Q | 2 | 0 | 0 | 0 | 0 |
| 61 | 2R | 3 | 0 | 0 | 0 | 0 |
| 61 | 2T | 5 | 0 | 0 | 0 | 0 |
| 61 | 2U | 2 | 0 | 0 | 0 | 0 |
| 61 | 2W | 3 | 0 | 0 | 0 | 0 |
| 61 | 2Z | 1 | 0 | 0 | 0 | 0 |
| 61 | 2a | 380 | 0 | 0 | 22 | 0 |
| 61 | 2d | 1 | 0 | 0 | 0 | 0 |
| 61 | 2g | 1 | 0 | 0 | 0 | 0 |
| 61 | 2i | 1 | 0 | 0 | 0 | 0 |
| 61 | 2j | 3 | 0 | 0 | 2 | 0 |
| 61 | 2l | 2 | 0 | 0 | 1 | 0 |
| 61 | 2p | 1 | 0 | 0 | 0 | 0 |
| 61 | 2r | 1 | 0 | 0 | 0 | 0 |
| 61 | 2t | 2 | 0 | 0 | 0 | 0 |
| 61 | 2x | 7 | 0 | 0 | 1 | 0 |
| 61 | 2y | 13 | 0 | 0 | 0 | 0 |
| All | All | 300833 | 0 | 196713 | 4469 | 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 10.

All (4469) 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) |
|---|---|---|---|
| 1:2A:2138:C:N4 | 1:2A:2153:G:H1 | 1.53 | 1.07 |
| 35:1d:22:LYS:HB2 | 35:1d:26:CYS:SG | 1.95 | 1.05 |
| 54:1w:7:A:N6 | 54:1w:66:U:H3 | 1.54 | 1.05 |
| 1:2A:2129:C:N4 | 1:2A:2159:G:H1 | 1.55 | 1.03 |
| 1:1A:1058:G:H1 | 1:1A:1080:C:N4 | 1.56 | 1.01 |
| 32:2a:1002:G:H1 | 32:2a:1038:C:N4 | 1.56 | 1.01 |
| 54:2y:52:G:H1 | 54:2y:62:C:H42 | 1.05 | 1.00 |
| 54:2w:50:U:H3 | 54:2w:64:A:N6 | 1.59 | 1.00 |
| 54:2w:50:U:H3 | 54:2w:64:A:H61 | 1.01 | 0.98 |
| 32:1a:998:G:H1 | 32:1a:1043:C:H42 | 1.06 | 0.97 |
| 32:2a:1132:C:H42 | 32:2a:1142:G:H1 | 1.11 | 0.97 |
| 1:1A:1082:U:O4 | 1:1A:1086:A:N1 | 1.96 | 0.97 |
| 1:1A:2100:G:H1 | 1:1A:2189:U:H3 | 1.11 | 0.96 |
| 32:2a:1000:U:H3 | 32:2a:1041:A:H61 | 1.09 | 0.96 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1A:2136:C:N4 | 1:1A:2155:G:H1 | 1.64 | 0.95 |
| 32:2a:1089:G:H1 | 32:2a:1096:C:H42 | 1.02 | 0.94 |
| 1:1A:2136:C:H42 | 1:1A:2155:G:H1 | 0.97 | 0.94 |
| 1:1A:1059:G:H1 | 1:1A:1079:C:N4 | 1.65 | 0.92 |
| 32:2a:1264:C:H42 | 32:2a:1271:G:H1 | 0.98 | 0.92 |
| 32:2a:997:U:H3 | 32:2a:1044:A:H61 | 0.97 | 0.92 |
| 1:2A:2136:C:N4 | 1:2A:2155:G:H1 | 1.68 | 0.92 |
| 1:2A:2121:G:H1 | 1:2A:2177:C:H42 | 0.99 | 0.92 |
| 1:2A:2099:U:H3 | 1:2A:2190:G:H1 | 1.18 | 0.91 |
| 32:2a:1011:G:H1 | 32:2a:1018:C:N4 | 1.68 | 0.91 |
| 1:1A:1082:U:H3 | 1:1A:1086:A:N6 | 1.68 | 0.91 |
| 32:1a:664:G:H22 | 32:1a:741:G:H1 | 1.18 | 0.91 |
| 1:1A:1059:G:H1 | 1:1A:1079:C:H42 | 0.92 | 0.91 |
| 1:1A:1082:U:H3 | 1:1A:1086:A:H61 | 0.92 | 0.91 |
| 55:2x:3:C:H42 | 55:2x:70:G:H1 | 0.94 | 0.91 |
| 55:2x:3:C:N4 | 55:2x:70:G:H1 | 1.68 | 0.91 |
| 32:2a:1089:G:H1 | 32:2a:1096:C:N4 | 1.70 | 0.90 |
| 32:2a:1133:G:H1 | 32:2a:1141:C:H42 | 0.98 | 0.90 |
| 54:1y:28:G:H1 | 54:1y:42:C:H42 | 1.19 | 0.90 |
| 32:2a:997:U:H3 | 32:2a:1044:A:N6 | 1.69 | 0.90 |
| 32:2a:1011:G:H1 | 32:2a:1018:C:H42 | 1.18 | 0.90 |
| 32:1a:1004:A:N6 | 32:1a:1037:C:N3 | 2.19 | 0.89 |
| 1:2A:2096:U:H3 | 1:2A:2193:G:H1 | 1.20 | 0.89 |
| 1:1A:1055:G:H1 | 1:1A:1104:C:H42 | 1.21 | 0.89 |
| 54:1w:6:G:H1 | 54:1w:67:C:H42 | 1.18 | 0.89 |
| 35:1d:31:CYS:SG | 60:1d:302:SF4:FE4 | 1.64 | 0.88 |
| 1:2A:2127:G:C2 | 1:2A:2161:C:N3 | 2.41 | 0.88 |
| 32:2a:1025:U:H3 | 32:2a:1036:G:H1 | 1.13 | 0.88 |
| 32:2a:1264:C:N4 | 32:2a:1271:G:H1 | 1.72 | 0.87 |
| 35:1d:26:CYS:SG | 60:1d:302:SF4:FE2 | 1.66 | 0.87 |
| 1:2A:2121:G:H1 | 1:2A:2177:C:N4 | 1.73 | 0.87 |
| 32:2a:1000:U:H3 | 32:2a:1041:A:N6 | 1.72 | 0.87 |
| 32:2a:1133:G:H1 | 32:2a:1141:C:N4 | 1.71 | 0.86 |
| 35:1d:9:CYS:SG | 60:1d:302:SF4:FE1 | 1.65 | 0.86 |
| 1:1A:2136:C:N3 | 1:1A:2155:G:N2 | 2.23 | 0.85 |
| 1:1A:1054:A:H61 | 1:1A:1105:U:H3 | 1.25 | 0.85 |
| 1:2A:2127:G:N1 | 1:2A:2161:C:C4 | 2.45 | 0.85 |
| 32:2a:559:A:H4' | 32:2a:560:U:H3' | 1.57 | 0.85 |
| 1:2A:2127:G:N2 | 1:2A:2161:C:C2 | 2.44 | 0.85 |
| 35:1d:9:CYS:HG | 60:1d:302:SF4:FE1 | 0.54 | 0.85 |
| 1:2A:2127:G:C6 | 1:2A:2161:C:N4 | 2.45 | 0.85 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:2A:2129:C:H42 | 1:2A:2159:G:H1 | 0.89 | 0.84 |
| 10:2O:35:VAL:HG11 | 10:2O:103:ALA:HB3 | 1.60 | 0.84 |
| 32:1a:998:G:H1 | 32:1a:1043:C:N4 | 1.76 | 0.84 |
| 54:2y:15:G:H22 | 54:2y:48:C:H42 | 1.26 | 0.84 |
| 22:10:10:THR:HG22 | 22:10:12:ASN:H | 1.43 | 0.83 |
| 1:1A:1058:G:N2 | 1:1A:1080:C:N3 | 2.24 | 0.83 |
| 1:1A:1054:A:N6 | 1:1A:1105:U:H3 | 1.76 | 0.83 |
| 11:1P:52:GLU:OE1 | 11:1P:55:ARG:NH1 | 2.11 | 0.83 |
| 54:2w:4:C:H42 | 54:2w:69:G:H1 | 1.26 | 0.83 |
| 54:2y:52:G:H1 | 54:2y:62:C:N4 | 1.75 | 0.83 |
| 11:1P:126:VAL:HG12 | 11:1P:148:LEU:HD23 | 1.60 | 0.83 |
| 1:2A:2127:G:C2 | 1:2A:2161:C:C4 | 2.67 | 0.83 |
| 1:1A:2690:C:OP1 | 13:1R:17:ARG:NH2 | 2.10 | 0.83 |
| 32:2a:1002:G:N2 | 32:2a:1038:C:N3 | 2.27 | 0.83 |
| 1:2A:2138:C:N3 | 1:2A:2153:G:N2 | 2.26 | 0.82 |
| 1:1A:1065:U:O2 | 1:1A:1073:A:N6 | 2.12 | 0.82 |
| 1:2A:878:A:H61 | 1:2A:899:A:H1' | 1.43 | 0.82 |
| 32:2a:1316:G:H22 | 32:2a:1319:A:H5" | 1.44 | 0.82 |
| 32:1a:1402:4OC:HM22 | 32:1a:1403:C:H5' | 1.62 | 0.82 |
| 1:2A:1566:A:OP1 | 3:2D:211:ARG:NH1 | 2.13 | 0.81 |
| 1:1A:1818:U:OP2 | 3:1D:157:ARG:NH1 | 2.13 | 0.81 |
| 1:2A:1607:C:N4 | 1:2A:1622:G:OP2 | 2.14 | 0.81 |
| 32:2a:1273:G:H3' | 32:2a:1274:G:H8 | 1.44 | 0.81 |
| 54:2w:7:A:H5' | 54:2w:8:4SU:H5 | 1.62 | 0.81 |
| 32:2a:266:G:H5" | 32:2a:268:C:H41 | 1.43 | 0.81 |
| 32:2a:1055:A:N7 | 32:2a:1200:C:N4 | 2.27 | 0.81 |
| 1:1A:2135:A:H5' | 1:1A:2160:G:H4' | 1.62 | 0.81 |
| 1:1A:1058:G:H1 | 1:1A:1080:C:H42 | 0.82 | 0.80 |
| 1:2A:2167:U:H2' | 1:2A:2168:G:H21 | 1.42 | 0.80 |
| 2:1B:33:G:H5' | 6:1G:2:PRO:HD3 | 1.64 | 0.80 |
| 32:1a:1027:C:C2 | 32:1a:1034:G:N2 | 2.50 | 0.80 |
| 33:2b:185:ILE:HG22 | 33:2b:199:TYR:HB2 | 1.61 | 0.80 |
| 50:1s:27:GLU:HB2 | 50:1s:28:LYS:HA | 1.62 | 0.80 |
| 1:2A:2129:C:N3 | 1:2A:2159:G:N2 | 2.29 | 0.80 |
| 32:2a:975:A:H4' | 32:2a:976:G:H5" | 1.62 | 0.80 |
| 32:1a:1008:C:N3 | 32:1a:1021:G:O6 | 2.15 | 0.80 |
| 1:1A:2099:U:H3 | 1:1A:2190:G:H1 | 1.27 | 0.79 |
| 1:2A:652(D):C:H42 | 1:2A:652(U):G:H1 | 1.28 | 0.79 |
| 1:1A:882:G:H1 | 1:1A:894:C:H42 | 1.26 | 0.79 |
| 3:2D:69:ARG:HE | 3:2D:130:ALA:HB2 | 1.47 | 0.79 |
| 31:29:25:VAL:HB | 31:29:34:GLN:HB2 | 1.64 | 0.79 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 33:1b:185:ILE:HG22 | 33:1b:199:TYR:HB2 | 1.65 | 0.79 |
| 33:2b:8:LYS:HG3 | 33:2b:9:GLU:HG3 | 1.65 | 0.79 |
| 41:2j:49:VAL:HG23 | 45:2n:41:ARG:HB2 | 1.63 | 0.79 |
| 1:1A:880:G:H2' | 1:1A:881:G:H8 | 1.48 | 0.78 |
| 32:1a:189(F):U:H3 | 48:1q:72:ARG:HH22 | 1.30 | 0.78 |
| 6:2G:38:VAL:HG22 | 6:2G:93:THR:HG23 | 1.65 | 0.78 |
| 1:1A:1817:G:OP1 | 3:1D:88:ARG:NH2 | 2.16 | 0.78 |
| 26:14:58:ARG:HB3 | 50:1s:67:VAL:HB | 1.63 | 0.78 |
| 35:1d:31:CYS:HG | 60:1d:302:SF4:FE4 | 0.52 | 0.78 |
| 32:2a:1047:G:H5" | 45:2n:4:LYS:HD3 | 1.65 | 0.78 |
| 36:1e:105:VAL:HG21 | 36:1e:128:PRO:HB3 | 1.66 | 0.78 |
| 35:2d:53:ASP:HB3 | 35:2d:57:ARG:HH12 | 1.49 | 0.78 |
| 32:2a:953:G:H5' | 32:2a:965:A:H61 | 1.47 | 0.77 |
| 54:1w:22:G:N7 | 54:1w:46:7MG:N2 | 2.30 | 0.77 |
| 1:2A:2206:G:H3' | 1:2A:2207:G:C8 | 2.19 | 0.77 |
| 4:2E:47:VAL:HG11 | 4:2E:86:PRO:HD2 | 1.67 | 0.77 |
| 10:1O:48:PRO:HB3 | 32:1a:1422:G:H5" | 1.66 | 0.77 |
| 1:2A:1689:A:H62 | 1:2A:1698:A:H2 | 1.31 | 0.77 |
| 1:2A:2595:G:N7 | 61:2A:6286:HOH:O | 2.17 | 0.77 |
| 32:2a:1086:U:H3 | 32:2a:1099:G:H22 | 1.30 | 0.77 |
| 32:2a:1350:A:N6 | 61:2a:3301:HOH:O | 2.16 | 0.77 |
| 33:2b:16:HIS:HB2 | 33:2b:204:ASN:HB3 | 1.66 | 0.77 |
| 54:2y:26:A:N6 | 54:2y:44:G:N1 | 2.33 | 0.77 |
| 44:2m:80:ARG:HH12 | 50:2s:69:HIS:HE1 | 1.29 | 0.76 |
| 33:2b:16:HIS:HB3 | 33:2b:210:SER:HB2 | 1.64 | 0.76 |
| 32:2a:1264:C:N3 | 32:2a:1271:G:N2 | 2.32 | 0.76 |
| 32:2a:1129:C:O2' | 32:2a:1130:A:N7 | 2.19 | 0.76 |
| 34:2c:78:GLY:HA3 | 34:2c:83:ARG:H | 1.51 | 0.76 |
| 1:2A:888:C:OP1 | 44:2m:93:ARG:NH1 | 2.18 | 0.76 |
| 8:2I:124:GLY:H | 8:2I:144:VAL:HG23 | 1.50 | 0.76 |
| 54:1w:6:G:H1 | 54:1w:67:C:N4 | 1.84 | 0.76 |
| 4:2E:28:ALA:HB3 | 4:2E:93:VAL:HG12 | 1.68 | 0.76 |
| 32:1a:559:A:H4' | 32:1a:560:U:H3' | 1.68 | 0.75 |
| 32:2a:782:A:OP1 | 32:2a:1521:G:N2 | 2.19 | 0.75 |
| 1:1A:2163:C:OP1 | 1:1A:2165:G:N2 | 2.19 | 0.75 |
| 32:1a:1133:G:H1 | 32:1a:1141:C:H42 | 1.34 | 0.75 |
| 1:2A:994:C:OP1 | 16:2U:53:ARG:NH2 | 2.19 | 0.75 |
| 1:2A:1818:U:OP2 | 3:2D:157:ARG:NH1 | 2.20 | 0.75 |
| 32:2a:664:G:H22 | 32:2a:741:G:H1 | 1.33 | 0.75 |
| 1:1A:1039:G:H1 | 1:1A:1116:C:H42 | 1.33 | 0.75 |
| 32:2a:993:G:O6 | 32:2a:1045:C:N4 | 2.18 | 0.75 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 32:2a:1002:G:H1 | 32:2a:1038:C:H42 | 0.81 | 0.74 |
| 32:1a:682:G:N7 | 61:1a:2309:HOH:O | 2.19 | 0.74 |
| 32:2a:673:G:H2' | 32:2a:674:G:C8 | 2.23 | 0.74 |
| 32:2a:1030:C:H42 | 32:2a:1031:G:H1 | 1.32 | 0.74 |
| 54:1y:28:G:H1 | 54:1y:42:C:N4 | 1.85 | 0.74 |
| 1:2A:143:G:H4' | 19:2X:35:THR:HG21 | 1.70 | 0.74 |
| 1:2A:775:G:O3' | 61:2A:4892:HOH:O | 2.06 | 0.74 |
| 11:2P:52:GLU:OE1 | 11:2P:55:ARG:NH1 | 2.21 | 0.74 |
| 33:2b:77:ALA:HB2 | 33:2b:211:ILE:HD13 | 1.70 | 0.74 |
| 54:2y:15:G:N2 | 54:2y:48:C:H42 | 1.86 | 0.74 |
| 1:2A:2127:G:C2 | 1:2A:2161:C:C2 | 2.75 | 0.74 |
| 32:2a:1132:C:N4 | 32:2a:1142:G:H1 | 1.84 | 0.74 |
| 44:2m:40:ASN:HB3 | 44:2m:43:THR:HG23 | 1.69 | 0.74 |
| 1:1A:2129:C:H42 | 1:1A:2159:G:H1 | 1.36 | 0.74 |
| 35:1d:26:CYS:HG | 60:1d:302:SF4:FE2 | 0.49 | 0.74 |
| 32:2a:324:G:OP1 | 51:2t:22:ARG:NH1 | 2.20 | 0.74 |
| 42:2k:22:HIS:HB3 | 42:2k:29:ILE:HB | 1.68 | 0.74 |
| 32:1a:976:G:N2 | 32:1a:1363:C:OP2 | 2.17 | 0.73 |
| 1:1A:510:C:OP1 | 61:1A:6777:HOH:O | 2.05 | 0.73 |
| 1:1A:2759:G:N7 | 61:1A:4924:HOH:O | 2.20 | 0.73 |
| 32:2a:1007:C:N3 | 32:2a:1022:G:O6 | 2.20 | 0.73 |
| 1:2A:2875:C:OP1 | 15:2T:3:ARG:NH1 | 2.22 | 0.73 |
| 1:1A:400:G:N7 | 61:1A:6131:HOH:O | 2.20 | 0.73 |
| 32:2a:1118:C:OP1 | 40:2i:104:ARG:NH1 | 2.22 | 0.73 |
| 1:1A:272(J):C:H2' | 1:1A:274:G:H8 | 1.52 | 0.73 |
| 4:2E:36:ARG:HG2 | 4:2E:47:VAL:HG12 | 1.71 | 0.73 |
| 32:2a:1030(A):G:N2 | 32:2a:1030(D):A:OP2 | 2.21 | 0.73 |
| 24:12:65:ASN:OD1 | 24:12:69:ARG:NH1 | 2.21 | 0.73 |
| 38:1g:78:ARG:NH1 | 38:1g:154:TYR:O | 2.21 | 0.73 |
| 7:2H:41:MET:HE2 | 7:2H:64:LEU:HB2 | 1.70 | 0.73 |
| 32:2a:1113:C:H42 | 32:2a:1187:G:H1 | 1.36 | 0.73 |
| 61:1a:2406:HOH:O | 52:1u:5:ASP:OD2 | 2.05 | 0.73 |
| 32:2a:1316:G:H5" | 45:2n:17:LYS:HE3 | 1.70 | 0.73 |
| 32:1a:148:G:H2' | 32:1a:149:A:H8 | 1.52 | 0.73 |
| 1:2A:1153:C:OP1 | 16:2U:92:ARG:NH2 | 2.21 | 0.73 |
| 54:1y:8:4SU:O2' | 54:1y:21:A:N1 | 2.20 | 0.73 |
| 1:2A:1011:G:OP2 | 16:2U:66:ASN:ND2 | 2.21 | 0.73 |
| 25:23:5:LYS:NZ | 25:23:34:GLU:OE2 | 2.21 | 0.72 |
| 32:2a:363:A:OP2 | 43:2l:34:ARG:NH1 | 2.22 | 0.72 |
| 11:1P:50:ARG:HD3 | 30:18:7:HIS:CD2 | 2.23 | 0.72 |
| 41:2j:6:ILE:HG12 | 41:2j:98:ILE:HG13 | 1.72 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 54:2w:51:U:H3 | 54:2w:63:G:H1 | 1.37 | 0.72 |
| 1:1A:1105:U:H2' | 1:1A:1106:G:H8 | 1.55 | 0.72 |
| 1:2A:89:G:H3' | 1:2A:90:U:H5" | 1.71 | 0.72 |
| 32:2a:829:G:N7 | 61:2a:3539:HOH:O | 2.22 | 0.72 |
| 20:2Y:77:PRO:HD2 | 20:2Y:106:LEU:HD22 | 1.70 | 0.72 |
| 30:28:32:LEU:O | 30:28:36:LYS:NZ | 2.21 | 0.72 |
| 38:2g:113:GLU:HG2 | 38:2g:119:ARG:HG2 | 1.69 | 0.72 |
| 32:1a:1086:U:H3 | 32:1a:1099:G:H22 | 1.36 | 0.72 |
| 4:1E:77:ILE:HG21 | 4:1E:195:LEU:HD11 | 1.72 | 0.72 |
| 1:1A:279:C:H42 | 1:1A:361:G:H1 | 1.36 | 0.71 |
| 54:1w:29:G:H1 | 54:1w:41:C:H42 | 1.38 | 0.71 |
| 32:2a:737:A:H1' | 37:2f:73:ASN:HD21 | 1.55 | 0.71 |
| 1:2A:698:C:O2' | 1:2A:734:A:N6 | 2.23 | 0.71 |
| 39:1h:14:ARG:NH1 | 39:1h:83:ILE:O | 2.23 | 0.71 |
| 43:1l:71:PRO:O | 43:1l:102:ARG:NH1 | 2.22 | 0.71 |
| 43:2l:117:ARG:HG2 | 43:2l:122:THR:HB | 1.72 | 0.71 |
| 1:1A:1783:A:N7 | 61:1A:6221:HOH:O | 2.24 | 0.71 |
| 32:1a:1006:C:H42 | 32:1a:1023:G:H1 | 1.36 | 0.71 |
| 32:2a:1010:G:N2 | 32:2a:1020:U:HO2' | 1.89 | 0.71 |
| 44:2m:91:ARG:NE | 44:2m:97:PRO:O | 2.22 | 0.71 |
| 54:2w:26:A:N1 | 54:2w:44:G:O6 | 2.22 | 0.71 |
| 32:2a:297:G:N2 | 32:2a:300:A:OP2 | 2.23 | 0.71 |
| 10:1O:63:VAL:HG12 | 10:1O:106:LEU:HD11 | 1.72 | 0.71 |
| 11:1P:59:LEU:HD11 | 30:18:10:ALA:HB2 | 1.73 | 0.71 |
| 12:1Q:10:ARG:HH11 | 12:1Q:11:LYS:HE2 | 1.56 | 0.71 |
| 32:2a:953:G:N7 | 44:2m:104:ARG:NH2 | 2.38 | 0.71 |
| 32:1a:324:G:OP1 | 51:1t:22:ARG:NH1 | 2.24 | 0.71 |
| 32:2a:1011:G:N2 | 32:2a:1018:C:N3 | 2.37 | 0.71 |
| 54:1w:7:A:H61 | 54:1w:66:U:H3 | 0.77 | 0.71 |
| 17:2V:40:LEU:HB2 | 17:2V:46:VAL:HG22 | 1.72 | 0.71 |
| 1:1A:1059:G:N2 | 1:1A:1079:C:N3 | 2.37 | 0.70 |
| 32:1a:324:G:N7 | 61:1a:1902:HOH:O | 2.22 | 0.70 |
| 1:2A:307:G:N1 | 1:2A:310:A:OP2 | 2.24 | 0.70 |
| 1:2A:309:G:N3 | 1:2A:329:G:O2' | 2.24 | 0.70 |
| 1:2A:1780:A:N7 | 61:2A:4441:HOH:O | 2.24 | 0.70 |
| 40:2i:23:ASN:N | 40:2i:23:ASN:OD1 | 2.24 | 0.70 |
| 1:1A:2153:G:H2' | 1:1A:2154:G:H8 | 1.56 | 0.70 |
| 1:2A:2121:G:N2 | 1:2A:2177:C:N3 | 2.33 | 0.70 |
| 1:2A:2502:G:N7 | 61:2A:5288:HOH:O | 2.23 | 0.70 |
| 1:2A:2683:C:O2 | 10:2O:70:LYS:NZ | 2.20 | 0.70 |
| 61:2a:3487:HOH:O | 52:2u:2:GLY:N | 2.24 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 33:2b:69:LEU:HB3 | 33:2b:162:ILE:HG22 | 1.72 | 0.70 |
| 1:1A:1023:U:OP2 | 61:1A:5955:HOH:O | 2.09 | 0.70 |
| 1:2A:897:C:H1' | 54:2w:56:C:H5 | 1.56 | 0.70 |
| 1:2A:2138:C:H42 | 1:2A:2153:G:H1 | 0.77 | 0.70 |
| 22:20:10:THR:HG22 | 22:20:12:ASN:H | 1.57 | 0.70 |
| 9:1N:67:LEU:HA | 9:1N:87:LEU:HD22 | 1.74 | 0.70 |
| 36:2e:31:LEU:HD11 | 36:2e:129:ILE:HA | 1.73 | 0.70 |
| 54:2y:46:7MG:O2' | 54:2y:48:C:OP2 | 2.09 | 0.70 |
| 1:1A:2722:G:OP2 | 61:1A:4900:HOH:O | 2.10 | 0.70 |
| 1:1A:1506:C:H2' | 1:1A:1507:A:H8 | 1.55 | 0.70 |
| 33:2b:134:GLU:HA | 33:2b:137:ARG:HE | 1.57 | 0.70 |
| 32:1a:975:A:H4' | 32:1a:976:G:H5" | 1.73 | 0.70 |
| 32:1a:1009:G:O6 | 32:1a:1020:U:O2 | 2.08 | 0.70 |
| 1:1A:2789:C:O2 | 1:1A:2894:G:N2 | 2.17 | 0.70 |
| 1:2A:500:G:N1 | 1:2A:503:A:OP2 | 2.25 | 0.70 |
| 6:2G:79:ASN:N | 6:2G:79:ASN:OD1 | 2.25 | 0.70 |
| 3:1D:125:ILE:HB | 37:1f:81:ILE:HD11 | 1.74 | 0.70 |
| 1:2A:947:G:OP2 | 61:2A:5952:HOH:O | 2.10 | 0.70 |
| 32:2a:501:C:H2' | 32:2a:502:G:H8 | 1.56 | 0.70 |
| 34:2c:20:SER:HB3 | 34:2c:22:TRP:HE1 | 1.57 | 0.70 |
| 1:1A:2810:A:N6 | 1:1A:2891:G:O2' | 2.23 | 0.69 |
| 34:1c:6:HIS:HD2 | 34:1c:8:ILE:H | 1.40 | 0.69 |
| 32:2a:662:G:H2' | 32:2a:663:A:C8 | 2.27 | 0.69 |
| 1:1A:2507:C:O2' | 54:1w:74:C:N4 | 2.25 | 0.69 |
| 30:18:6:THR:HG22 | 30:18:63:PRO:HD2 | 1.72 | 0.69 |
| 1:2A:630:G:OP2 | 30:28:15:LYS:NZ | 2.24 | 0.69 |
| 32:2a:1010:G:N2 | 32:2a:1020:U:O2' | 2.25 | 0.69 |
| 32:2a:1020:U:H2' | 32:2a:1021:G:C8 | 2.28 | 0.69 |
| 42:2k:54:ARG:NH1 | 54:2y:39:PSU:O2' | 2.25 | 0.69 |
| 1:2A:1204:A:H2 | 1:2A:1241:A:H62 | 1.40 | 0.69 |
| 12:1Q:111:GLU:OE2 | 12:1Q:133:ARG:NH2 | 2.24 | 0.69 |
| 1:2A:854:G:H2' | 1:2A:855:G:H8 | 1.57 | 0.69 |
| 9:2N:34:LEU:HD21 | 9:2N:120:LEU:HB2 | 1.73 | 0.69 |
| 14:2S:27:SER:HA | 14:2S:88:ASP:HB3 | 1.75 | 0.69 |
| 32:2a:1203:C:H2' | 32:2a:1204:A:H8 | 1.57 | 0.69 |
| 54:1w:6:G:N2 | 54:1w:67:C:N3 | 2.39 | 0.69 |
| 1:2A:962:G:OP1 | 61:2A:4963:HOH:O | 2.11 | 0.69 |
| 32:2a:380:G:N7 | 61:2a:3596:HOH:O | 2.24 | 0.69 |
| 32:2a:1040:U:H2' | 32:2a:1041:A:H8 | 1.57 | 0.69 |
| 33:2b:87:ARG:NH2 | 33:2b:220:ASP:OD1 | 2.23 | 0.69 |
| 17:2V:46:VAL:HG23 | 17:2V:52:VAL:HG11 | 1.73 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 28:26:10:LEU:HD13 | 28:26:19:ARG:HD3 | 1.75 | 0.69 |
| 32:2a:25:C:H5' | 32:2a:524:G:H1' | 1.73 | 0.69 |
| 1:1A:1311:G:H2' | 29:17:47:ARG:HH22 | 1.57 | 0.69 |
| 28:26:34:LEU:H | 28:26:51:GLU:HG2 | 1.58 | 0.69 |
| 36:2e:74:GLY:HA3 | 36:2e:116:THR:HG22 | 1.75 | 0.69 |
| 1:1A:1055:G:H1 | 1:1A:1104:C:N4 | 1.89 | 0.69 |
| 40:1i:128:ARG:NH2 | 55:1x:33:U:OP2 | 2.26 | 0.69 |
| 1:2A:84:A:N1 | 1:2A:98:G:O2' | 2.24 | 0.69 |
| 6:2G:64:THR:HB | 6:2G:94:LEU:HD21 | 1.74 | 0.68 |
| 55:2x:3:C:N3 | 55:2x:70:G:N2 | 2.38 | 0.68 |
| 41:1j:49:VAL:HG23 | 45:1n:41:ARG:HB2 | 1.75 | 0.68 |
| 6:2G:18:GLU:OE1 | 6:2G:21:ARG:NH1 | 2.26 | 0.68 |
| 32:2a:542:G:OP1 | 35:2d:10:ARG:NH2 | 2.25 | 0.68 |
| 32:2a:976:G:H5' | 32:2a:1358:U:O2' | 1.93 | 0.68 |
| 1:1A:1053:C:H42 | 1:1A:1106:G:H1 | 1.40 | 0.68 |
| 33:2b:212:GLN:NE2 | 33:2b:234:PRO:O | 2.25 | 0.68 |
| 1:1A:2683:C:O2 | 10:1O:70:LYS:NZ | 2.20 | 0.68 |
| 1:2A:2805:G:H2' | 1:2A:2807:G:C8 | 2.29 | 0.68 |
| 35:2d:98:GLU:HG3 | 35:2d:194:LEU:HD11 | 1.74 | 0.68 |
| 1:1A:1009:A:OP2 | 9:1N:37:LYS:NZ | 2.27 | 0.68 |
| 46:2o:25:THR:HG21 | 46:2o:70:LEU:HB2 | 1.74 | 0.68 |
| 34:1c:131:ARG:NH1 | 34:1c:166:GLU:OE2 | 2.26 | 0.68 |
| 35:1d:18:LYS:NZ | 35:1d:31:CYS:SG | 2.66 | 0.68 |
| 1:2A:2136:C:N3 | 1:2A:2155:G:N2 | 2.36 | 0.68 |
| 1:2A:2431:U:OP1 | 61:2A:4426:HOH:O | 2.12 | 0.68 |
| 34:2c:11:ARG:HB3 | 34:2c:15:THR:HB | 1.74 | 0.68 |
| 47:2p:14:ASN:OD1 | 47:2p:42:ARG:NH2 | 2.27 | 0.68 |
| 12:1Q:10:ARG:HH12 | 12:1Q:90:VAL:H | 1.40 | 0.68 |
| 1:2A:586:A:N1 | 1:2A:809:G:O2' | 2.25 | 0.68 |
| 1:2A:987:G:O2' | 1:2A:1000:A:N3 | 2.24 | 0.68 |
| 32:2a:1209:C:O2' | 32:2a:1214:C:N4 | 2.25 | 0.68 |
| 41:2j:5:ARG:N | 61:2j:303:HOH:O | 2.27 | 0.68 |
| 1:2A:2355:C:H1' | 22:20:39:ARG:HH21 | 1.57 | 0.68 |
| 9:2N:40:PRO:HB3 | 16:2U:68:ALA:HB2 | 1.76 | 0.68 |
| 23:21:59:THR:O | 23:21:91:LYS:NZ | 2.27 | 0.68 |
| 32:2a:1133:G:N2 | 32:2a:1141:C:N3 | 2.42 | 0.68 |
| 43:2l:86:ARG:NH1 | 61:2l:301:HOH:O | 2.26 | 0.68 |
| 1:1A:272(G):C:H42 | 1:1A:363(C):G:H1 | 1.40 | 0.68 |
| 40:1i:50:LEU:HD13 | 40:1i:56:LEU:HA | 1.76 | 0.68 |
| 1:1A:9:U:H3 | 1:1A:2629:A:H2 | 1.40 | 0.68 |
| 32:1a:1133:G:H1 | 32:1a:1141:C:N4 | 1.91 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1A:1773:A:OP2 | 61:1A:5760:HOH:O | 2.12 | 0.67 |
| 1:2A:81:G:N7 | 61:2A:4126:HOH:O | 2.27 | 0.67 |
| 1:2A:2126:A:N6 | 1:2A:2162:G:O2' | 2.26 | 0.67 |
| 1:1A:1026:U:OP1 | 61:1A:5955:HOH:O | 2.11 | 0.67 |
| 40:1i:16:ARG:HB2 | 40:1i:64:THR:HB | 1.76 | 0.67 |
| 1:2A:857:C:OP2 | 22:20:77:ARG:NH2 | 2.28 | 0.67 |
| 19:2X:8:ILE:O | 24:22:36:ARG:NH2 | 2.27 | 0.67 |
| 26:24:64:GLY:O | 26:24:66:SER:N | 2.26 | 0.67 |
| 55:2x:7:G:H5" | 55:2x:8:4SU:H5 | 1.75 | 0.67 |
| 1:1A:2121:G:H1 | 1:1A:2177:C:H42 | 1.42 | 0.67 |
| 7:2H:113:VAL:HG11 | 7:2H:151:ILE:HG21 | 1.76 | 0.67 |
| 15:2T:41:ARG:NH2 | 32:2a:346:G:OP1 | 2.27 | 0.67 |
| 23:21:50:ARG:HG2 | 23:21:59:THR:HG22 | 1.76 | 0.67 |
| 5:1F:101:LEU:O | 5:1F:106:ARG:NH1 | 2.27 | 0.67 |
| 10:1O:97:ARG:NH1 | 32:1a:339:C:OP2 | 2.27 | 0.67 |
| 32:1a:946:A:H2' | 32:1a:947:G:C8 | 2.28 | 0.67 |
| 1:2A:2136:C:N4 | 1:2A:2155:G:N1 | 2.41 | 0.67 |
| 32:2a:429:U:OP1 | 35:2d:13:ARG:NH1 | 2.27 | 0.67 |
| 32:2a:1312:G:H1 | 32:2a:1325:C:H42 | 1.43 | 0.67 |
| 54:2y:15:G:H22 | 54:2y:48:C:N4 | 1.93 | 0.67 |
| 1:1A:1077:A:H2' | 1:1A:1078:U:H4' | 1.75 | 0.67 |
| 1:1A:2022:U:OP1 | 61:1A:7049:HOH:O | 2.12 | 0.67 |
| 32:1a:1166:G:N2 | 32:1a:1170:A:OP2 | 2.28 | 0.67 |
| 1:2A:882:G:H2' | 1:2A:883:G:C8 | 2.29 | 0.67 |
| 1:2A:922:U:O2' | 22:20:29:GLN:NE2 | 2.26 | 0.67 |
| 32:2a:974:A:OP2 | 45:2n:29:ARG:NH2 | 2.28 | 0.67 |
| 35:2d:8:VAL:HG22 | 35:2d:21:LEU:HD13 | 1.76 | 0.67 |
| 5:1F:158:THR:O | 5:1F:164:ARG:NH1 | 2.28 | 0.67 |
| 18:1W:25:ARG:NH2 | 18:1W:74:ALA:O | 2.27 | 0.67 |
| 23:21:50:ARG:NH1 | 23:21:57:GLU:OE2 | 2.28 | 0.67 |
| 44:2m:3:ARG:NH2 | 44:2m:9:ILE:O | 2.27 | 0.67 |
| 34:1c:150:LYS:HE3 | 34:1c:152:ILE:HD11 | 1.77 | 0.67 |
| 36:1e:8:GLU:HG2 | 36:1e:34:VAL:HG23 | 1.76 | 0.67 |
| 6:2G:105:LYS:NZ | 26:24:25:TYR:O | 2.28 | 0.67 |
| 32:2a:107:G:N7 | 51:2t:15:ARG:NH2 | 2.43 | 0.67 |
| 8:1I:92:VAL:HG13 | 8:1I:120:ILE:HB | 1.77 | 0.66 |
| 32:1a:299:G:O6 | 61:1a:2088:HOH:O | 2.09 | 0.66 |
| 34:1c:82:GLU:OE2 | 34:1c:85:ARG:NH1 | 2.28 | 0.66 |
| 35:1d:205:GLU:OE2 | 36:1e:107:ARG:NH1 | 2.28 | 0.66 |
| 8:1I:77:LEU:HB3 | 8:1I:142:VAL:HG12 | 1.75 | 0.66 |
| 25:13:5:LYS:NZ | 25:13:34:GLU:OE2 | 2.28 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 32:1a:184:G:H2' | 32:1a:185:A:H8 | 1.60 | 0.66 |
| 61:2A:4822:HOH:O | 11:2P:42:SER:O | 2.13 | 0.66 |
| 51:2t:56:MET:HE3 | 51:2t:85:MET:HG2 | 1.77 | 0.66 |
| 32:1a:954:G:N7 | 61:1a:2359:HOH:O | 2.28 | 0.66 |
| 1:2A:1817:G:OP1 | 3:2D:88:ARG:NH2 | 2.28 | 0.66 |
| 1:2A:2296:U:OP2 | 14:2S:9:ARG:NH2 | 2.28 | 0.66 |
| 1:1A:2632:A:HO2' | 1:1A:2811:G:HO2' | 1.39 | 0.66 |
| 32:1a:584:G:H5' | 48:1q:91:ARG:HH22 | 1.61 | 0.66 |
| 41:1j:35:SER:HB3 | 41:1j:73:ASP:HB2 | 1.77 | 0.66 |
| 1:2A:1771:C:OP1 | 61:2A:6272:HOH:O | 2.14 | 0.66 |
| 1:2A:2049:G:N7 | 61:2A:6105:HOH:O | 2.26 | 0.66 |
| 1:1A:500:G:N7 | 61:1A:6883:HOH:O | 2.27 | 0.66 |
| 1:1A:530:G:N1 | 1:1A:2023:G:OP1 | 2.25 | 0.66 |
| 32:1a:1435:G:H2' | 32:1a:1436:U:C6 | 2.30 | 0.66 |
| 34:1c:3:ASN:OD1 | 34:1c:3:ASN:N | 2.28 | 0.66 |
| 1:2A:271(H):G:H2' | 1:2A:271(I):G:H8 | 1.61 | 0.66 |
| 35:2d:205:GLU:OE2 | 36:2e:107:ARG:NH1 | 2.29 | 0.66 |
| 4:1E:105:THR:OG1 | 4:1E:199:ARG:NH2 | 2.29 | 0.66 |
| 32:1a:1000:U:O4 | 32:1a:1041:A:N1 | 2.28 | 0.66 |
| 1:2A:392:C:H5" | 1:2A:409:C:H5" | 1.76 | 0.66 |
| 4:2E:18:ASP:OD2 | 15:2T:33:LYS:NZ | 2.28 | 0.66 |
| 7:2H:59:ARG:O | 7:2H:63:SER:OG | 2.14 | 0.66 |
| 32:2a:289:G:OP2 | 61:2a:3917:HOH:O | 2.13 | 0.66 |
| 55:2x:14:A:N6 | 55:2x:21:A:C2 | 2.63 | 0.66 |
| 1:1A:1176:G:H1' | 1:1A:1177:A:H5" | 1.78 | 0.66 |
| 46:1o:54:ARG:HG2 | 46:1o:58:MET:HE2 | 1.77 | 0.66 |
| 11:2P:59:LEU:HD11 | 30:28:10:ALA:HB2 | 1.77 | 0.66 |
| 26:24:14:ILE:HB | 26:24:22:ILE:HB | 1.78 | 0.66 |
| 3:1D:242:ARG:HG3 | 3:1D:242:ARG:HH11 | 1.61 | 0.66 |
| 37:1f:9:VAL:HB | 37:1f:87:ARG:HB2 | 1.78 | 0.66 |
| 1:2A:299:A:H5" | 20:2Y:86:ARG:HH21 | 1.60 | 0.66 |
| 32:2a:1119:C:H2' | 32:2a:1120:G:C8 | 2.30 | 0.66 |
| 41:2j:98:ILE:O | 61:2j:301:HOH:O | 2.13 | 0.66 |
| 1:1A:392:C:OP1 | 61:1A:6959:HOH:O | 2.13 | 0.65 |
| 1:2A:1537:G:H2' | 1:2A:1538:G:H8 | 1.60 | 0.65 |
| 40:2i:105:ASP:HB2 | 40:2i:107:ARG:HG3 | 1.77 | 0.65 |
| 43:1l:28:LYS:HD3 | 43:1l:62:SER:HB2 | 1.77 | 0.65 |
| 1:2A:2577:A:OP1 | 61:2A:4831:HOH:O | 2.13 | 0.65 |
| 13:2R:97:VAL:HG22 | 13:2R:114:VAL:HG13 | 1.78 | 0.65 |
| 32:2a:1027:C:C2 | 32:2a:1034:G:N2 | 2.61 | 0.65 |
| 40:2i:31:GLN:HE21 | 40:2i:36:TYR:HD1 | 1.44 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1A:483:A:H5" | 20:1Y:50:ARG:HG2 | 1.78 | 0.65 |
| 32:2a:576:G:OP1 | 61:2a:3629:HOH:O | 2.13 | 0.65 |
| 35:2d:57:ARG:HB3 | 35:2d:206:PHE:HB2 | 1.77 | 0.65 |
| 50:2s:50:ALA:HB1 | 50:2s:57:HIS:HB3 | 1.77 | 0.65 |
| 1:1A:2053:G:OP1 | 61:1A:7036:HOH:O | 2.14 | 0.65 |
| 10:2O:24:VAL:HG13 | 10:2O:33:ALA:HB2 | 1.78 | 0.65 |
| 55:2x:28:C:H2' | 55:2x:29:G:H8 | 1.61 | 0.65 |
| 1:1A:250:G:OP2 | 30:18:13:ARG:NH2 | 2.30 | 0.65 |
| 18:1W:1:MET:HE2 | 18:1W:62:HIS:HB3 | 1.78 | 0.65 |
| 33:1b:201:ILE:HG21 | 33:1b:214:ILE:HG21 | 1.78 | 0.65 |
| 51:2t:9:ASN:O | 51:2t:10:LEU:HB2 | 1.96 | 0.65 |
| 1:1A:1447:G:N7 | 61:1A:6819:HOH:O | 2.29 | 0.65 |
| 1:2A:1514:U:H2' | 1:2A:1515:G:H8 | 1.61 | 0.65 |
| 44:2m:14:ARG:HE | 44:2m:42:ALA:HA | 1.61 | 0.65 |
| 54:2w:18:G:O2' | 54:2w:57:G:N2 | 2.25 | 0.65 |
| 1:1A:2646:C:OP2 | 1:1A:2732:G:O2' | 2.10 | 0.65 |
| 1:2A:72:U:OP1 | 61:2A:6029:HOH:O | 2.14 | 0.65 |
| 61:2A:6386:HOH:O | 4:2E:127:ASP:OD2 | 2.14 | 0.65 |
| 32:2a:1266:G:N2 | 32:2a:1269:A:OP2 | 2.22 | 0.65 |
| 5:1F:157:VAL:HB | 5:1F:194:MET:HG2 | 1.77 | 0.65 |
| 20:1Y:14:LEU:HB2 | 20:1Y:75:ILE:HD11 | 1.79 | 0.65 |
| 32:1a:1355:G:N7 | 61:1a:2283:HOH:O | 2.29 | 0.65 |
| 1:2A:1798:U:H5' | 3:2D:259:THR:HG22 | 1.78 | 0.65 |
| 51:2t:57:ARG:HH12 | 51:2t:100:ILE:HD12 | 1.62 | 0.65 |
| 1:1A:1173:G:N1 | 1:1A:1176:G:OP2 | 2.30 | 0.65 |
| 32:1a:1035:A:H2' | 32:1a:1036:G:H21 | 1.60 | 0.65 |
| 32:1a:1385:G:N7 | 61:1a:2460:HOH:O | 2.30 | 0.65 |
| 1:2A:2815:C:H5' | 27:25:29:THR:HG21 | 1.78 | 0.65 |
| 1:1A:1267:U:OP1 | 61:1A:6299:HOH:O | 2.15 | 0.65 |
| 1:1A:631:A:OP1 | 11:1P:65:ARG:NE | 2.30 | 0.64 |
| 1:1A:1113:U:H2' | 1:1A:1114:G:H8 | 1.62 | 0.64 |
| 23:11:50:ARG:HG2 | 23:11:59:THR:HG22 | 1.80 | 0.64 |
| 12:2Q:16:ARG:HG2 | 12:2Q:18:LYS:HG3 | 1.78 | 0.64 |
| 43:2l:71:PRO:O | 43:2l:102:ARG:NH1 | 2.26 | 0.64 |
| 1:1A:192:C:OP1 | 61:1A:4755:HOH:O | 2.14 | 0.64 |
| 1:1A:1469:A:OP2 | 61:1A:6789:HOH:O | 2.13 | 0.64 |
| 12:1Q:18:LYS:O | 12:1Q:98:LYS:NZ | 2.22 | 0.64 |
| 36:1e:74:GLY:HA3 | 36:1e:116:THR:HG22 | 1.78 | 0.64 |
| 44:1m:3:ARG:HG3 | 44:1m:4:ILE:H | 1.61 | 0.64 |
| 32:2a:236:G:OP1 | 48:2q:40:LYS:NZ | 2.31 | 0.64 |
| 32:2a:1402:4OC:HM22 | 32:2a:1403:C:H5' | 1.78 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1A:2153:G:H2' | 1:1A:2154:G:C8 | 2.32 | 0.64 |
| 1:2A:2127:G:C6 | 1:2A:2161:C:C4 | 2.85 | 0.64 |
| 30:28:6:THR:HG22 | 30:28:63:PRO:HD2 | 1.80 | 0.64 |
| 32:2a:1166:G:N2 | 32:2a:1170:A:OP2 | 2.30 | 0.64 |
| 1:1A:2422:A:O4' | 54:1y:76:A:N6 | 2.29 | 0.64 |
| 1:1A:2839:G:OP1 | 61:1A:6632:HOH:O | 2.15 | 0.64 |
| 21:1Z:41:LEU:HD11 | 21:1Z:83:PRO:HG2 | 1.79 | 0.64 |
| 32:1a:510:A:OP2 | 35:1d:49:ARG:NH1 | 2.27 | 0.64 |
| 32:1a:582:U:OP1 | 46:1o:64:ARG:NH1 | 2.30 | 0.64 |
| 32:1a:974:A:OP2 | 45:1n:29:ARG:NH2 | 2.30 | 0.64 |
| 34:1c:58:GLU:HB3 | 41:1j:92:THR:HG21 | 1.78 | 0.64 |
| 35:1d:26:CYS:HB3 | 60:1d:302:SF4:S1 | 2.37 | 0.64 |
| 54:1w:9:A:O2' | 54:1w:10:G:N7 | 2.30 | 0.64 |
| 1:2A:2280:G:N7 | 61:20:206:HOH:O | 2.29 | 0.64 |
| 32:2a:640:A:N6 | 61:2a:3427:HOH:O | 2.30 | 0.64 |
| 43:1l:39:VAL:HG11 | 43:1l:41:ARG:HH11 | 1.61 | 0.64 |
| 1:2A:1557:C:OP2 | 1:2A:1558:A:O2' | 2.15 | 0.64 |
| 1:2A:2151:G:H2' | 1:2A:2152:G:H8 | 1.63 | 0.64 |
| 10:2O:115:VAL:HG13 | 10:2O:121:VAL:HG21 | 1.78 | 0.64 |
| 32:1a:161:A:N1 | 32:1a:347:G:O2' | 2.31 | 0.64 |
| 32:1a:542:G:OP1 | 35:1d:10:ARG:NH2 | 2.31 | 0.64 |
| 32:1a:1147:C:O2 | 40:1i:16:ARG:NH1 | 2.30 | 0.64 |
| 1:2A:307:G:H21 | 1:2A:330:A:H62 | 1.46 | 0.64 |
| 48:2q:66:SER:O | 48:2q:70:ARG:NH1 | 2.31 | 0.64 |
| 1:1A:307:G:N7 | 61:1A:5169:HOH:O | 2.30 | 0.64 |
| 4:1E:47:VAL:HG11 | 4:1E:86:PRO:HD2 | 1.78 | 0.64 |
| 7:1H:86:GLU:OE2 | 7:1H:132:ARG:NH2 | 2.31 | 0.64 |
| 32:1a:1518:MA6:N6 | 32:1a:1519:MA6:H103 | 2.13 | 0.64 |
| 38:1g:113:GLU:HG2 | 38:1g:119:ARG:HG2 | 1.79 | 0.64 |
| 8:2I:4:ILE:HG12 | 8:2I:18:VAL:HG22 | 1.78 | 0.64 |
| 41:2j:40:LEU:HB2 | 41:2j:69:ASN:HB2 | 1.78 | 0.64 |
| 1:2A:1264:G:OP1 | 27:25:19:ARG:NH2 | 2.31 | 0.64 |
| 32:2a:922:G:H4' | 36:2e:20:GLN:HA | 1.80 | 0.64 |
| 34:2c:79:ARG:H | 34:2c:82:GLU:HB3 | 1.63 | 0.64 |
| 32:2a:790:A:N6 | 32:2a:1498:UR3:OP1 | 2.31 | 0.64 |
| 54:2y:67:C:H2' | 54:2y:68:C:C6 | 2.32 | 0.64 |
| 5:1F:70:THR:HG23 | 5:1F:72:ARG:H | 1.63 | 0.64 |
| 33:1b:24:TRP:CD1 | 33:1b:24:TRP:H | 2.16 | 0.64 |
| 35:2d:18:LYS:NZ | 35:2d:31:CYS:SG | 2.71 | 0.64 |
| 41:2j:26:ALA:O | 41:2j:84:GLN:NE2 | 2.31 | 0.64 |
| 1:1A:517:C:OP1 | 27:15:16:ARG:NH2 | 2.30 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:2A:1007:C:OP1 | 9:2N:35:ARG:NH1 | 2.31 | 0.63 |
| 1:2A:1226:A:OP1 | 17:2V:84:LYS:NZ | 2.21 | 0.63 |
| 1:2A:2507:C:O2' | 54:2w:74:C:N4 | 2.30 | 0.63 |
| 1:2A:2624:G:N7 | 61:2A:6351:HOH:O | 2.30 | 0.63 |
| 5:2F:157:VAL:HB | 5:2F:194:MET:HG2 | 1.80 | 0.63 |
| 20:2Y:86:ARG:HD2 | 20:2Y:100:ALA:HA | 1.80 | 0.63 |
| 1:1A:822:U:OP2 | 61:1A:6645:HOH:O | 2.15 | 0.63 |
| 1:1A:994:C:OP1 | 16:1U:53:ARG:NH2 | 2.31 | 0.63 |
| 6:1G:41:GLN:HB3 | 6:1G:43:LEU:HD13 | 1.79 | 0.63 |
| 32:1a:1074:G:O2' | 32:1a:1101:A:N1 | 2.31 | 0.63 |
| 32:2a:78:G:O6 | 32:2a:91:C:N3 | 2.32 | 0.63 |
| 32:2a:1104:G:H4' | 33:2b:111:ARG:HH21 | 1.62 | 0.63 |
| 32:1a:107:G:N7 | 51:1t:15:ARG:NH2 | 2.46 | 0.63 |
| 32:1a:1027:C:C4 | 32:1a:1034:G:C2 | 2.86 | 0.63 |
| 1:2A:1025:G:O2' | 61:2A:5647:HOH:O | 2.15 | 0.63 |
| 19:2X:53:LYS:HB3 | 19:2X:82:GLN:HB3 | 1.79 | 0.63 |
| 54:2w:4:C:N4 | 54:2w:69:G:H1 | 1.95 | 0.63 |
| 32:1a:1004:A:H5' | 32:1a:1024:G:H1 | 1.63 | 0.63 |
| 32:2a:585:G:OP1 | 48:2q:37:LYS:NZ | 2.30 | 0.63 |
| 32:2a:1007:C:O2 | 32:2a:1022:G:N1 | 2.27 | 0.63 |
| 33:2b:162:ILE:HD11 | 33:2b:184:VAL:HG22 | 1.79 | 0.63 |
| 36:2e:102:ALA:O | 36:2e:107:ARG:NH2 | 2.32 | 0.63 |
| 39:2h:49:GLU:OE2 | 39:2h:62:TYR:OH | 2.17 | 0.63 |
| 1:1A:882:G:H4' | 54:1w:19:G:C6 | 2.33 | 0.63 |
| 29:17:8:ASN:HB3 | 29:17:11:LYS:HB3 | 1.79 | 0.63 |
| 1:2A:2839:G:H5' | 13:2R:46:GLY:HA2 | 1.81 | 0.63 |
| 1:1A:1309:G:H4' | 29:17:7:PRO:HB2 | 1.81 | 0.63 |
| 1:1A:1840:G:N7 | 61:1A:5163:HOH:O | 2.31 | 0.63 |
| 32:1a:1305:G:N2 | 32:1a:1331:G:H1' | 2.13 | 0.63 |
| 54:1y:19:G:N2 | 54:1y:56:C:N3 | 2.46 | 0.63 |
| 15:2T:39:ARG:NH2 | 32:2a:345:C:OP2 | 2.31 | 0.63 |
| 6:1G:18:GLU:OE2 | 6:1G:21:ARG:NH1 | 2.32 | 0.63 |
| 13:1R:97:VAL:HG22 | 13:1R:114:VAL:HG13 | 1.81 | 0.63 |
| 54:1w:29:G:H1 | 54:1w:41:C:N4 | 1.96 | 0.63 |
| 1:2A:2287:A:H62 | 1:2A:2344:U:H3 | 1.46 | 0.63 |
| 54:2w:9:A:OP2 | 54:2w:13:C:N4 | 2.31 | 0.63 |
| 1:1A:2328:A:H2' | 1:1A:2329:G:C8 | 2.34 | 0.63 |
| 1:1A:2727:G:O2' | 10:1O:70:LYS:NZ | 2.30 | 0.63 |
| 1:1A:1048:A:OP2 | 1:1A:1109:C:N4 | 2.23 | 0.62 |
| 34:1c:131:ARG:HE | 34:1c:135:LYS:HE3 | 1.64 | 0.62 |
| 40:1i:21:PRO:HA | 40:1i:59:PHE:HA | 1.81 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 23:21:51:VAL:HG11 | 23:21:74:VAL:HG21 | 1.80 | 0.62 |
| 1:1A:2140:C:N3 | 1:1A:2151:G:O6 | 2.32 | 0.62 |
| 33:1b:82:ARG:NH1 | 33:1b:92:TYR:OH | 2.32 | 0.62 |
| 49:1r:32:ARG:HA | 49:1r:69:THR:HG21 | 1.81 | 0.62 |
| 1:2A:1141:U:OP2 | 9:2N:63:THR:OG1 | 2.16 | 0.62 |
| 5:2F:143:ALA:HB1 | 5:2F:148:LEU:HB2 | 1.80 | 0.62 |
| 32:2a:67:C:H2' | 32:2a:68:G:C8 | 2.33 | 0.62 |
| 32:2a:1020:U:H2' | 32:2a:1021:G:H8 | 1.63 | 0.62 |
| 54:2y:26:A:N6 | 54:2y:44:G:C6 | 2.67 | 0.62 |
| 50:1s:77:THR:HG23 | 50:1s:78:ARG:HG3 | 1.81 | 0.62 |
| 1:2A:652(B):A:H61 | 1:2A:655:A:H1' | 1.64 | 0.62 |
| 1:2A:2849:U:OP2 | 15:2T:95:ARG:NH1 | 2.32 | 0.62 |
| 32:1a:911:U:OP2 | 43:1l:97:ARG:NH2 | 2.24 | 0.62 |
| 32:2a:975:A:H5" | 32:2a:1363(A):A:H62 | 1.65 | 0.62 |
| 32:2a:1145:C:H4' | 32:2a:1146:A:H5' | 1.81 | 0.62 |
| 54:2y:52:G:N2 | 54:2y:62:C:N3 | 2.46 | 0.62 |
| 17:1V:74:LYS:HB2 | 17:1V:83:ARG:HB2 | 1.80 | 0.62 |
| 32:1a:1006:C:N3 | 32:1a:1023:G:N2 | 2.47 | 0.62 |
| 1:2A:1378:A:O2' | 1:2A:1380:G:N7 | 2.28 | 0.62 |
| 6:2G:15:VAL:HG22 | 6:2G:175:LEU:HB3 | 1.82 | 0.62 |
| 33:2b:166:ASP:HB3 | 33:2b:169:LYS:HB3 | 1.81 | 0.62 |
| 1:1A:1509(A):A:H3' | 1:1A:1509(B):A:H8 | 1.65 | 0.62 |
| 6:1G:38:VAL:HG22 | 6:1G:93:THR:HG23 | 1.81 | 0.62 |
| 3:2D:108:PRO:HB3 | 3:2D:143:HIS:CE1 | 2.34 | 0.62 |
| 24:22:39:ALA:HB2 | 24:22:44:LEU:HD23 | 1.81 | 0.62 |
| 32:2a:405:U:O4 | 35:2d:2:GLY:N | 2.33 | 0.62 |
| 36:2e:148:VAL:HG21 | 39:2h:107:LEU:HD22 | 1.81 | 0.62 |
| 39:2h:83:ILE:HB | 39:2h:137:VAL:HG13 | 1.82 | 0.62 |
| 42:2k:51:LYS:HA | 42:2k:55:LYS:HE3 | 1.81 | 0.62 |
| 6:1G:142:PRO:HB2 | 26:14:31:ILE:HD13 | 1.81 | 0.62 |
| 46:1o:11:VAL:HG21 | 46:1o:34:LEU:HD22 | 1.82 | 0.62 |
| 1:2A:531:C:OP1 | 1:2A:561:G:N1 | 2.31 | 0.62 |
| 5:2F:167:ALA:HB1 | 5:2F:173:VAL:HG11 | 1.81 | 0.62 |
| 18:2W:88:ARG:NH1 | 18:2W:94:ASP:OD2 | 2.33 | 0.62 |
| 32:2a:1368:G:OP1 | 40:2i:111:ARG:NH2 | 2.32 | 0.62 |
| 54:2w:12:U:H3' | 54:2w:13:C:H5" | 1.82 | 0.62 |
| 1:1A:1798:U:H5' | 3:1D:259:THR:HG22 | 1.82 | 0.62 |
| 54:1w:51:U:H2' | 54:1w:52:G:C8 | 2.35 | 0.62 |
| 5:2F:64:ILE:HG21 | 5:2F:78:ILE:HG23 | 1.80 | 0.62 |
| 35:2d:116:GLN:HE21 | 35:2d:157:LEU:HD21 | 1.65 | 0.62 |
| 3:1D:17:THR:O | 3:1D:211:ARG:NH2 | 2.33 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 32:1a:1202:G:H1' | 45:1n:29:ARG:HD2 | 1.81 | 0.62 |
| 1:2A:2317:C:N4 | 1:2A:2318:G:O6 | 2.33 | 0.62 |
| 26:14:58:ARG:HG3 | 50:1s:68:GLY:H | 1.65 | 0.62 |
| 1:2A:1266:G:O5' | 18:2W:15:ARG:NH2 | 2.33 | 0.62 |
| 32:2a:959:A:O2' | 32:2a:984:C:O2' | 2.17 | 0.62 |
| 34:2c:131:ARG:HH21 | 36:2e:50:GLU:HG3 | 1.65 | 0.62 |
| 1:2A:322:A:OP2 | 5:2F:169:ASN:HB2 | 2.00 | 0.61 |
| 1:2A:2136:C:H42 | 1:2A:2155:G:H1 | 1.45 | 0.61 |
| 3:2D:125:ILE:HB | 37:2f:81:ILE:HD11 | 1.82 | 0.61 |
| 10:2O:63:VAL:HG11 | 10:2O:85:VAL:HG23 | 1.82 | 0.61 |
| 44:2m:82:MET:O | 44:2m:93:ARG:NH2 | 2.33 | 0.61 |
| 1:1A:833:U:O2 | 11:1P:55:ARG:NH2 | 2.33 | 0.61 |
| 1:1A:1105:U:H2' | 1:1A:1106:G:C8 | 2.35 | 0.61 |
| 34:1c:11:ARG:HB3 | 34:1c:15:THR:HB | 1.81 | 0.61 |
| 51:1t:57:ARG:HH12 | 51:1t:100:ILE:HD12 | 1.65 | 0.61 |
| 1:2A:889:C:O2' | 1:2A:890:A:O4' | 2.17 | 0.61 |
| 1:2A:2134:A:OP2 | 1:2A:2135:A:N6 | 2.32 | 0.61 |
| 32:2a:420:U:O2' | 32:2a:423:G:O6 | 2.09 | 0.61 |
| 32:2a:521:G:N7 | 43:2l:53:ARG:NH2 | 2.47 | 0.61 |
| 32:2a:1052:U:O2' | 32:2a:1055:A:OP2 | 2.15 | 0.61 |
| 32:2a:1089:G:N2 | 32:2a:1096:C:N3 | 2.40 | 0.61 |
| 39:2h:51:VAL:HG11 | 39:2h:60:ARG:HH12 | 1.64 | 0.61 |
| 43:2l:124:LYS:HD2 | 43:2l:125:PRO:HD2 | 1.81 | 0.61 |
| 50:2s:27:GLU:HG3 | 50:2s:47:HIS:CE1 | 2.35 | 0.61 |
| 32:1a:67:C:H2' | 32:1a:68:G:C8 | 2.34 | 0.61 |
| 1:2A:2657:A:O3' | 7:2H:160:LYS:NZ | 2.26 | 0.61 |
| 2:2B:48:A:H4' | 14:2S:95:HIS:HD2 | 1.63 | 0.61 |
| 33:2b:55:PHE:O | 33:2b:59:GLU:N | 2.25 | 0.61 |
| 7:1H:149:ARG:NH1 | 7:1H:167:GLU:OE2 | 2.33 | 0.61 |
| 33:1b:77:ALA:HB2 | 33:1b:211:ILE:HD13 | 1.82 | 0.61 |
| 1:2A:764:A:H5' | 3:2D:210:GLY:HA2 | 1.83 | 0.61 |
| 12:2Q:16:ARG:HE | 12:2Q:18:LYS:HD3 | 1.65 | 0.61 |
| 33:2b:74:LYS:NZ | 33:2b:205:ASP:O | 2.33 | 0.61 |
| 1:1A:2142:C:N3 | 1:1A:2149:G:O6 | 2.32 | 0.61 |
| 1:1A:2801(A):A:H1' | 1:1A:2895:U:H1' | 1.83 | 0.61 |
| 12:1Q:35:VAL:HG13 | 12:1Q:130:LYS:HB3 | 1.82 | 0.61 |
| 32:1a:559:A:OP2 | 36:1e:126:ARG:NH2 | 2.34 | 0.61 |
| 1:2A:132:G:O6 | 61:2A:5539:HOH:O | 2.15 | 0.61 |
| 9:2N:32:THR:HG23 | 9:2N:37:LYS:HB2 | 1.82 | 0.61 |
| 32:1a:1077:G:N2 | 32:1a:1080:A:OP2 | 2.33 | 0.61 |
| 1:2A:1434:A:H61 | 1:2A:1558:A:H62 | 1.48 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:2A:2022:U:O2' | 1:2A:2617:C:H5' | 2.00 | 0.61 |
| 1:2A:2151:G:H2' | 1:2A:2152:G:C8 | 2.35 | 0.61 |
| 13:2R:2:ARG:NH1 | 13:2R:5:LYS:O | 2.33 | 0.61 |
| 51:2t:50:GLU:HB2 | 51:2t:99:LEU:HD22 | 1.83 | 0.61 |
| 54:2w:68:C:N4 | 54:2w:69:G:O6 | 2.34 | 0.61 |
| 8:1I:130:TYR:HB3 | 8:1I:138:ILE:HB | 1.82 | 0.61 |
| 32:1a:356:A:N3 | 32:1a:368:U:O2' | 2.29 | 0.61 |
| 32:1a:1047:G:H5" | 45:1n:4:LYS:HD3 | 1.82 | 0.61 |
| 1:2A:700:G:O2' | 1:2A:1632:A:N3 | 2.31 | 0.61 |
| 1:2A:1507:A:O2' | 1:2A:1508:A:O5' | 2.18 | 0.61 |
| 1:2A:2336:A:H61 | 22:20:43:THR:HG22 | 1.66 | 0.61 |
| 33:2b:100:GLY:N | 33:2b:176:GLU:OE2 | 2.32 | 0.61 |
| 35:2d:57:ARG:HD3 | 35:2d:205:GLU:HB3 | 1.82 | 0.61 |
| 44:2m:37:THR:O | 44:2m:55:ARG:NH1 | 2.34 | 0.61 |
| 1:1A:859:G:O2' | 1:1A:916:G:O6 | 2.17 | 0.61 |
| 1:1A:1176:G:N2 | 1:1A:1178:C:OP1 | 2.34 | 0.61 |
| 35:1d:187:ARG:NH1 | 35:1d:190:ASP:OD1 | 2.32 | 0.61 |
| 1:2A:18:C:O2' | 1:2A:554:U:OP1 | 2.19 | 0.61 |
| 1:2A:276:A:H5" | 1:2A:277:C:H5' | 1.83 | 0.61 |
| 1:2A:2035:G:O6 | 61:2A:4288:HOH:O | 2.15 | 0.61 |
| 1:2A:2316:C:O2' | 6:2G:128:ARG:NH2 | 2.33 | 0.61 |
| 3:2D:108:PRO:HG2 | 3:2D:111:LEU:HB2 | 1.81 | 0.61 |
| 5:2F:156:LEU:HD21 | 5:2F:163:VAL:HG12 | 1.82 | 0.61 |
| 18:1W:11:ARG:NH1 | 18:1W:99:ARG:O | 2.33 | 0.61 |
| 23:11:51:VAL:HG11 | 23:11:74:VAL:HG21 | 1.83 | 0.61 |
| 32:1a:1030:C:N4 | 32:1a:1030(A):G:N3 | 2.49 | 0.61 |
| 54:1w:23:A:H3' | 54:1w:24:G:H8 | 1.65 | 0.61 |
| 1:2A:2127:G:C5 | 1:2A:2161:C:N4 | 2.68 | 0.61 |
| 32:2a:426:G:OP1 | 35:2d:38:TYR:OH | 2.17 | 0.61 |
| 1:1A:1385:G:O2' | 1:1A:1396:U:O2 | 2.19 | 0.60 |
| 29:27:2:LYS:NZ | 61:27:201:HOH:O | 2.34 | 0.60 |
| 32:2a:1367:C:OP2 | 40:2i:112:LYS:NZ | 2.25 | 0.60 |
| 36:2e:7:GLU:OE1 | 36:2e:37:ARG:NE | 2.31 | 0.60 |
| 47:2p:51:VAL:HG12 | 47:2p:53:VAL:H | 1.64 | 0.60 |
| 1:1A:674:G:OP2 | 61:1A:7223:HOH:O | 2.17 | 0.60 |
| 1:1A:2788:C:OP1 | 4:1E:61:ARG:NH2 | 2.34 | 0.60 |
| 32:1a:1030(A):G:O2' | 32:1a:1031:G:N2 | 2.34 | 0.60 |
| 1:2A:458:G:O2' | 1:2A:469:G:O6 | 2.19 | 0.60 |
| 5:2F:103:LYS:HA | 5:2F:106:ARG:HG3 | 1.82 | 0.60 |
| 32:2a:437:U:O2 | 35:2d:119:GLN:NE2 | 2.35 | 0.60 |
| 33:2b:60:ASP:OD1 | 33:2b:64:ARG:NH1 | 2.34 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 11:1P:63:PRO:HD3 | 30:18:27:THR:HG22 | 1.83 | 0.60 |
| 2:2B:110:G:H2' | 2:2B:111:G:H5' | 1.82 | 0.60 |
| 32:2a:643:C:H2' | 32:2a:644:G:H8 | 1.66 | 0.60 |
| 32:2a:1346:A:OP1 | 40:2i:120:ARG:NH1 | 2.31 | 0.60 |
| 2:1B:92:C:OP1 | 21:1Z:79:ARG:NH1 | 2.35 | 0.60 |
| 43:1l:124:LYS:HD2 | 43:1l:125:PRO:HD2 | 1.84 | 0.60 |
| 1:2A:2143:C:H2' | 1:2A:2144:U:O4' | 2.01 | 0.60 |
| 1:2A:2836:U:H2' | 1:2A:2837:G:C8 | 2.36 | 0.60 |
| 5:2F:108:LYS:HG2 | 5:2F:112:MET:HE2 | 1.83 | 0.60 |
| 7:2H:149:ARG:NH1 | 7:2H:167:GLU:OE2 | 2.34 | 0.60 |
| 32:2a:1357:A:N6 | 32:2a:1363(A):A:N1 | 2.50 | 0.60 |
| 34:2c:131:ARG:NH2 | 36:2e:50:GLU:HG3 | 2.17 | 0.60 |
| 54:2w:6:G:O6 | 54:2w:67:C:N3 | 2.35 | 0.60 |
| 1:1A:586:A:H5' | 5:1F:89:VAL:HG21 | 1.84 | 0.60 |
| 1:1A:1693:U:O2' | 3:1D:14:ARG:NH2 | 2.34 | 0.60 |
| 18:1W:82:LEU:HB2 | 18:1W:98:LYS:HB2 | 1.83 | 0.60 |
| 32:1a:953:G:H5' | 32:1a:965:A:H61 | 1.64 | 0.60 |
| 32:1a:1028:C:H42 | 32:1a:1033:G:H1 | 1.50 | 0.60 |
| 54:1y:58:A:O2' | 54:1y:59:U:OP1 | 2.18 | 0.60 |
| 1:2A:568:U:H5' | 1:2A:945:A:N1 | 2.16 | 0.60 |
| 1:2A:2882:A:OP1 | 13:2R:96:ARG:NH1 | 2.33 | 0.60 |
| 3:1D:242:ARG:HD2 | 3:1D:246:PRO:HG3 | 1.82 | 0.60 |
| 32:1a:1095:U:P | 32:1a:1108:G:H1 | 2.24 | 0.60 |
| 37:1f:35:ALA:HB2 | 37:1f:67:MET:HE2 | 1.83 | 0.60 |
| 39:1h:10:LEU:HD22 | 39:1h:83:ILE:HD11 | 1.82 | 0.60 |
| 40:1i:111:ARG:O | 40:1i:113:LYS:NZ | 2.34 | 0.60 |
| 1:2A:223:A:O2' | 1:2A:420:C:O2 | 2.18 | 0.60 |
| 32:2a:157:G:H1 | 32:2a:164:U:H3 | 1.50 | 0.60 |
| 32:2a:532:A:N6 | 32:2a:1206:G:O2' | 2.34 | 0.60 |
| 1:1A:1754:C:OP1 | 15:1T:96:ARG:NH1 | 2.35 | 0.60 |
| 8:1I:5:LEU:HD11 | 8:1I:19:VAL:HG22 | 1.82 | 0.60 |
| 32:1a:972:C:O2' | 41:1j:55:LYS:O | 2.20 | 0.60 |
| 1:2A:2079:U:O3' | 23:21:35:THR:OG1 | 2.19 | 0.60 |
| 25:23:7:LYS:HB2 | 25:23:34:GLU:HG3 | 1.82 | 0.60 |
| 32:2a:532:A:N1 | 34:2c:156:ARG:NH1 | 2.48 | 0.60 |
| 32:2a:1239:A:H4' | 32:2a:1240:U:H5" | 1.84 | 0.60 |
| 33:2b:74:LYS:HD2 | 33:2b:166:ASP:HB2 | 1.82 | 0.60 |
| 33:2b:158:LEU:HD21 | 33:2b:180:LEU:HD13 | 1.82 | 0.60 |
| 1:1A:1025:G:C4 | 1:1A:1135:C:H1' | 2.36 | 0.60 |
| 1:1A:2596:U:OP1 | 61:1A:4205:HOH:O | 2.17 | 0.60 |
| 11:1P:63:PRO:HG2 | 30:18:25:MET:HB2 | 1.83 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 32:1a:328:C:H4' | 32:1a:329:A:H5' | 1.82 | 0.60 |
| 32:1a:1503:A:O2' | 53:1v:13:A:N1 | 2.33 | 0.60 |
| 50:1s:27:GLU:OE1 | 50:1s:27:GLU:N | 2.29 | 0.60 |
| 1:2A:666:G:H1' | 30:28:4:MET:HE3 | 1.84 | 0.60 |
| 48:2q:9:VAL:HG12 | 48:2q:56:VAL:HG22 | 1.83 | 0.60 |
| 1:1A:581:C:OP1 | 16:1U:33:ARG:HG3 | 2.02 | 0.60 |
| 1:2A:1420:U:O2' | 1:2A:1421:G:OP1 | 2.19 | 0.60 |
| 8:2I:3:VAL:HG12 | 8:2I:38:LEU:HA | 1.83 | 0.60 |
| 34:2c:3:ASN:N | 34:2c:3:ASN:OD1 | 2.32 | 0.60 |
| 54:2w:50:U:O2 | 54:2w:64:A:N1 | 2.35 | 0.60 |
| 10:1O:35:VAL:HG11 | 10:1O:103:ALA:HB3 | 1.82 | 0.60 |
| 36:1e:6:PHE:HB3 | 36:1e:34:VAL:HG22 | 1.83 | 0.60 |
| 4:2E:48:GLN:NE2 | 4:2E:78:LEU:HD23 | 2.17 | 0.60 |
| 11:2P:63:PRO:HD3 | 30:28:27:THR:HG22 | 1.84 | 0.60 |
| 32:1a:557:G:N7 | 61:1a:2490:HOH:O | 2.30 | 0.59 |
| 1:2A:1652:A:OP1 | 13:2R:8:ARG:NH1 | 2.34 | 0.59 |
| 1:2A:1796:U:H2' | 1:2A:1797:C:C6 | 2.37 | 0.59 |
| 1:2A:2126:A:H61 | 1:2A:2162:G:HO2' | 1.49 | 0.59 |
| 32:2a:1048:G:N2 | 32:2a:1214:C:O2 | 2.31 | 0.59 |
| 32:2a:1147:C:O2 | 40:2i:16:ARG:NH1 | 2.36 | 0.59 |
| 1:1A:272(F):C:H42 | 1:1A:363(D):G:H1 | 1.51 | 0.59 |
| 1:1A:566:U:H5" | 11:1P:29:LYS:HE3 | 1.85 | 0.59 |
| 1:1A:1165:U:H2' | 1:1A:1166:C:C6 | 2.37 | 0.59 |
| 1:1A:1226:A:OP1 | 17:1V:84:LYS:NZ | 2.26 | 0.59 |
| 1:1A:1359:A:H2' | 1:1A:1360:A:H5' | 1.84 | 0.59 |
| 1:2A:927:G:O6 | 1:2A:928:G:N2 | 2.36 | 0.59 |
| 1:2A:2537:U:H2' | 1:2A:2538:C:C6 | 2.37 | 0.59 |
| 32:2a:45:U:H2' | 32:2a:46:G:C8 | 2.37 | 0.59 |
| 32:2a:1027:C:N4 | 32:2a:1036:G:O6 | 2.35 | 0.59 |
| 32:2a:1239:A:H62 | 32:2a:1299:A:H62 | 1.49 | 0.59 |
| 35:2d:79:PHE:HE1 | 35:2d:204:ILE:HD13 | 1.66 | 0.59 |
| 3:1D:108:PRO:HB3 | 3:1D:143:HIS:CE1 | 2.37 | 0.59 |
| 12:1Q:60:ARG:NH1 | 54:1w:54:5MU:OP2 | 2.35 | 0.59 |
| 1:1A:1452:A:OP2 | 61:1A:4749:HOH:O | 2.17 | 0.59 |
| 1:2A:1803:A:O2' | 3:2D:259:THR:HG21 | 2.02 | 0.59 |
| 1:2A:2343:C:O2' | 1:2A:2373:G:O2' | 2.15 | 0.59 |
| 32:2a:656:C:O2' | 46:2o:28:GLN:OE1 | 2.10 | 0.59 |
| 1:1A:2023:G:H5' | 1:1A:2617:C:H4' | 1.84 | 0.59 |
| 6:1G:131:TYR:HB3 | 6:1G:159:VAL:HG13 | 1.85 | 0.59 |
| 14:1S:11:LYS:HE2 | 14:1S:15:ARG:HH12 | 1.67 | 0.59 |
| 21:1Z:151:HIS:HA | 21:1Z:170:THR:HA | 1.84 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:1j:81:THR:HA | 41:1j:84:GLN:HB3 | 1.83 | 0.59 |
| 1:2A:2136:C:O2' | 1:2A:2137:C:O5' | 2.21 | 0.59 |
| 12:2Q:60:ARG:NH1 | 54:2w:54:5MU:OP2 | 2.36 | 0.59 |
| 32:2a:54:C:N4 | 32:2a:353:A:OP2 | 2.35 | 0.59 |
| 50:2s:70:LYS:HB2 | 50:2s:73:GLU:HG3 | 1.85 | 0.59 |
| 32:1a:1002:G:H3' | 32:1a:1003:G:H4' | 1.84 | 0.59 |
| 36:1e:8:GLU:OE2 | 36:1e:63:ARG:NH2 | 2.35 | 0.59 |
| 48:1q:66:SER:O | 48:1q:70:ARG:NH1 | 2.36 | 0.59 |
| 1:2A:860:U:H1' | 1:2A:2268:A:H5' | 1.83 | 0.59 |
| 1:2A:1169:G:H1 | 1:2A:1180:C:H42 | 1.51 | 0.59 |
| 10:2O:48:PRO:HB3 | 32:2a:1422:G:H5" | 1.84 | 0.59 |
| 32:2a:1151:A:N3 | 41:2j:39:PRO:HG3 | 2.17 | 0.59 |
| 32:2a:1376:U:H2' | 32:2a:1377:A:C8 | 2.37 | 0.59 |
| 34:2c:43:LEU:HD21 | 34:2c:91:LEU:HD13 | 1.85 | 0.59 |
| 1:1A:1153:C:OP2 | 61:1A:5679:HOH:O | 2.17 | 0.59 |
| 32:2a:1315:U:O2' | 32:2a:1360:A:N3 | 2.26 | 0.59 |
| 37:2f:97:PHE:HE2 | 49:2r:62:GLU:HG2 | 1.66 | 0.59 |
| 40:2i:85:LEU:HB3 | 40:2i:92:TYR:HD2 | 1.68 | 0.59 |
| 50:2s:19:VAL:O | 50:2s:23:ASN:ND2 | 2.35 | 0.59 |
| 32:1a:8:A:N6 | 35:1d:205:GLU:O | 2.35 | 0.59 |
| 1:2A:882:G:H1 | 1:2A:894:C:H42 | 1.50 | 0.59 |
| 1:2A:1865:G:OP1 | 61:2A:3902:HOH:O | 2.17 | 0.59 |
| 21:2Z:4:ARG:HG2 | 21:2Z:58:VAL:HB | 1.84 | 0.59 |
| 32:2a:450:G:H4' | 47:2p:41:PRO:HB2 | 1.85 | 0.59 |
| 1:1A:2822:G:OP2 | 61:1A:6915:HOH:O | 2.16 | 0.59 |
| 32:1a:53:A:N6 | 61:1a:2342:HOH:O | 2.35 | 0.59 |
| 32:1a:343:U:O2' | 32:1a:346:G:O6 | 2.18 | 0.59 |
| 1:2A:668:G:H5' | 1:2A:669:G:OP2 | 2.03 | 0.59 |
| 20:2Y:64:GLU:OE1 | 20:2Y:64:GLU:N | 2.29 | 0.59 |
| 32:2a:815:A:N7 | 32:2a:1509:C:O2' | 2.36 | 0.59 |
| 32:2a:946:A:H2' | 32:2a:947:G:C8 | 2.37 | 0.59 |
| 48:2q:53:LEU:HD23 | 48:2q:82:MET:HE1 | 1.85 | 0.59 |
| 10:1O:64:ARG:HB2 | 10:1O:79:PHE:CG | 2.38 | 0.59 |
| 25:13:6:VAL:HG12 | 25:13:28:LEU:HD11 | 1.84 | 0.59 |
| 33:1b:88:ALA:HB2 | 33:1b:219:VAL:HG13 | 1.84 | 0.59 |
| 37:1f:99:ALA:HB1 | 49:1r:23:LYS:HE3 | 1.84 | 0.59 |
| 61:2A:6385:HOH:O | 4:2E:127:ASP:OD2 | 2.17 | 0.59 |
| 32:2a:331:G:N7 | 61:2a:3368:HOH:O | 2.32 | 0.59 |
| 32:2a:818:G:N2 | 32:2a:873:A:OP1 | 2.36 | 0.59 |
| 32:2a:1275:A:H3' | 32:2a:1276:G:H8 | 1.67 | 0.59 |
| 32:2a:1338:G:H21 | 55:2x:41:C:H1' | 1.67 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 36:2e:31:LEU:HD22 | 36:2e:43:LEU:HD11 | 1.85 | 0.59 |
| 37:2f:9:VAL:HB | 37:2f:87:ARG:HB2 | 1.84 | 0.59 |
| 44:2m:58:GLU:O | 44:2m:62:ASN:ND2 | 2.33 | 0.59 |
| 1:1A:624:C:O2' | 1:1A:657:U:OP1 | 2.19 | 0.58 |
| 1:1A:1094:U:H1' | 1:1A:1097:U:H5 | 1.68 | 0.58 |
| 8:1I:12:LEU:HD22 | 8:1I:19:VAL:HG21 | 1.85 | 0.58 |
| 1:2A:2880:C:O3' | 13:2R:90:ARG:NH1 | 2.35 | 0.58 |
| 34:2c:152:ILE:HG13 | 34:2c:167:TRP:HB3 | 1.83 | 0.58 |
| 35:2d:31:CYS:CB | 60:2d:302:SF4:S3 | 2.91 | 0.58 |
| 33:1b:62:ALA:HB1 | 33:1b:226:ARG:HG3 | 1.84 | 0.58 |
| 11:2P:121:LYS:HG2 | 11:2P:123:LEU:HG | 1.85 | 0.58 |
| 1:1A:764:A:H5" | 3:1D:210:GLY:HA2 | 1.83 | 0.58 |
| 4:1E:48:GLN:HE21 | 4:1E:78:LEU:HG | 1.68 | 0.58 |
| 4:1E:128:SER:OG | 4:1E:129:HIS:N | 2.34 | 0.58 |
| 32:1a:890:G:O2' | 32:1a:906:G:O6 | 2.20 | 0.58 |
| 32:1a:1353:G:OP1 | 52:1u:10:ARG:NH1 | 2.37 | 0.58 |
| 1:2A:2144:U:H1' | 1:2A:2148:G:N2 | 2.17 | 0.58 |
| 12:2Q:111:GLU:O | 12:2Q:115:MET:HG2 | 2.03 | 0.58 |
| 32:2a:592:G:H1 | 32:2a:647:C:H42 | 1.51 | 0.58 |
| 54:2w:8:4SU:S4 | 54:2w:13:C:O2' | 2.61 | 0.58 |
| 1:1A:452:G:OP2 | 61:1A:7439:HOH:O | 2.17 | 0.58 |
| 1:1A:878:A:N6 | 1:1A:899:A:O2' | 2.34 | 0.58 |
| 4:1E:8:LYS:HG2 | 4:1E:192:ASN:HA | 1.85 | 0.58 |
| 15:2T:50:ILE:HG22 | 15:2T:102:ILE:HD11 | 1.83 | 0.58 |
| 21:2Z:72:ARG:NH2 | 21:2Z:97:GLU:O | 2.36 | 0.58 |
| 32:2a:717:C:H4' | 42:2k:117:ASN:HD22 | 1.67 | 0.58 |
| 33:2b:78:GLN:NE2 | 33:2b:94:ASN:O | 2.36 | 0.58 |
| 35:2d:31:CYS:HB2 | 60:2d:302:SF4:S3 | 2.42 | 0.58 |
| 44:1m:23:TYR:HB3 | 44:1m:67:GLU:HA | 1.85 | 0.58 |
| 1:2A:90:U:H1' | 1:2A:92:A:C8 | 2.37 | 0.58 |
| 1:2A:481:G:N7 | 61:2A:3913:HOH:O | 2.32 | 0.58 |
| 15:2T:127:ALA:C | 15:2T:129:ARG:H | 2.12 | 0.58 |
| 21:2Z:91:LEU:HD11 | 21:2Z:96:VAL:HG11 | 1.83 | 0.58 |
| 1:1A:744:G:OP1 | 61:1A:5723:HOH:O | 2.16 | 0.58 |
| 1:1A:2723:C:OP1 | 13:1R:3:HIS:ND1 | 2.33 | 0.58 |
| 32:1a:581:G:OP1 | 46:1o:65:ARG:NH2 | 2.36 | 0.58 |
| 32:1a:1467:G:O6 | 61:1a:2150:HOH:O | 2.16 | 0.58 |
| 33:1b:60:ASP:HA | 33:1b:63:MET:HE3 | 1.85 | 0.58 |
| 61:2A:5566:HOH:O | 19:2X:44:GLU:OE2 | 2.17 | 0.58 |
| 2:2B:22:U:H3 | 2:2B:61:G:H1 | 1.51 | 0.58 |
| 1:1A:946:G:OP1 | 61:1A:5865:HOH:O | 2.17 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1A:1702:G:N7 | 61:1A:6157:HOH:O | 2.32 | 0.58 |
| 32:1a:783:C:OP1 | 32:1a:1515:C:O2' | 2.20 | 0.58 |
| 41:1j:54:PHE:O | 41:1j:56:HIS:N | 2.31 | 0.58 |
| 54:1w:7:A:N1 | 54:1w:66:U:O2 | 2.37 | 0.58 |
| 28:26:35:GLU:OE2 | 28:26:50:ARG:NH1 | 2.36 | 0.58 |
| 32:2a:748:C:H4' | 32:2a:749:C:O5' | 2.04 | 0.58 |
| 32:1a:1196:U:H3 | 34:1c:162:GLN:HE22 | 1.51 | 0.58 |
| 1:2A:1309:G:H4' | 29:27:7:PRO:HB2 | 1.85 | 0.58 |
| 1:2A:1568:G:N7 | 61:2A:5809:HOH:O | 2.32 | 0.58 |
| 15:2T:26:ASP:OD1 | 15:2T:120:ARG:NH2 | 2.26 | 0.58 |
| 21:2Z:151:HIS:HA | 21:2Z:170:THR:HA | 1.84 | 0.58 |
| 36:2e:18:ARG:HH11 | 36:2e:27:ARG:HH12 | 1.51 | 0.58 |
| 43:2l:71:PRO:HG2 | 43:2l:102:ARG:HG2 | 1.86 | 0.58 |
| 15:1T:127:ALA:C | 15:1T:129:ARG:H | 2.12 | 0.58 |
| 21:1Z:21:ALA:O | 21:1Z:23:LYS:NZ | 2.35 | 0.58 |
| 32:1a:1104:G:H4' | 33:1b:111:ARG:HH21 | 1.68 | 0.58 |
| 32:2a:134:A:H61 | 47:2p:25:ARG:HH12 | 1.52 | 0.58 |
| 32:2a:390:C:H2' | 32:2a:391:G:C8 | 2.39 | 0.58 |
| 32:2a:646:U:H2' | 32:2a:647:C:C6 | 2.39 | 0.58 |
| 32:2a:1029:C:C4 | 32:2a:1032:G:N1 | 2.71 | 0.58 |
| 32:2a:1189:C:OP1 | 41:2j:51:ARG:NH2 | 2.35 | 0.58 |
| 1:1A:1429:G:H2' | 1:1A:1430:C:C6 | 2.38 | 0.58 |
| 32:1a:390:C:H2' | 32:1a:391:G:C8 | 2.39 | 0.58 |
| 32:1a:1411:C:N4 | 61:1a:2396:HOH:O | 2.30 | 0.58 |
| 1:2A:111:A:O2' | 24:22:65:ASN:ND2 | 2.37 | 0.58 |
| 1:2A:566:U:H5" | 11:2P:29:LYS:HE3 | 1.86 | 0.58 |
| 1:2A:2010:G:H5" | 18:2W:42:ARG:HB2 | 1.85 | 0.58 |
| 1:2A:2176:A:H2' | 1:2A:2177:C:C6 | 2.39 | 0.58 |
| 12:2Q:38:GLU:HG3 | 12:2Q:127:ILE:HB | 1.84 | 0.58 |
| 33:2b:101:MET:HG2 | 33:2b:108:ILE:HG21 | 1.85 | 0.58 |
| 18:1W:71:VAL:HA | 18:1W:107:LEU:HD12 | 1.86 | 0.57 |
| 32:1a:1221:G:OP1 | 32:1a:1320:C:N4 | 2.37 | 0.57 |
| 32:2a:1077:G:N2 | 32:2a:1080:A:OP2 | 2.36 | 0.57 |
| 32:2a:1404:5MC:O2 | 32:2a:1519:MA6:O2' | 2.19 | 0.57 |
| 33:2b:200:ILE:HG22 | 33:2b:202:PRO:HD3 | 1.87 | 0.57 |
| 44:2m:80:ARG:HH12 | 50:2s:69:HIS:CE1 | 2.16 | 0.57 |
| 55:2x:76:A:O2' | 61:2x:201:HOH:O | 2.17 | 0.57 |
| 1:1A:2038:G:O6 | 61:1A:5710:HOH:O | 2.16 | 0.57 |
| 1:1A:2336:A:H61 | 22:10:43:THR:CG2 | 2.17 | 0.57 |
| 1:1A:2706:G:N7 | 61:1A:5748:HOH:O | 2.32 | 0.57 |
| 22:10:70:GLN:OE1 | 22:10:80:HIS:NE2 | 2.36 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 34:1c:78:GLY:HA3 | 34:1c:83:ARG:H | 1.69 | 0.57 |
| 61:2A:4994:HOH:O | 11:2P:54:GLY:O | 2.17 | 0.57 |
| 32:2a:1004:A:N6 | 32:2a:1037:C:O2 | 2.34 | 0.57 |
| 32:2a:1305:G:N2 | 32:2a:1331:G:H1' | 2.19 | 0.57 |
| 33:2b:15:VAL:HG21 | 33:2b:213:LEU:HD22 | 1.86 | 0.57 |
| 50:2s:27:GLU:HG2 | 50:2s:28:LYS:HD2 | 1.86 | 0.57 |
| 54:2y:55:PSU:N3 | 54:2y:57:G:H5' | 2.17 | 0.57 |
| 1:1A:2105:C:H2' | 1:1A:2106:G:C8 | 2.40 | 0.57 |
| 32:1a:532:A:N6 | 32:1a:1206:G:O2' | 2.37 | 0.57 |
| 41:1j:30:SER:O | 41:1j:81:THR:OG1 | 2.23 | 0.57 |
| 1:2A:140:G:H1' | 1:2A:141:A:H2 | 1.68 | 0.57 |
| 1:2A:873:G:H1 | 1:2A:904:C:H42 | 1.50 | 0.57 |
| 16:2U:92:ARG:HA | 16:2U:95:LEU:HB2 | 1.86 | 0.57 |
| 1:1A:570:G:O6 | 61:1A:6393:HOH:O | 2.17 | 0.57 |
| 1:1A:588:U:H2' | 1:1A:589:C:C6 | 2.39 | 0.57 |
| 1:1A:897:C:N3 | 1:1A:898:C:N4 | 2.52 | 0.57 |
| 1:1A:1913:A:H4' | 1:1A:1914:C:H5" | 1.86 | 0.57 |
| 44:1m:34:LEU:HD13 | 44:1m:41:PRO:HA | 1.87 | 0.57 |
| 5:2F:154:VAL:HG22 | 5:2F:191:ARG:HB2 | 1.85 | 0.57 |
| 32:2a:9:G:H2' | 32:2a:10:A:H8 | 1.68 | 0.57 |
| 32:2a:376:G:H5" | 47:2p:5:ARG:HB2 | 1.87 | 0.57 |
| 32:2a:444:C:H2' | 32:2a:445:G:H8 | 1.69 | 0.57 |
| 32:2a:501:C:H2' | 32:2a:502:G:C8 | 2.38 | 0.57 |
| 32:2a:1000:U:H2' | 32:2a:1001:A:C8 | 2.39 | 0.57 |
| 32:2a:1119:C:H2' | 32:2a:1120:G:H8 | 1.66 | 0.57 |
| 32:2a:1273:G:H3' | 32:2a:1274:G:C8 | 2.32 | 0.57 |
| 46:2o:11:VAL:HG21 | 46:2o:34:LEU:HD22 | 1.86 | 0.57 |
| 54:2w:72:C:H2' | 54:2w:73:A:C8 | 2.39 | 0.57 |
| 1:1A:662:G:H5" | 11:1P:16:ARG:HG2 | 1.85 | 0.57 |
| 1:1A:883:G:H22 | 1:1A:893:C:H42 | 1.51 | 0.57 |
| 1:1A:2331:G:O2' | 1:1A:2336:A:N1 | 2.35 | 0.57 |
| 1:1A:2522:U:O2' | 1:1A:2647:U:OP1 | 2.16 | 0.57 |
| 32:1a:7:G:O2' | 36:1e:120:THR:O | 2.23 | 0.57 |
| 32:1a:1027:C:N4 | 32:1a:1034:G:C6 | 2.73 | 0.57 |
| 1:2A:1021:A:H62 | 1:2A:1141:U:H3 | 1.52 | 0.57 |
| 1:2A:2630:G:H2' | 1:2A:2631:G:C8 | 2.40 | 0.57 |
| 32:2a:67:C:H2' | 32:2a:68:G:H8 | 1.69 | 0.57 |
| 51:2t:60:GLU:HG3 | 51:2t:81:LYS:HD2 | 1.85 | 0.57 |
| 1:1A:1199:U:OP1 | 61:1A:5824:HOH:O | 2.17 | 0.57 |
| 1:1A:2430:A:N3 | 1:1A:2430:A:H2' | 2.19 | 0.57 |
| 4:1E:11:MET:HG2 | 4:1E:24:THR:HB | 1.87 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 9:1N:70:LYS:HD3 | 9:1N:87:LEU:HD12 | 1.87 | 0.57 |
| 32:1a:1236:A:H4' | 32:1a:1304:G:H4' | 1.86 | 0.57 |
| 36:1e:78:HIS:HE1 | 36:1e:143:ARG:H | 1.51 | 0.57 |
| 39:1h:83:ILE:HB | 39:1h:137:VAL:HG13 | 1.86 | 0.57 |
| 1:2A:1028:A:N6 | 1:2A:1125:G:H2' | 2.20 | 0.57 |
| 3:2D:108:PRO:HD2 | 3:2D:111:LEU:HD22 | 1.85 | 0.57 |
| 5:2F:195:ASP:HB3 | 5:2F:198:ALA:H | 1.69 | 0.57 |
| 32:2a:1183:A:O2' | 32:2a:1184:G:OP1 | 2.23 | 0.57 |
| 38:2g:59:LEU:HG | 38:2g:63:LYS:HE2 | 1.85 | 0.57 |
| 38:2g:69:VAL:HG21 | 38:2g:104:LEU:HD11 | 1.86 | 0.57 |
| 1:1A:2001:A:OP1 | 13:1R:9:LYS:NZ | 2.38 | 0.57 |
| 1:1A:2112:G:H1' | 54:1y:19:G:O2' | 2.05 | 0.57 |
| 33:1b:124:SER:HB3 | 33:1b:125:PRO:HA | 1.87 | 0.57 |
| 32:2a:1113:C:N4 | 32:2a:1187:G:H1 | 2.03 | 0.57 |
| 1:1A:441:U:O2 | 5:1F:46:ARG:NH2 | 2.34 | 0.57 |
| 5:1F:11:VAL:HB | 5:1F:18:ARG:HG3 | 1.85 | 0.57 |
| 7:1H:17:VAL:HG22 | 7:1H:26:VAL:HG22 | 1.86 | 0.57 |
| 32:1a:164:U:H2' | 32:1a:165:C:C6 | 2.40 | 0.57 |
| 32:1a:410:G:OP1 | 35:1d:30:LYS:NZ | 2.36 | 0.57 |
| 1:2A:247:G:H4' | 1:2A:386:G:C5 | 2.39 | 0.57 |
| 1:2A:1383:C:O2 | 61:2A:6037:HOH:O | 2.17 | 0.57 |
| 13:2R:51:LEU:HD22 | 13:2R:66:VAL:HG13 | 1.86 | 0.57 |
| 32:2a:1314:C:N4 | 50:2s:2:PRO:O | 2.31 | 0.57 |
| 36:2e:145:LYS:HA | 36:2e:148:VAL:HB | 1.86 | 0.57 |
| 38:2g:16:LEU:HD21 | 40:2i:45:ALA:HB2 | 1.86 | 0.57 |
| 54:2w:8:4SU:H1' | 54:2w:48:C:H1' | 1.86 | 0.57 |
| 2:1B:1:U:O2' | 2:1B:2:C:OP1 | 2.20 | 0.57 |
| 32:1a:1136:U:H5" | 32:1a:1137:C:C4 | 2.40 | 0.57 |
| 1:2A:686:G:N2 | 1:2A:788:A:H61 | 2.02 | 0.57 |
| 5:2F:101:LEU:O | 5:2F:106:ARG:NH1 | 2.38 | 0.57 |
| 13:2R:44:LEU:HD22 | 13:2R:48:VAL:HG23 | 1.87 | 0.57 |
| 32:2a:1333:A:H3' | 32:2a:1334:G:H8 | 1.69 | 0.57 |
| 1:1A:615:G:OP1 | 5:1F:40:GLN:NE2 | 2.38 | 0.57 |
| 1:1A:1406:U:H2' | 1:1A:1407:C:C6 | 2.40 | 0.57 |
| 29:17:12:ARG:NH2 | 29:17:44:PRO:HB3 | 2.20 | 0.57 |
| 32:1a:68:G:H1 | 32:1a:101:A:H61 | 1.53 | 0.57 |
| 32:1a:1414:U:H3 | 32:1a:1486:G:H1 | 1.52 | 0.57 |
| 33:1b:166:ASP:HB3 | 33:1b:169:LYS:HB3 | 1.85 | 0.57 |
| 36:1e:152:ARG:NH2 | 39:1h:107:LEU:O | 2.37 | 0.57 |
| 48:1q:75:ARG:NH1 | 48:1q:76:LEU:O | 2.38 | 0.57 |
| 1:2A:1769:G:O2' | 1:2A:1958:C:OP1 | 2.18 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 32:2a:1148:U:H2' | 32:2a:1149:C:O4' | 2.05 | 0.57 |
| 1:1A:560:C:H5' | 16:1U:52:ARG:HH21 | 1.69 | 0.56 |
| 32:1a:1001(A):G:C2 | 32:1a:1002:G:H1' | 2.40 | 0.56 |
| 32:1a:1118:C:OP1 | 40:1i:104:ARG:NH1 | 2.34 | 0.56 |
| 1:2A:1688:U:O2 | 1:2A:1700:A:H5' | 2.04 | 0.56 |
| 8:2I:123:LEU:HD22 | 8:2I:144:VAL:HB | 1.87 | 0.56 |
| 32:2a:719:C:H1' | 49:2r:49:LYS:HB3 | 1.86 | 0.56 |
| 35:2d:11:LEU:HD23 | 35:2d:66:ARG:HB3 | 1.87 | 0.56 |
| 54:2w:8:4SU:HN3 | 54:2w:14:A:H62 | 1.51 | 0.56 |
| 2:1B:13:A:N1 | 2:1B:69:G:O2' | 2.36 | 0.56 |
| 6:1G:7:LEU:HD11 | 6:1G:107:LEU:HD12 | 1.87 | 0.56 |
| 2:2B:51:G:N7 | 14:2S:62:LYS:NZ | 2.52 | 0.56 |
| 33:2b:102:LEU:HD23 | 33:2b:182:ILE:HD12 | 1.85 | 0.56 |
| 1:1A:642:G:N2 | 1:1A:645:C:OP2 | 2.36 | 0.56 |
| 1:1A:2136:C:N4 | 1:1A:2155:G:N1 | 2.29 | 0.56 |
| 7:1H:3:ARG:HE | 7:1H:54:ARG:HH12 | 1.53 | 0.56 |
| 20:1Y:20:TYR:CE2 | 20:1Y:43:ASN:HA | 2.39 | 0.56 |
| 22:10:11:ARG:O | 22:10:14:ARG:NH2 | 2.37 | 0.56 |
| 32:1a:1356:G:H2' | 32:1a:1357:A:C8 | 2.41 | 0.56 |
| 32:1a:1445:C:O2' | 32:1a:1447:A:N6 | 2.38 | 0.56 |
| 33:1b:19:HIS:NE2 | 33:1b:206:ASP:OD2 | 2.33 | 0.56 |
| 33:1b:52:GLU:HG2 | 33:1b:56:ARG:HH12 | 1.70 | 0.56 |
| 39:1h:121:ASP:OD2 | 39:1h:125:ARG:NH2 | 2.36 | 0.56 |
| 46:1o:29:VAL:HG13 | 46:1o:63:ARG:HG3 | 1.87 | 0.56 |
| 49:1r:52:PRO:HB2 | 49:1r:54:ARG:HG2 | 1.87 | 0.56 |
| 32:2a:328:C:H4' | 32:2a:329:A:H5' | 1.87 | 0.56 |
| 1:1A:1688:U:O2 | 1:1A:1700:A:H5' | 2.05 | 0.56 |
| 20:1Y:102:CYS:SG | 20:1Y:103:GLY:N | 2.77 | 0.56 |
| 26:14:64:GLY:C | 26:14:66:SER:H | 2.13 | 0.56 |
| 32:1a:108:G:N1 | 51:1t:15:ARG:HG2 | 2.20 | 0.56 |
| 32:1a:978:A:O2' | 32:1a:1322:C:N3 | 2.35 | 0.56 |
| 32:1a:1007:C:N3 | 32:1a:1022:G:O6 | 2.38 | 0.56 |
| 54:1w:4:C:H2' | 54:1w:5:G:C8 | 2.39 | 0.56 |
| 1:2A:1645:G:H5" | 1:2A:1646:C:H5' | 1.87 | 0.56 |
| 1:2A:2206:G:H3' | 1:2A:2207:G:H8 | 1.65 | 0.56 |
| 11:2P:36:LYS:O | 61:2P:305:HOH:O | 2.17 | 0.56 |
| 26:24:64:GLY:C | 26:24:66:SER:H | 2.13 | 0.56 |
| 32:2a:1030(A):G:N2 | 32:2a:1030(C):G:H3' | 2.21 | 0.56 |
| 32:2a:1274:G:N2 | 32:2a:1275:A:N7 | 2.47 | 0.56 |
| 32:2a:1366:C:H2' | 32:2a:1367:C:C6 | 2.41 | 0.56 |
| 50:2s:28:LYS:HB3 | 50:2s:29:ARG:CB | 2.34 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1A:919:G:N2 | 1:1A:2269:A:OP2 | 2.39 | 0.56 |
| 1:1A:2022:U:O2' | 1:1A:2617:C:H5' | 2.06 | 0.56 |
| 1:1A:2853:C:H2' | 1:1A:2854:G:C8 | 2.41 | 0.56 |
| 21:1Z:69:THR:HG22 | 21:1Z:90:VAL:HA | 1.88 | 0.56 |
| 32:1a:929:G:H1 | 32:1a:1388:C:H42 | 1.52 | 0.56 |
| 32:1a:1021:G:O2' | 32:1a:1022:G:O5' | 2.24 | 0.56 |
| 33:1b:28:PHE:HD1 | 33:1b:194:PRO:HG3 | 1.70 | 0.56 |
| 1:2A:122:G:N3 | 61:2A:3915:HOH:O | 2.33 | 0.56 |
| 2:2B:117:G:N7 | 61:2B:301:HOH:O | 2.33 | 0.56 |
| 5:2F:53:THR:HG23 | 5:2F:55:GLY:H | 1.69 | 0.56 |
| 12:2Q:125:LEU:HD12 | 12:2Q:129:THR:HG21 | 1.88 | 0.56 |
| 1:2A:2343:C:HO2' | 1:2A:2373:G:HO2' | 1.48 | 0.56 |
| 32:2a:174:C:H2' | 32:2a:175:C:H6 | 1.70 | 0.56 |
| 32:2a:1062:U:H2' | 32:2a:1063:C:C6 | 2.41 | 0.56 |
| 32:2a:1190:G:H5' | 34:2c:176:HIS:CE1 | 2.40 | 0.56 |
| 32:2a:1479:C:H2' | 32:2a:1480:G:H8 | 1.69 | 0.56 |
| 1:1A:668:G:H5' | 1:1A:669:G:OP2 | 2.06 | 0.56 |
| 32:1a:1036:G:H5" | 32:1a:1037:C:C5 | 2.41 | 0.56 |
| 15:2T:118:ARG:HG2 | 32:2a:1442(A):G:C8 | 2.41 | 0.56 |
| 21:2Z:33:LEU:HD11 | 21:2Z:90:VAL:HG21 | 1.88 | 0.56 |
| 32:2a:537:G:H5" | 43:2l:113:ARG:NH1 | 2.21 | 0.56 |
| 1:1A:1796:U:H2' | 1:1A:1797:C:C6 | 2.40 | 0.56 |
| 1:1A:2478:A:OP2 | 31:19:2:LYS:NZ | 2.24 | 0.56 |
| 4:1E:111:ARG:HG3 | 4:1E:160:TYR:CD2 | 2.41 | 0.56 |
| 12:1Q:10:ARG:NH1 | 12:1Q:90:VAL:H | 2.04 | 0.56 |
| 12:1Q:16:ARG:HG3 | 12:1Q:18:LYS:HG3 | 1.88 | 0.56 |
| 32:1a:790:A:OP1 | 55:1x:38:A:O2' | 2.20 | 0.56 |
| 54:1w:2:C:N3 | 54:1w:71:G:N2 | 2.54 | 0.56 |
| 32:2a:1412:C:H2' | 32:2a:1413:A:C8 | 2.41 | 0.56 |
| 43:2l:32:PHE:HB3 | 43:2l:84:LEU:HD11 | 1.86 | 0.56 |
| 1:1A:616:G:H5' | 5:1F:205:ARG:HD3 | 1.88 | 0.56 |
| 1:1A:1113:U:H2' | 1:1A:1114:G:C8 | 2.40 | 0.56 |
| 1:1A:1862:G:H2' | 1:1A:1863:G:H8 | 1.71 | 0.56 |
| 5:1F:178:PRO:HB2 | 5:1F:201:VAL:HG21 | 1.88 | 0.56 |
| 32:1a:636:U:H2' | 32:1a:637:G:H8 | 1.71 | 0.56 |
| 32:1a:1008:C:O2 | 32:1a:1021:G:N1 | 2.25 | 0.56 |
| 1:2A:581:C:H2' | 1:2A:582:G:C8 | 2.41 | 0.56 |
| 1:2A:2693:A:H2' | 1:2A:2694:G:H8 | 1.71 | 0.56 |
| 6:2G:44:GLY:N | 6:2G:88:ILE:O | 2.39 | 0.56 |
| 32:2a:28:G:O2' | 32:2a:296:U:OP1 | 2.21 | 0.56 |
| 33:2b:80:ILE:HG12 | 33:2b:215:LEU:HD23 | 1.88 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1A:2567:G:H2' | 1:1A:2568:C:C6 | 2.41 | 0.56 |
| 33:1b:80:ILE:HG12 | 33:1b:215:LEU:HD23 | 1.87 | 0.56 |
| 1:2A:631:A:OP1 | 11:2P:65:ARG:NE | 2.26 | 0.56 |
| 2:2B:14:U:O3' | 2:2B:108:U:O2' | 2.23 | 0.56 |
| 6:2G:122:PRO:HB3 | 6:2G:170:ARG:HH12 | 1.71 | 0.56 |
| 8:2I:130:TYR:HB3 | 8:2I:138:ILE:HB | 1.87 | 0.56 |
| 32:2a:259:G:OP2 | 51:2t:83:ARG:NH1 | 2.39 | 0.56 |
| 32:2a:952:U:H2' | 32:2a:953:G:C8 | 2.41 | 0.56 |
| 32:2a:1040:U:H2' | 32:2a:1041:A:C8 | 2.41 | 0.56 |
| 35:2d:119:GLN:HE21 | 35:2d:123:HIS:CD2 | 2.24 | 0.56 |
| 35:2d:148:VAL:HB | 35:2d:181:MET:HG3 | 1.87 | 0.56 |
| 50:2s:20:LEU:HA | 50:2s:23:ASN:HD22 | 1.71 | 0.56 |
| 54:2w:8:4SU:S4 | 54:2w:14:A:N7 | 2.79 | 0.56 |
| 1:1A:740:U:OP2 | 61:1A:5734:HOH:O | 2.18 | 0.55 |
| 1:1A:2243:U:H2' | 1:1A:2244:U:C6 | 2.40 | 0.55 |
| 12:1Q:85:LYS:HG2 | 22:10:7:LEU:HB3 | 1.87 | 0.55 |
| 13:1R:28:LEU:HD23 | 13:1R:48:VAL:HG21 | 1.88 | 0.55 |
| 32:1a:1027:C:N3 | 32:1a:1034:G:N2 | 2.54 | 0.55 |
| 33:1b:15:VAL:HG23 | 33:1b:16:HIS:ND1 | 2.22 | 0.55 |
| 33:1b:158:LEU:HD21 | 33:1b:180:LEU:HD13 | 1.88 | 0.55 |
| 39:1h:21:LYS:O | 39:1h:65:TYR:OH | 2.20 | 0.55 |
| 1:2A:1839:G:C8 | 1:2A:1927:A:H1' | 2.41 | 0.55 |
| 32:2a:1106:G:H5" | 34:2c:172:ARG:HG2 | 1.88 | 0.55 |
| 33:2b:91:PRO:HG2 | 33:2b:155:LEU:HD13 | 1.87 | 0.55 |
| 15:1T:49:VAL:HG12 | 15:1T:63:VAL:HG22 | 1.88 | 0.55 |
| 32:1a:73:G:H1 | 32:1a:96:U:H3 | 1.55 | 0.55 |
| 32:1a:1060:C:H5" | 41:1j:51:ARG:HG2 | 1.88 | 0.55 |
| 34:2c:32:LEU:HD23 | 34:2c:59:ARG:HD3 | 1.87 | 0.55 |
| 34:2c:77:ILE:HG13 | 34:2c:78:GLY:H | 1.72 | 0.55 |
| 55:2x:23:C:H2' | 55:2x:24:U:C6 | 2.40 | 0.55 |
| 1:1A:2390:U:P | 30:18:35:GLN:HE22 | 2.29 | 0.55 |
| 19:1X:53:LYS:HB3 | 19:1X:82:GLN:HB3 | 1.89 | 0.55 |
| 34:1c:15:THR:HG22 | 34:1c:16:ARG:HG2 | 1.87 | 0.55 |
| 1:2A:2646:C:OP2 | 1:2A:2732:G:O2' | 2.21 | 0.55 |
| 12:2Q:68:ILE:HG22 | 12:2Q:101:ARG:HE | 1.71 | 0.55 |
| 20:2Y:97:ARG:NH1 | 20:2Y:107:ASP:O | 2.40 | 0.55 |
| 32:2a:157:G:H2' | 32:2a:158:G:H8 | 1.72 | 0.55 |
| 32:2a:515:G:H2' | 32:2a:516:PSU:H6 | 1.71 | 0.55 |
| 32:2a:581:G:N1 | 32:2a:759:A:OP2 | 2.32 | 0.55 |
| 32:2a:1269:A:OP1 | 52:2u:24:ARG:NH2 | 2.37 | 0.55 |
| 33:2b:28:PHE:HD1 | 33:2b:194:PRO:HG3 | 1.71 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 35:2d:76:ARG:NE | 35:2d:80:GLU:OE2 | 2.34 | 0.55 |
| 54:2w:27:G:H1 | 54:2w:43:C:N4 | 2.05 | 0.55 |
| 18:1W:77:ASP:OD1 | 61:1W:301:HOH:O | 2.18 | 0.55 |
| 40:1i:20:ARG:O | 40:1i:60:ASP:N | 2.33 | 0.55 |
| 1:2A:236:C:H2' | 1:2A:237:C:C6 | 2.42 | 0.55 |
| 32:2a:967:5MC:H2' | 32:2a:968:A:C8 | 2.41 | 0.55 |
| 37:2f:67:MET:HE1 | 37:2f:75:LEU:HD22 | 1.89 | 0.55 |
| 1:1A:579:G:OP1 | 61:1A:7016:HOH:O | 2.18 | 0.55 |
| 1:1A:2467:C:H4' | 12:1Q:123:HIS:CD2 | 2.41 | 0.55 |
| 32:1a:576:G:O6 | 32:1a:880:C:O2' | 2.23 | 0.55 |
| 32:1a:976:G:H5' | 32:1a:1358:U:O2' | 2.06 | 0.55 |
| 1:2A:1580:A:H3' | 1:2A:1581:G:H8 | 1.71 | 0.55 |
| 32:2a:584:G:OP2 | 48:2q:87:LYS:NZ | 2.39 | 0.55 |
| 32:2a:1033:G:H2' | 32:2a:1034:G:H8 | 1.71 | 0.55 |
| 32:2a:1240:U:N3 | 38:2g:30:ILE:O | 2.28 | 0.55 |
| 32:2a:1342:C:H2' | 32:2a:1343:G:H8 | 1.71 | 0.55 |
| 42:2k:43:SER:HA | 42:2k:47:VAL:HG21 | 1.88 | 0.55 |
| 1:1A:1507:A:O2' | 1:1A:1509(A):A:N6 | 2.40 | 0.55 |
| 1:1A:1786:A:H1' | 1:1A:1938:A:N6 | 2.21 | 0.55 |
| 1:1A:2128:C:H42 | 1:1A:2160:G:H1 | 1.55 | 0.55 |
| 1:1A:2787:C:H1' | 4:1E:62:PRO:HG3 | 1.89 | 0.55 |
| 32:1a:1378:C:O2 | 38:1g:76:ARG:NH2 | 2.40 | 0.55 |
| 40:1i:17:VAL:HG11 | 40:1i:81:ILE:HA | 1.89 | 0.55 |
| 54:1y:15:G:H22 | 54:1y:48:C:H42 | 1.52 | 0.55 |
| 1:2A:819:A:OP2 | 1:2A:1187:G:N2 | 2.30 | 0.55 |
| 1:2A:2104:G:H1 | 1:2A:2185:C:H42 | 1.54 | 0.55 |
| 2:2B:41:U:H5 | 6:2G:70:VAL:H | 1.55 | 0.55 |
| 3:2D:108:PRO:HB3 | 3:2D:143:HIS:HE1 | 1.70 | 0.55 |
| 6:2G:106:LEU:HA | 6:2G:110:ALA:HB3 | 1.88 | 0.55 |
| 32:2a:1406:U:O2 | 32:2a:1517:G:N2 | 2.40 | 0.55 |
| 32:2a:1517:G:N7 | 32:2a:1518:MA6:H103 | 2.21 | 0.55 |
| 39:2h:110:ALA:HB3 | 39:2h:121:ASP:HB3 | 1.88 | 0.55 |
| 1:1A:793:A:OP2 | 1:1A:2071:A:O2' | 2.23 | 0.55 |
| 1:1A:1057:A:H61 | 1:1A:1081:U:H3 | 1.54 | 0.55 |
| 1:1A:1537:G:OP1 | 61:1A:4207:HOH:O | 2.18 | 0.55 |
| 3:1D:274:ARG:NH1 | 61:1D:401:HOH:O | 2.40 | 0.55 |
| 4:1E:181:LEU:HD11 | 15:1T:6:LEU:HD23 | 1.88 | 0.55 |
| 32:1a:103:C:OP2 | 51:1t:14:LYS:NZ | 2.31 | 0.55 |
| 32:1a:430:A:OP1 | 35:1d:9:CYS:HB2 | 2.07 | 0.55 |
| 28:26:9:LEU:HD22 | 28:26:25:LYS:HD2 | 1.89 | 0.55 |
| 32:2a:662:G:H2' | 32:2a:663:A:H8 | 1.72 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 33:2b:187:LEU:HA | 33:2b:201:ILE:HB | 1.88 | 0.55 |
| 35:2d:164:ALA:HB1 | 35:2d:168:ARG:HH11 | 1.71 | 0.55 |
| 39:2h:28:ALA:HB3 | 39:2h:57:PRO:HB2 | 1.88 | 0.55 |
| 44:2m:5:ALA:HB3 | 44:2m:22:ILE:HD13 | 1.88 | 0.55 |
| 1:1A:1779:U:H2' | 61:1A:6221:HOH:O | 2.06 | 0.55 |
| 1:1A:2537:U:H2' | 1:1A:2538:C:C6 | 2.42 | 0.55 |
| 2:1B:106:G:H5' | 21:1Z:31:ARG:HG2 | 1.88 | 0.55 |
| 31:19:17:ILE:HD13 | 31:19:26:ILE:HD13 | 1.89 | 0.55 |
| 32:1a:45:U:H2' | 32:1a:46:G:C8 | 2.42 | 0.55 |
| 36:1e:144:THR:OG1 | 36:1e:147:ASP:OD2 | 2.21 | 0.55 |
| 50:1s:27:GLU:CB | 50:1s:28:LYS:HA | 2.35 | 0.55 |
| 1:2A:800:A:H8 | 1:2A:800:A:OP1 | 1.90 | 0.55 |
| 1:2A:981:A:N1 | 1:2A:2027:G:O2' | 2.38 | 0.55 |
| 1:2A:1311:G:H2' | 29:27:47:ARG:HH22 | 1.70 | 0.55 |
| 2:2B:113:G:N2 | 14:2S:45:GLY:O | 2.26 | 0.55 |
| 32:2a:64:G:H4' | 32:2a:65:U:H3' | 1.88 | 0.55 |
| 32:2a:537:G:H2' | 32:2a:538:G:C8 | 2.41 | 0.55 |
| 38:2g:78:ARG:HG2 | 38:2g:79:ARG:H | 1.71 | 0.55 |
| 25:13:18:ASP:OD1 | 25:13:18:ASP:N | 2.40 | 0.55 |
| 32:1a:452:A:O2' | 32:1a:453:A:OP2 | 2.24 | 0.55 |
| 1:2A:2273:A:H2' | 1:2A:2274:A:C8 | 2.42 | 0.55 |
| 5:2F:184:TYR:CE2 | 5:2F:188:ARG:HD2 | 2.42 | 0.55 |
| 21:2Z:98:MET:O | 21:2Z:126:VAL:N | 2.39 | 0.55 |
| 41:2j:65:LEU:HD13 | 45:2n:56:VAL:HG22 | 1.89 | 0.55 |
| 16:1U:52:ARG:HH11 | 16:1U:55:ARG:HH21 | 1.55 | 0.55 |
| 32:1a:453:A:O2' | 47:1p:68:ASP:O | 2.24 | 0.55 |
| 1:2A:2788:C:OP1 | 4:2E:61:ARG:NH2 | 2.40 | 0.55 |
| 32:2a:538:G:H5" | 43:2l:114:LYS:HB2 | 1.89 | 0.55 |
| 34:2c:108:ASN:HB3 | 34:2c:111:LEU:HB2 | 1.88 | 0.55 |
| 44:2m:11:ARG:HA | 44:2m:45:VAL:HB | 1.88 | 0.55 |
| 24:12:32:LEU:HD22 | 24:12:36:ARG:HH11 | 1.72 | 0.54 |
| 25:13:6:VAL:HG13 | 25:13:54:VAL:HG11 | 1.89 | 0.54 |
| 25:13:37:LEU:HB3 | 25:13:43:ILE:HD13 | 1.89 | 0.54 |
| 34:1c:155:GLY:HA3 | 34:1c:196:LEU:HD22 | 1.88 | 0.54 |
| 54:1y:53:G:H1 | 54:1y:61:C:H42 | 1.56 | 0.54 |
| 1:2A:1113:U:H2' | 1:2A:1114:G:C8 | 2.42 | 0.54 |
| 10:2O:73:ASP:OD2 | 15:2T:32:TYR:OH | 2.20 | 0.54 |
| 29:27:5:TRP:NE1 | 29:27:7:PRO:HG3 | 2.22 | 0.54 |
| 38:2g:68:ASN:ND2 | 38:2g:127:ALA:O | 2.38 | 0.54 |
| 1:1A:2125:G:N1 | 1:1A:2172:U:OP1 | 2.29 | 0.54 |
| 10:1O:64:ARG:HG2 | 10:1O:83:ALA:HB3 | 1.89 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 39:1h:81:HIS:N | 39:1h:138:TRP:O | 2.40 | 0.54 |
| 1:2A:740:U:H2' | 1:2A:741:G:C8 | 2.43 | 0.54 |
| 1:2A:955:C:OP1 | 12:2Q:87:LYS:NZ | 2.27 | 0.54 |
| 1:2A:2144:U:H1' | 1:2A:2148:G:H22 | 1.73 | 0.54 |
| 32:2a:565:U:OP2 | 32:2a:566:G:O2' | 2.22 | 0.54 |
| 32:2a:947:G:O3' | 44:2m:109:THR:OG1 | 2.25 | 0.54 |
| 32:2a:1323:G:H4' | 32:2a:1363:C:C2 | 2.42 | 0.54 |
| 1:1A:729:G:C6 | 3:1D:208:LYS:HB2 | 2.41 | 0.54 |
| 1:1A:857:C:H4' | 22:10:23:VAL:HG21 | 1.88 | 0.54 |
| 1:1A:2377:A:H2' | 1:1A:2378:A:C8 | 2.42 | 0.54 |
| 10:1O:35:VAL:HG21 | 10:1O:69:ILE:HD13 | 1.89 | 0.54 |
| 17:1V:76:LYS:HB2 | 17:1V:81:TYR:HB3 | 1.88 | 0.54 |
| 39:1h:11:THR:O | 39:1h:15:ASN:ND2 | 2.41 | 0.54 |
| 39:1h:34:GLU:OE1 | 39:1h:37:ARG:NH2 | 2.41 | 0.54 |
| 50:1s:38:SER:HB2 | 50:1s:71:LEU:HD23 | 1.89 | 0.54 |
| 1:2A:136:G:H1 | 1:2A:143(A):C:H42 | 1.53 | 0.54 |
| 1:2A:2753:A:N3 | 31:29:15:LYS:NZ | 2.55 | 0.54 |
| 15:2T:11:GLU:O | 15:2T:15:VAL:HG23 | 2.07 | 0.54 |
| 32:2a:975:A:H5" | 32:2a:1363(A):A:N6 | 2.21 | 0.54 |
| 54:2w:28:G:H2' | 54:2w:29:G:O4' | 2.06 | 0.54 |
| 1:1A:323:G:C8 | 5:1F:171:PRO:HG3 | 2.43 | 0.54 |
| 32:1a:1401:G:C2 | 32:1a:1402:4OC:H1' | 2.43 | 0.54 |
| 51:1t:60:GLU:HG3 | 51:1t:81:LYS:HD2 | 1.88 | 0.54 |
| 1:2A:99:U:O4 | 20:2Y:8:LYS:NZ | 2.40 | 0.54 |
| 1:2A:517:C:OP1 | 27:25:16:ARG:NH2 | 2.41 | 0.54 |
| 1:2A:551:G:O2' | 1:2A:1220:A:N3 | 2.37 | 0.54 |
| 1:2A:2499:C:OP1 | 61:2A:6007:HOH:O | 2.17 | 0.54 |
| 6:2G:11:TYR:HA | 6:2G:15:VAL:HB | 1.89 | 0.54 |
| 7:2H:28:GLY:HA3 | 7:2H:79:VAL:HB | 1.88 | 0.54 |
| 12:2Q:85:LYS:HG2 | 22:20:7:LEU:HB3 | 1.88 | 0.54 |
| 19:2X:43:VAL:HG21 | 19:2X:81:VAL:HG11 | 1.89 | 0.54 |
| 32:2a:1007:C:N3 | 32:2a:1022:G:C6 | 2.76 | 0.54 |
| 32:2a:1239:A:H62 | 32:2a:1299:A:N6 | 2.05 | 0.54 |
| 45:2n:37:PHE:HZ | 45:2n:56:VAL:HG21 | 1.71 | 0.54 |
| 1:1A:1750:G:O2' | 1:1A:2860:A:N1 | 2.40 | 0.54 |
| 32:1a:1027:C:N4 | 32:1a:1034:G:N1 | 2.56 | 0.54 |
| 32:1a:1030:C:N3 | 32:1a:1031:G:C2 | 2.76 | 0.54 |
| 32:1a:1510:U:H2' | 32:1a:1511:G:C8 | 2.43 | 0.54 |
| 50:1s:22:LEU:HB3 | 50:1s:27:GLU:HB3 | 1.90 | 0.54 |
| 32:2a:1387:G:H2' | 32:2a:1388:C:C6 | 2.42 | 0.54 |
| 26:14:58:ARG:HE | 50:1s:68:GLY:HA3 | 1.73 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 32:1a:254:G:O2' | 48:1q:16:GLN:O | 2.25 | 0.54 |
| 44:1m:37:THR:O | 44:1m:55:ARG:NH1 | 2.40 | 0.54 |
| 1:2A:441:U:O2 | 5:2F:46:ARG:NH2 | 2.36 | 0.54 |
| 1:2A:1159:U:H2' | 1:2A:1160:G:H8 | 1.71 | 0.54 |
| 32:2a:396:G:O2' | 32:2a:398:C:OP1 | 2.16 | 0.54 |
| 32:2a:1485:U:H2' | 32:2a:1486:G:C8 | 2.43 | 0.54 |
| 33:2b:88:ALA:HB2 | 33:2b:219:VAL:HG13 | 1.89 | 0.54 |
| 35:2d:60:GLU:HG2 | 35:2d:202:LEU:HB2 | 1.89 | 0.54 |
| 35:2d:119:GLN:HG2 | 35:2d:123:HIS:CD2 | 2.42 | 0.54 |
| 41:2j:49:VAL:HG11 | 45:2n:45:ARG:HD2 | 1.90 | 0.54 |
| 51:2t:59:ALA:O | 51:2t:63:ILE:HG13 | 2.07 | 0.54 |
| 1:1A:1094:U:H1' | 1:1A:1097:U:C5 | 2.43 | 0.54 |
| 1:1A:1668:A:O2' | 1:1A:1674:G:N7 | 2.38 | 0.54 |
| 1:1A:1937:A:H1' | 1:1A:1939:5MU:H72 | 1.88 | 0.54 |
| 6:1G:43:LEU:HD11 | 6:1G:153:ARG:HD2 | 1.90 | 0.54 |
| 12:1Q:51:ARG:HD3 | 12:1Q:66:ILE:HD11 | 1.89 | 0.54 |
| 21:1Z:150:LEU:HB3 | 21:1Z:171:ILE:HD11 | 1.89 | 0.54 |
| 35:1d:61:LYS:NZ | 35:1d:72:GLU:OE1 | 2.40 | 0.54 |
| 47:1p:22:THR:HA | 47:1p:33:ILE:HG13 | 1.90 | 0.54 |
| 32:2a:274:A:N6 | 61:2a:3617:HOH:O | 2.26 | 0.54 |
| 32:2a:707:C:H2' | 32:2a:708:C:H6 | 1.72 | 0.54 |
| 32:2a:1030(A):G:H21 | 32:2a:1030(C):G:H3' | 1.71 | 0.54 |
| 5:1F:167:ALA:HB1 | 5:1F:173:VAL:HG11 | 1.89 | 0.54 |
| 32:1a:1062:U:H2' | 32:1a:1063:C:C6 | 2.42 | 0.54 |
| 41:1j:38:ILE:HG13 | 41:1j:71:LEU:HB3 | 1.89 | 0.54 |
| 54:1w:44:G:C5 | 54:1w:45:U:H1' | 2.43 | 0.54 |
| 1:2A:223:A:N1 | 1:2A:407:G:O2' | 2.41 | 0.54 |
| 1:2A:630:G:N2 | 1:2A:633:A:OP2 | 2.36 | 0.54 |
| 1:2A:900:A:O2' | 1:2A:901:A:OP1 | 2.20 | 0.54 |
| 3:2D:3:VAL:HG13 | 3:2D:17:THR:HB | 1.89 | 0.54 |
| 32:2a:782:A:OP1 | 61:2a:3642:HOH:O | 2.18 | 0.54 |
| 36:2e:110:LEU:HD13 | 36:2e:118:ILE:HG21 | 1.90 | 0.54 |
| 38:2g:69:VAL:HG22 | 38:2g:135:VAL:HG22 | 1.90 | 0.54 |
| 1:1A:1069:A:H2' | 1:1A:1073:A:N7 | 2.23 | 0.54 |
| 1:1A:2747:G:O6 | 1:1A:2755:C:H5" | 2.08 | 0.54 |
| 1:1A:2815:C:H5' | 27:15:29:THR:HG21 | 1.89 | 0.54 |
| 6:1G:67:LYS:HD3 | 26:14:5:ILE:HD12 | 1.90 | 0.54 |
| 8:1I:65:ALA:HB1 | 8:1I:136:VAL:HG11 | 1.89 | 0.54 |
| 32:1a:676:A:H1' | 42:1k:115:PRO:HB3 | 1.90 | 0.54 |
| 1:2A:2127:G:N1 | 1:2A:2161:C:C5 | 2.75 | 0.54 |
| 4:2E:116:VAL:HG13 | 4:2E:122:PHE:HB2 | 1.90 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:2H:9:ILE:HB | 7:2H:50:VAL:HB | 1.90 | 0.54 |
| 32:2a:1142:G:H2' | 32:2a:1143:G:O4' | 2.08 | 0.54 |
| 32:2a:1203:C:H2' | 32:2a:1204:A:C8 | 2.41 | 0.54 |
| 37:2f:70:ASP:OD1 | 37:2f:70:ASP:N | 2.40 | 0.54 |
| 41:2j:47:PHE:HB2 | 41:2j:63:PHE:HB2 | 1.90 | 0.54 |
| 1:1A:576:U:H2' | 1:1A:577:G:C8 | 2.42 | 0.54 |
| 7:1H:40:GLU:OE1 | 7:1H:61:HIS:NE2 | 2.40 | 0.54 |
| 33:1b:93:VAL:HG21 | 33:1b:97:TRP:HD1 | 1.73 | 0.54 |
| 34:1c:15:THR:HG21 | 34:1c:181:ASN:HA | 1.90 | 0.54 |
| 35:1d:81:GLU:OE1 | 35:1d:139:ARG:NH2 | 2.40 | 0.54 |
| 36:1e:78:HIS:CE1 | 36:1e:143:ARG:H | 2.26 | 0.54 |
| 46:1o:25:THR:HG21 | 46:1o:70:LEU:HB2 | 1.89 | 0.54 |
| 1:2A:789:A:N1 | 61:2A:4447:HOH:O | 2.33 | 0.54 |
| 1:2A:882:G:H2' | 1:2A:883:G:H8 | 1.73 | 0.54 |
| 1:2A:2619:C:OP1 | 4:2E:152:LYS:NZ | 2.28 | 0.54 |
| 32:2a:375:U:OP1 | 47:2p:69:THR:HG21 | 2.07 | 0.54 |
| 32:2a:1005:A:OP1 | 32:2a:1006:C:N4 | 2.41 | 0.54 |
| 1:1A:721:C:H2' | 1:1A:722:A:C8 | 2.43 | 0.53 |
| 1:1A:2130:U:H2' | 1:1A:2158:A:N1 | 2.23 | 0.53 |
| 32:1a:662:G:H2' | 32:1a:663:A:C8 | 2.43 | 0.53 |
| 32:1a:1133:G:N2 | 32:1a:1141:C:N3 | 2.57 | 0.53 |
| 33:1b:21:ARG:O | 33:1b:23:ARG:N | 2.35 | 0.53 |
| 33:1b:162:ILE:O | 33:1b:185:ILE:HG12 | 2.07 | 0.53 |
| 50:1s:50:ALA:HB1 | 50:1s:57:HIS:HB3 | 1.89 | 0.53 |
| 1:2A:271(G):C:H2' | 1:2A:271(H):G:C8 | 2.42 | 0.53 |
| 1:2A:1826:G:H4' | 3:2D:242:ARG:NH1 | 2.23 | 0.53 |
| 32:2a:189(B):C:H42 | 32:2a:189(I):G:H1 | 1.56 | 0.53 |
| 32:2a:986:A:N3 | 50:2s:52:TYR:OH | 2.40 | 0.53 |
| 32:2a:1330:U:H4' | 44:2m:23:TYR:CE1 | 2.43 | 0.53 |
| 49:2r:32:ARG:HA | 49:2r:69:THR:HG21 | 1.90 | 0.53 |
| 55:2x:40:C:H2' | 55:2x:41:C:H6 | 1.73 | 0.53 |
| 32:1a:1033:G:H2' | 32:1a:1034:G:H8 | 1.73 | 0.53 |
| 35:1d:26:CYS:SG | 60:1d:302:SF4:S1 | 3.07 | 0.53 |
| 1:2A:686:G:H21 | 1:2A:788:A:H61 | 1.55 | 0.53 |
| 1:2A:2117:A:O2' | 1:2A:2118:U:H5" | 2.07 | 0.53 |
| 1:2A:2126:A:N6 | 1:2A:2162:G:HO2' | 2.05 | 0.53 |
| 1:2A:2646:C:H2' | 1:2A:2647:U:O4' | 2.08 | 0.53 |
| 1:2A:2751:G:O2' | 1:2A:2752:C:O4' | 2.26 | 0.53 |
| 32:2a:447:G:O6 | 32:2a:485:G:O2' | 2.24 | 0.53 |
| 32:2a:585:G:O2' | 32:2a:879:C:OP1 | 2.23 | 0.53 |
| 32:2a:1435:G:H2' | 32:2a:1436:U:C6 | 2.44 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 33:2b:15:VAL:HG11 | 33:2b:213:LEU:HD13 | 1.88 | 0.53 |
| 1:1A:84:A:H5" | 20:1Y:8:LYS:HG2 | 1.90 | 0.53 |
| 34:1c:35:GLU:CD | 34:1c:59:ARG:HH22 | 2.16 | 0.53 |
| 42:1k:15:ALA:HA | 42:1k:76:GLY:O | 2.09 | 0.53 |
| 1:2A:1991:U:H2' | 1:2A:1992:G:H5" | 1.90 | 0.53 |
| 32:2a:662:G:H1 | 32:2a:743:U:H3 | 1.55 | 0.53 |
| 32:2a:1456:G:O6 | 51:2t:54:LYS:NZ | 2.32 | 0.53 |
| 1:1A:2305:A:H5" | 6:1G:134:GLY:HA3 | 1.89 | 0.53 |
| 1:1A:2312:U:H5' | 6:1G:88:ILE:HD11 | 1.91 | 0.53 |
| 30:18:15:LYS:NZ | 61:18:211:HOH:O | 2.37 | 0.53 |
| 32:1a:731:G:H5' | 32:1a:766:A:H4' | 1.89 | 0.53 |
| 1:2A:845:G:OP2 | 1:2A:845:G:N2 | 2.36 | 0.53 |
| 1:2A:1231:G:H2' | 1:2A:1232:G:C8 | 2.43 | 0.53 |
| 5:2F:95:ARG:NH1 | 5:2F:97:TYR:OH | 2.42 | 0.53 |
| 8:2I:14:ASP:OD1 | 8:2I:15:VAL:N | 2.41 | 0.53 |
| 12:2Q:81:VAL:HG12 | 22:20:5:LYS:HD2 | 1.90 | 0.53 |
| 13:2R:33:ARG:NH1 | 13:2R:115:GLU:OE1 | 2.35 | 0.53 |
| 26:24:24:THR:OG1 | 26:24:25:TYR:N | 2.33 | 0.53 |
| 32:2a:834:C:H2' | 32:2a:835:U:H6 | 1.73 | 0.53 |
| 32:2a:1347:G:N2 | 32:2a:1373:G:H2' | 2.23 | 0.53 |
| 32:2a:1492:A:H4' | 43:2l:47:LYS:HE3 | 1.91 | 0.53 |
| 32:2a:1513:A:H2' | 32:2a:1514:C:C6 | 2.44 | 0.53 |
| 45:2n:24:CYS:HB3 | 45:2n:29:ARG:H | 1.73 | 0.53 |
| 1:1A:271(M):G:O2' | 1:1A:271(N):U:H5" | 2.08 | 0.53 |
| 1:1A:1264:G:OP1 | 27:15:19:ARG:NH2 | 2.29 | 0.53 |
| 1:1A:1619:G:N7 | 61:1A:6580:HOH:O | 2.34 | 0.53 |
| 1:1A:2627:G:O2' | 1:1A:2781:A:N1 | 2.30 | 0.53 |
| 7:1H:164:TYR:HB2 | 7:1H:167:GLU:HB2 | 1.89 | 0.53 |
| 8:1I:116:LEU:HD21 | 8:1I:119:PRO:HA | 1.91 | 0.53 |
| 32:1a:262:A:H2' | 32:1a:263:A:C8 | 2.43 | 0.53 |
| 32:1a:998:G:N2 | 32:1a:1043:C:N3 | 2.46 | 0.53 |
| 1:2A:400:G:N7 | 61:2A:5225:HOH:O | 2.33 | 0.53 |
| 1:2A:577:G:O2' | 1:2A:1254:A:OP1 | 2.25 | 0.53 |
| 1:2A:1204:A:H5' | 1:2A:1206:G:H1' | 1.90 | 0.53 |
| 1:2A:2168:G:H8 | 1:2A:2170:A:N7 | 2.07 | 0.53 |
| 4:2E:26:ILE:HD11 | 4:2E:188:VAL:HG21 | 1.91 | 0.53 |
| 10:2O:68:GLU:HB3 | 10:2O:78:ARG:HG3 | 1.90 | 0.53 |
| 26:24:48:ARG:HE | 26:24:52:THR:HA | 1.74 | 0.53 |
| 32:2a:17:U:H2' | 32:2a:18:C:C6 | 2.43 | 0.53 |
| 54:2w:53:G:H1 | 54:2w:61:C:H42 | 1.56 | 0.53 |
| 1:1A:1426:G:O2' | 1:1A:1572:A:N6 | 2.42 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1A:1675:C:O2 | 4:1E:128:SER:OG | 2.27 | 0.53 |
| 1:1A:2483:C:OP1 | 54:1w:64:A:H4' | 2.08 | 0.53 |
| 61:1A:6915:HOH:O | 13:1R:3:HIS:NE2 | 2.34 | 0.53 |
| 7:1H:24:VAL:HG22 | 7:1H:35:VAL:HB | 1.89 | 0.53 |
| 28:16:8:LYS:HD3 | 30:18:34:TRP:CD2 | 2.44 | 0.53 |
| 1:2A:2408:U:H2' | 1:2A:2409:G:C8 | 2.44 | 0.53 |
| 18:2W:17:VAL:HG11 | 18:2W:103:ILE:HD11 | 1.90 | 0.53 |
| 32:2a:9:G:H2' | 32:2a:10:A:C8 | 2.43 | 0.53 |
| 35:2d:114:ARG:O | 35:2d:118:ARG:N | 2.35 | 0.53 |
| 35:2d:173:TRP:CD1 | 35:2d:174:LEU:HG | 2.44 | 0.53 |
| 36:2e:33:VAL:HG22 | 36:2e:112:LEU:HD12 | 1.90 | 0.53 |
| 6:1G:106:LEU:HA | 6:1G:110:ALA:HB3 | 1.91 | 0.53 |
| 12:1Q:30:GLY:HA2 | 12:1Q:107:ALA:HB2 | 1.90 | 0.53 |
| 32:1a:1412:C:H2' | 32:1a:1413:A:C8 | 2.44 | 0.53 |
| 48:1q:24:GLU:HA | 48:1q:39:SER:HA | 1.91 | 0.53 |
| 1:2A:212:G:H2' | 1:2A:213:A:O4' | 2.09 | 0.53 |
| 1:2A:296:C:O3' | 20:2Y:95:LYS:NZ | 2.42 | 0.53 |
| 1:2A:851:U:H5' | 25:23:49:LYS:HD2 | 1.91 | 0.53 |
| 1:2A:979:G:H5" | 1:2A:980:A:H5" | 1.90 | 0.53 |
| 1:2A:1188:U:H4' | 17:2V:79:VAL:HG22 | 1.89 | 0.53 |
| 3:2D:17:THR:O | 3:2D:211:ARG:NH2 | 2.42 | 0.53 |
| 20:2Y:28:LYS:HB3 | 20:2Y:38:ILE:HG22 | 1.91 | 0.53 |
| 37:2f:30:LEU:HD23 | 37:2f:75:LEU:HD11 | 1.91 | 0.53 |
| 40:2i:85:LEU:HB3 | 40:2i:92:TYR:CD2 | 2.44 | 0.53 |
| 1:1A:278:A:H2' | 1:1A:279:C:C6 | 2.43 | 0.53 |
| 7:1H:98:LEU:HD13 | 7:1H:125:VAL:HG23 | 1.89 | 0.53 |
| 12:1Q:20:ALA:HB2 | 21:1Z:79:ARG:HG3 | 1.90 | 0.53 |
| 26:14:57:GLU:HG2 | 26:14:58:ARG:HH11 | 1.73 | 0.53 |
| 26:14:58:ARG:O | 26:14:61:ARG:N | 2.28 | 0.53 |
| 32:1a:1027:C:C4 | 32:1a:1034:G:N1 | 2.76 | 0.53 |
| 34:1c:22:TRP:NE1 | 34:1c:36:ASP:OD2 | 2.40 | 0.53 |
| 36:1e:33:VAL:HG21 | 36:1e:109:ILE:HA | 1.91 | 0.53 |
| 39:1h:7:ALA:HB2 | 39:1h:85:ARG:HG3 | 1.90 | 0.53 |
| 39:1h:124:ALA:O | 39:1h:128:GLY:N | 2.42 | 0.53 |
| 1:2A:1567:A:OP2 | 3:2D:84:TYR:OH | 2.18 | 0.53 |
| 1:2A:2572:A:OP1 | 1:2A:2574:G:O2' | 2.27 | 0.53 |
| 7:2H:80:SER:OG | 7:2H:81:GLU:OE1 | 2.26 | 0.53 |
| 32:1a:333:G:H4' | 51:1t:16:HIS:CE1 | 2.44 | 0.53 |
| 33:1b:24:TRP:H | 33:1b:24:TRP:HD1 | 1.56 | 0.53 |
| 33:1b:91:PRO:HG2 | 33:1b:155:LEU:HD13 | 1.91 | 0.53 |
| 42:1k:84:VAL:HG11 | 42:1k:91:ARG:HD2 | 1.91 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:2H:24:VAL:HG13 | 7:2H:37:VAL:HG21 | 1.90 | 0.53 |
| 32:2a:560:U:OP2 | 61:2a:3572:HOH:O | 2.18 | 0.53 |
| 32:2a:1117:G:N2 | 32:2a:1180:A:O2' | 2.42 | 0.53 |
| 40:2i:46:ALA:HA | 40:2i:78:LYS:HB2 | 1.91 | 0.53 |
| 41:2j:21:GLN:O | 41:2j:21:GLN:NE2 | 2.40 | 0.53 |
| 1:1A:2590:A:H2' | 1:1A:2591:C:C6 | 2.42 | 0.53 |
| 1:1A:2791:C:H2' | 1:1A:2792:G:C8 | 2.44 | 0.53 |
| 1:1A:2839:G:H5' | 13:1R:46:GLY:HA2 | 1.90 | 0.53 |
| 32:1a:1277:C:O2' | 32:1a:1279:A:H1' | 2.09 | 0.53 |
| 3:2D:182:LEU:HB2 | 3:2D:272:ALA:HB3 | 1.91 | 0.53 |
| 13:2R:33:ARG:NH2 | 27:25:57:VAL:O | 2.26 | 0.53 |
| 35:2d:63:LYS:HD2 | 35:2d:198:VAL:HG22 | 1.90 | 0.53 |
| 40:2i:9:ARG:HG2 | 40:2i:14:VAL:HG12 | 1.91 | 0.53 |
| 1:1A:910:A:N3 | 1:1A:2264:C:O2' | 2.35 | 0.52 |
| 1:1A:2386:C:O2' | 61:1A:4208:HOH:O | 2.19 | 0.52 |
| 32:1a:1347:G:H5" | 40:1i:107:ARG:HB3 | 1.91 | 0.52 |
| 1:2A:817:C:O2' | 1:2A:839:U:H5" | 2.09 | 0.52 |
| 1:2A:1899:G:H2' | 1:2A:1899:G:N3 | 2.25 | 0.52 |
| 2:2B:110:G:C2' | 2:2B:111:G:H5' | 2.39 | 0.52 |
| 3:2D:26:LYS:HB3 | 3:2D:83:GLU:HG2 | 1.90 | 0.52 |
| 32:2a:1030:C:N3 | 32:2a:1031:G:N2 | 2.57 | 0.52 |
| 41:2j:81:THR:HA | 41:2j:84:GLN:HB3 | 1.91 | 0.52 |
| 46:2o:26:GLU:N | 46:2o:26:GLU:OE1 | 2.42 | 0.52 |
| 1:1A:800:A:H8 | 1:1A:800:A:OP1 | 1.92 | 0.52 |
| 1:1A:1420:U:O2' | 1:1A:1421:G:O5' | 2.21 | 0.52 |
| 1:1A:2728:U:H5' | 10:1O:70:LYS:HZ3 | 1.73 | 0.52 |
| 5:1F:140:LEU:HD11 | 5:1F:170:LEU:HD11 | 1.91 | 0.52 |
| 32:1a:69:G:H2' | 32:1a:70:G:C8 | 2.45 | 0.52 |
| 32:1a:183:G:N2 | 32:1a:223:U:O2' | 2.37 | 0.52 |
| 32:1a:1030:C:C4 | 32:1a:1030(A):G:H1' | 2.44 | 0.52 |
| 33:1b:60:ASP:O | 33:1b:64:ARG:HG2 | 2.10 | 0.52 |
| 54:1w:13:C:H2' | 54:1w:14:A:H5" | 1.90 | 0.52 |
| 1:2A:642:G:H21 | 1:2A:646:A:H2 | 1.57 | 0.52 |
| 1:2A:856:C:H2' | 1:2A:857:C:C6 | 2.44 | 0.52 |
| 1:2A:2114:A:N6 | 1:2A:2115:G:H21 | 2.07 | 0.52 |
| 1:2A:2773:C:OP1 | 4:2E:166:THR:OG1 | 2.21 | 0.52 |
| 32:2a:537:G:H2' | 32:2a:538:G:H8 | 1.74 | 0.52 |
| 42:2k:43:SER:HB3 | 42:2k:68:ALA:HB2 | 1.91 | 0.52 |
| 43:2l:33:ARG:HG2 | 43:2l:60:LEU:HD23 | 1.92 | 0.52 |
| 1:1A:72:U:H5' | 24:12:61:LEU:HD12 | 1.91 | 0.52 |
| 1:1A:124:G:OP1 | 1:1A:1376:C:O2' | 2.24 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 32:1a:1148:U:H2' | 32:1a:1149:C:O4' | 2.09 | 0.52 |
| 38:1g:47:CYS:HA | 38:1g:50:ILE:HG22 | 1.90 | 0.52 |
| 1:2A:796:C:H2' | 1:2A:797:C:C6 | 2.44 | 0.52 |
| 5:2F:12:LEU:HB2 | 5:2F:124:LEU:HD11 | 1.92 | 0.52 |
| 36:2e:146:ALA:O | 36:2e:150:ARG:HG2 | 2.09 | 0.52 |
| 1:1A:1453:U:OP1 | 13:1R:77:ARG:NH1 | 2.32 | 0.52 |
| 6:1G:179:PRO:HG3 | 26:14:43:TYR:OH | 2.10 | 0.52 |
| 12:1Q:10:ARG:NH1 | 12:1Q:11:LYS:HE2 | 2.24 | 0.52 |
| 30:18:23:VAL:HG11 | 30:18:47:LYS:HD3 | 1.90 | 0.52 |
| 32:1a:192:U:H2' | 32:1a:193:C:H6 | 1.75 | 0.52 |
| 32:1a:1286:A:H2' | 32:1a:1287:A:H4' | 1.92 | 0.52 |
| 32:1a:1376:U:OP1 | 38:1g:98:SER:HB3 | 2.09 | 0.52 |
| 41:1j:40:LEU:HD12 | 41:1j:69:ASN:HB3 | 1.92 | 0.52 |
| 1:2A:112:U:H5' | 24:22:65:ASN:ND2 | 2.24 | 0.52 |
| 1:2A:492:A:H2' | 1:2A:493:G:O4' | 2.08 | 0.52 |
| 1:2A:538:G:H5' | 9:2N:5:VAL:HG11 | 1.92 | 0.52 |
| 1:2A:2134:A:H2' | 1:2A:2134:A:N3 | 2.24 | 0.52 |
| 1:2A:2712:U:OP1 | 1:2A:2714:G:H4' | 2.10 | 0.52 |
| 10:2O:15:GLY:O | 10:2O:47:ILE:HG12 | 2.10 | 0.52 |
| 32:2a:1353:G:H2' | 32:2a:1354:C:C6 | 2.45 | 0.52 |
| 1:1A:534:U:H2' | 1:1A:535:C:C6 | 2.44 | 0.52 |
| 1:1A:637:A:OP1 | 11:1P:133:SER:OG | 2.26 | 0.52 |
| 1:1A:971:C:O2' | 1:1A:983:A:N3 | 2.36 | 0.52 |
| 1:1A:2121:G:H1 | 1:1A:2177:C:N4 | 2.07 | 0.52 |
| 32:1a:811:C:O2' | 32:1a:901:A:N1 | 2.40 | 0.52 |
| 32:1a:1346:A:N1 | 32:1a:1374:A:H5" | 2.24 | 0.52 |
| 39:1h:11:THR:HG22 | 39:1h:15:ASN:HD21 | 1.74 | 0.52 |
| 1:2A:1462:C:H4' | 1:2A:2703:C:H5' | 1.91 | 0.52 |
| 1:2A:1693:U:H1' | 3:2D:14:ARG:NH2 | 2.25 | 0.52 |
| 1:2A:2524:G:N7 | 61:2A:6346:HOH:O | 2.34 | 0.52 |
| 1:1A:272(J):C:H2' | 1:1A:274:G:C8 | 2.39 | 0.52 |
| 1:1A:1419:A:O2' | 1:1A:1421:G:N7 | 2.33 | 0.52 |
| 1:1A:2171:A:O2' | 1:1A:2172:U:H5" | 2.09 | 0.52 |
| 1:1A:2271:G:OP1 | 22:10:18:ALA:HB1 | 2.10 | 0.52 |
| 13:1R:12:ARG:O | 13:1R:17:ARG:NH1 | 2.42 | 0.52 |
| 20:1Y:99:CYS:HB2 | 20:1Y:106:LEU:HD21 | 1.91 | 0.52 |
| 26:14:58:ARG:HG3 | 50:1s:68:GLY:N | 2.25 | 0.52 |
| 32:1a:1237:C:O2' | 32:1a:1300:G:N2 | 2.41 | 0.52 |
| 1:2A:2478:A:OP2 | 31:29:2:LYS:NZ | 2.34 | 0.52 |
| 7:2H:11:VAL:HG21 | 7:2H:50:VAL:HG23 | 1.90 | 0.52 |
| 25:23:7:LYS:NZ | 25:23:32:GLN:O | 2.42 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 32:2a:857:C:H2' | 32:2a:858:G:O4' | 2.08 | 0.52 |
| 32:2a:1157:A:H5' | 32:2a:1158:C:C6 | 2.45 | 0.52 |
| 33:2b:30:ARG:HH21 | 33:2b:194:PRO:HB2 | 1.74 | 0.52 |
| 35:2d:187:ARG:NH1 | 35:2d:190:ASP:OD1 | 2.42 | 0.52 |
| 51:2t:16:HIS:O | 51:2t:19:SER:OG | 2.25 | 0.52 |
| 1:1A:1045:A:H5' | 1:1A:1046:A:H5' | 1.91 | 0.52 |
| 1:1A:1358:G:O2' | 1:1A:1373:A:N6 | 2.41 | 0.52 |
| 1:1A:2129:C:N4 | 1:1A:2159:G:H1 | 2.04 | 0.52 |
| 8:1I:75:LEU:HD22 | 8:1I:105:HIS:CD2 | 2.45 | 0.52 |
| 26:14:64:GLY:O | 26:14:66:SER:N | 2.42 | 0.52 |
| 32:1a:673:G:H2' | 32:1a:674:G:C8 | 2.45 | 0.52 |
| 1:2A:1865:G:N2 | 1:2A:1877:A:OP2 | 2.38 | 0.52 |
| 1:2A:2061:G:N2 | 1:2A:2062:A:N1 | 2.57 | 0.52 |
| 1:2A:2162:G:H4' | 1:2A:2172:U:H2' | 1.91 | 0.52 |
| 1:1A:1292:U:H2' | 1:1A:1293:C:C6 | 2.45 | 0.52 |
| 1:1A:2343:C:O2' | 1:1A:2373:G:O2' | 2.28 | 0.52 |
| 39:1h:82:HIS:NE2 | 39:1h:136:GLU:OE2 | 2.41 | 0.52 |
| 1:2A:861:A:N3 | 2:2B:79:C:O2' | 2.37 | 0.52 |
| 10:2O:64:ARG:HB2 | 10:2O:79:PHE:CG | 2.45 | 0.52 |
| 20:2Y:43:ASN:HD22 | 20:2Y:67:LEU:HD23 | 1.75 | 0.52 |
| 26:24:16:CYS:SG | 26:24:17:GLY:N | 2.83 | 0.52 |
| 32:2a:401:C:P | 35:2d:73:ARG:HH21 | 2.33 | 0.52 |
| 32:2a:925:G:H1 | 32:2a:1391:U:H3 | 1.57 | 0.52 |
| 32:2a:1053:G:H4' | 32:2a:1054:C:H3' | 1.91 | 0.52 |
| 35:2d:173:TRP:CD1 | 35:2d:189:PRO:HG3 | 2.44 | 0.52 |
| 40:2i:3:GLN:HE21 | 40:2i:20:ARG:HE | 1.57 | 0.52 |
| 43:2l:88:GLY:HA3 | 43:2l:99:HIS:HD2 | 1.75 | 0.52 |
| 1:1A:1022:G:N7 | 9:1N:66:LYS:HE2 | 2.25 | 0.52 |
| 1:1A:1653:G:H3' | 13:1R:2:ARG:HD3 | 1.91 | 0.52 |
| 1:1A:1826:G:H4' | 3:1D:242:ARG:CZ | 2.39 | 0.52 |
| 6:1G:108:ASN:HD22 | 26:14:22:ILE:HG21 | 1.75 | 0.52 |
| 35:1d:111:ALA:HB2 | 35:1d:120:LEU:HD12 | 1.91 | 0.52 |
| 38:1g:69:VAL:HG21 | 38:1g:104:LEU:HD11 | 1.92 | 0.52 |
| 54:1w:2:C:N4 | 54:1w:71:G:N1 | 2.58 | 0.52 |
| 1:2A:860:U:OP2 | 61:2A:6253:HOH:O | 2.19 | 0.52 |
| 1:2A:2129:C:H5' | 1:2A:2130:U:OP2 | 2.10 | 0.52 |
| 1:2A:2392:A:OP2 | 30:28:31:HIS:NE2 | 2.42 | 0.52 |
| 14:2S:14:VAL:O | 14:2S:18:ILE:HG12 | 2.10 | 0.52 |
| 31:29:29:ASN:HD22 | 31:29:32:HIS:CE1 | 2.28 | 0.52 |
| 32:2a:1226:C:H4' | 50:2s:80:TYR:CZ | 2.45 | 0.52 |
| 32:2a:1256:A:H5' | 32:2a:1258:G:O4' | 2.09 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 34:2c:70:VAL:HG12 | 34:2c:72:LYS:H | 1.75 | 0.52 |
| 38:2g:27:ILE:HA | 38:2g:30:ILE:HD12 | 1.92 | 0.52 |
| 42:2k:34:ASP:HB3 | 42:2k:40:ILE:HD11 | 1.92 | 0.52 |
| 1:1A:922:U:H2' | 1:1A:923:C:C6 | 2.45 | 0.52 |
| 1:1A:1153:C:H2' | 1:1A:1154:G:O4' | 2.10 | 0.52 |
| 32:1a:69:G:H2' | 32:1a:70:G:H8 | 1.75 | 0.52 |
| 34:1c:87:LEU:O | 34:1c:91:LEU:N | 2.41 | 0.52 |
| 1:2A:973:A:H8 | 1:2A:973:A:OP1 | 1.93 | 0.52 |
| 1:2A:2285:C:OP2 | 28:26:6:ARG:HD3 | 2.10 | 0.52 |
| 32:2a:421:U:O2' | 32:2a:423:G:N7 | 2.42 | 0.52 |
| 44:2m:101:GLN:OE1 | 44:2m:101:GLN:N | 2.42 | 0.52 |
| 54:2y:19:G:O4' | 54:2y:57:G:N1 | 2.40 | 0.52 |
| 1:1A:1278:A:OP1 | 13:1R:36:THR:HG23 | 2.10 | 0.51 |
| 1:1A:2108:C:H2' | 1:1A:2109:U:H6 | 1.74 | 0.51 |
| 3:1D:21:PHE:HB3 | 3:1D:24:ILE:HD12 | 1.91 | 0.51 |
| 11:1P:65:ARG:HD2 | 30:18:25:MET:SD | 2.50 | 0.51 |
| 32:1a:192:U:H2' | 32:1a:193:C:C6 | 2.45 | 0.51 |
| 32:1a:1359:C:OP1 | 45:1n:22:THR:OG1 | 2.25 | 0.51 |
| 35:1d:19:LEU:H | 35:1d:19:LEU:HD12 | 1.75 | 0.51 |
| 36:1e:140:ARG:O | 36:1e:143:ARG:NH1 | 2.40 | 0.51 |
| 1:2A:1658:C:OP1 | 4:2E:135:HIS:NE2 | 2.37 | 0.51 |
| 1:2A:2552:2MU:OP2 | 61:2A:5426:HOH:O | 2.19 | 0.51 |
| 32:2a:966:M2G:HM22 | 55:2x:34:C:H5' | 1.92 | 0.51 |
| 33:2b:115:LEU:HB2 | 33:2b:145:LEU:HD13 | 1.92 | 0.51 |
| 1:1A:1754:C:H5 | 15:1T:96:ARG:HH21 | 1.58 | 0.51 |
| 3:1D:26:LYS:HE2 | 3:1D:28:GLU:O | 2.09 | 0.51 |
| 8:1I:38:LEU:HD13 | 8:1I:40:THR:HG23 | 1.92 | 0.51 |
| 12:1Q:42:ILE:HD11 | 12:1Q:127:ILE:HD13 | 1.92 | 0.51 |
| 32:1a:148:G:H2' | 32:1a:149:A:C8 | 2.40 | 0.51 |
| 32:1a:438:G:O2' | 32:1a:494:U:O4 | 2.22 | 0.51 |
| 32:1a:584:G:H5' | 48:1q:91:ARG:NH2 | 2.24 | 0.51 |
| 32:1a:742:G:OP2 | 46:1o:35:ARG:NH2 | 2.37 | 0.51 |
| 1:2A:2121:G:N1 | 1:2A:2177:C:N4 | 2.42 | 0.51 |
| 6:2G:120:LEU:N | 6:2G:179:PRO:O | 2.32 | 0.51 |
| 9:2N:54:VAL:HB | 9:2N:122:VAL:HG22 | 1.93 | 0.51 |
| 18:2W:71:VAL:HA | 18:2W:107:LEU:HD12 | 1.92 | 0.51 |
| 32:2a:1067:A:O2' | 32:2a:1093:A:O2' | 2.24 | 0.51 |
| 32:2a:1173:G:H2' | 32:2a:1174:G:H8 | 1.75 | 0.51 |
| 32:2a:1342:C:H2' | 32:2a:1343:G:C8 | 2.44 | 0.51 |
| 33:2b:50:GLU:HB3 | 33:2b:200:ILE:O | 2.11 | 0.51 |
| 36:2e:33:VAL:HG21 | 36:2e:109:ILE:HA | 1.93 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:2j:38:ILE:HD11 | 41:2j:71:LEU:HD23 | 1.92 | 0.51 |
| 1:1A:1379:A:H4' | 1:1A:1380:G:OP2 | 2.09 | 0.51 |
| 5:1F:117:ARG:NH2 | 5:1F:189:THR:O | 2.41 | 0.51 |
| 6:1G:4:ASP:OD1 | 6:1G:9:ARG:NH1 | 2.41 | 0.51 |
| 9:1N:73:THR:HG23 | 9:1N:82:LEU:HD11 | 1.93 | 0.51 |
| 32:1a:407:G:H5" | 35:1d:115:ARG:HG2 | 1.91 | 0.51 |
| 32:1a:674:G:H2' | 32:1a:675:A:H8 | 1.75 | 0.51 |
| 32:1a:1070:U:H2' | 32:1a:1071:C:C6 | 2.45 | 0.51 |
| 36:1e:31:LEU:HD11 | 36:1e:129:ILE:HA | 1.93 | 0.51 |
| 1:2A:586:A:H5' | 5:2F:89:VAL:HG21 | 1.93 | 0.51 |
| 1:2A:1128:A:N7 | 1:2A:2489:G:O2' | 2.43 | 0.51 |
| 32:2a:862:C:H1' | 32:2a:874:G:H5" | 1.92 | 0.51 |
| 52:2u:3:LYS:HA | 52:2u:10:ARG:HG3 | 1.92 | 0.51 |
| 1:1A:2286:A:H4' | 1:1A:2287:A:O4' | 2.10 | 0.51 |
| 5:1F:184:TYR:CE2 | 5:1F:188:ARG:HD2 | 2.45 | 0.51 |
| 32:1a:1002:G:H3' | 32:1a:1003:G:C4' | 2.40 | 0.51 |
| 35:1d:64:LEU:HB2 | 35:1d:198:VAL:HG11 | 1.92 | 0.51 |
| 39:1h:25:ASP:OD2 | 39:1h:60:ARG:NH2 | 2.43 | 0.51 |
| 48:1q:4:LYS:HG3 | 48:1q:6:LEU:HD13 | 1.92 | 0.51 |
| 1:2A:790:C:OP2 | 61:2A:4442:HOH:O | 2.19 | 0.51 |
| 1:2A:2615:U:C2 | 27:25:7:PRO:HA | 2.45 | 0.51 |
| 32:2a:1026:G:H5' | 32:2a:1027:C:O5' | 2.11 | 0.51 |
| 32:2a:1132:C:N3 | 32:2a:1142:G:N2 | 2.52 | 0.51 |
| 1:1A:1066:U:N3 | 1:1A:1069:A:OP2 | 2.43 | 0.51 |
| 1:1A:1256:G:H1' | 5:1F:82:ILE:HD11 | 1.93 | 0.51 |
| 1:1A:2238:G:N3 | 1:1A:2238:G:H2' | 2.25 | 0.51 |
| 5:1F:53:THR:CG2 | 5:1F:55:GLY:H | 2.24 | 0.51 |
| 1:2A:340:A:H2' | 1:2A:341:G:O4' | 2.10 | 0.51 |
| 1:2A:2280:G:O2' | 1:2A:2388:A:N1 | 2.43 | 0.51 |
| 41:2j:32:ALA:HB3 | 41:2j:76:ASN:H | 1.75 | 0.51 |
| 1:1A:1899:G:N3 | 1:1A:1899:G:H2' | 2.24 | 0.51 |
| 1:1A:2276:G:N7 | 61:1A:7102:HOH:O | 2.33 | 0.51 |
| 2:1B:91:C:OP2 | 12:1Q:16:ARG:NH1 | 2.43 | 0.51 |
| 32:1a:748:C:H4' | 32:1a:749:C:O5' | 2.10 | 0.51 |
| 32:1a:750:G:O2' | 46:1o:21:ASP:OD1 | 2.29 | 0.51 |
| 32:1a:1029:C:N3 | 32:1a:1032:G:O6 | 2.43 | 0.51 |
| 38:1g:78:ARG:HG2 | 38:1g:79:ARG:H | 1.76 | 0.51 |
| 41:1j:65:LEU:HD13 | 45:1n:56:VAL:HG22 | 1.93 | 0.51 |
| 1:2A:1187:G:H5' | 17:2V:81:TYR:CE1 | 2.46 | 0.51 |
| 32:2a:56:U:H2' | 32:2a:57:G:H8 | 1.76 | 0.51 |
| 32:2a:148:G:H2' | 32:2a:149:A:C8 | 2.45 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 32:2a:582:U:H5" | 46:2o:64:ARG:HH12 | 1.76 | 0.51 |
| 32:2a:1006:C:H2' | 32:2a:1007:C:C6 | 2.45 | 0.51 |
| 32:2a:1058:G:H1 | 32:2a:1199:U:H3 | 1.58 | 0.51 |
| 32:2a:1510:U:H2' | 32:2a:1511:G:C8 | 2.45 | 0.51 |
| 36:2e:83:GLU:HA | 36:2e:88:LYS:HA | 1.93 | 0.51 |
| 39:2h:19:VAL:HG23 | 39:2h:21:LYS:HG2 | 1.92 | 0.51 |
| 39:2h:60:ARG:HG2 | 39:2h:62:TYR:CZ | 2.46 | 0.51 |
| 39:2h:91:ARG:HD3 | 48:2q:32:TYR:O | 2.10 | 0.51 |
| 1:1A:1054:A:H3' | 1:1A:1055:G:C8 | 2.46 | 0.51 |
| 1:1A:1405:U:H2' | 1:1A:1406:U:C6 | 2.45 | 0.51 |
| 1:1A:1783:A:H5' | 1:1A:2608:G:H4' | 1.93 | 0.51 |
| 1:1A:2150:U:H2' | 1:1A:2151:G:C8 | 2.46 | 0.51 |
| 1:1A:2168:G:O6 | 1:1A:2171:A:H5" | 2.10 | 0.51 |
| 17:1V:60:GLU:HB2 | 17:1V:97:LYS:HE2 | 1.92 | 0.51 |
| 32:1a:401:C:O2' | 32:1a:621:A:N3 | 2.41 | 0.51 |
| 32:1a:1104:G:H4' | 33:1b:111:ARG:HE | 1.76 | 0.51 |
| 33:1b:71:VAL:N | 33:1b:163:PHE:O | 2.39 | 0.51 |
| 34:1c:73:PRO:HB3 | 34:1c:103:VAL:HG11 | 1.92 | 0.51 |
| 1:2A:10:G:O2' | 1:2A:2801(A):A:N7 | 2.40 | 0.51 |
| 1:2A:271(G):C:H2' | 1:2A:271(H):G:H8 | 1.75 | 0.51 |
| 1:2A:2693:A:H2' | 1:2A:2694:G:C8 | 2.46 | 0.51 |
| 1:2A:2870:C:H2' | 1:2A:2871:C:O4' | 2.11 | 0.51 |
| 13:2R:87:TYR:OH | 13:2R:117:VAL:O | 2.26 | 0.51 |
| 32:2a:1126:U:H3 | 41:2j:40:LEU:HD11 | 1.76 | 0.51 |
| 7:1H:51:ARG:NH2 | 7:1H:53:GLU:OE2 | 2.43 | 0.51 |
| 32:1a:200:G:H1 | 32:1a:217:C:H42 | 1.58 | 0.51 |
| 32:1a:973:G:H3' | 32:1a:974:A:H5" | 1.91 | 0.51 |
| 33:1b:174:VAL:HG13 | 33:1b:184:VAL:HG11 | 1.93 | 0.51 |
| 1:2A:2379:G:O2' | 14:2S:17:ARG:NH2 | 2.44 | 0.51 |
| 32:2a:72:C:N3 | 32:2a:97:G:O6 | 2.43 | 0.51 |
| 32:2a:263:A:OP1 | 51:2t:79:ARG:NH1 | 2.43 | 0.51 |
| 33:2b:81:VAL:HA | 33:2b:215:LEU:HD21 | 1.93 | 0.51 |
| 39:2h:7:ALA:HB2 | 39:2h:85:ARG:HG3 | 1.92 | 0.51 |
| 52:2u:5:ASP:O | 52:2u:11:GLY:HA3 | 2.10 | 0.51 |
| 1:1A:1301:A:O2' | 1:1A:1302:A:H3' | 2.10 | 0.51 |
| 32:1a:1006:C:N4 | 32:1a:1023:G:N1 | 2.52 | 0.51 |
| 32:1a:1095:U:OP1 | 32:1a:1108:G:N1 | 2.42 | 0.51 |
| 32:1a:1442:G:H2' | 32:1a:1442:G:N3 | 2.25 | 0.51 |
| 40:1i:7:THR:O | 40:1i:83:ARG:NH1 | 2.44 | 0.51 |
| 41:1j:21:GLN:HE21 | 41:1j:25:GLU:HG3 | 1.76 | 0.51 |
| 1:2A:661:C:H2' | 1:2A:662:G:C8 | 2.45 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:2A:821:A:N1 | 61:2A:4694:HOH:O | 2.33 | 0.51 |
| 1:2A:1604:C:OP2 | 61:2A:5432:HOH:O | 2.20 | 0.51 |
| 1:2A:1697:G:OP2 | 1:2A:1698:A:O2' | 2.18 | 0.51 |
| 32:2a:839:U:H3' | 32:2a:840:C:C6 | 2.46 | 0.51 |
| 32:2a:1071:C:H2' | 32:2a:1072:G:C8 | 2.46 | 0.51 |
| 32:2a:1189:C:H5' | 34:2c:5:ILE:HD12 | 1.92 | 0.51 |
| 32:2a:1323:G:H4' | 32:2a:1363:C:N3 | 2.26 | 0.51 |
| 35:2d:76:ARG:O | 35:2d:80:GLU:HG2 | 2.11 | 0.51 |
| 1:1A:278:A:H4' | 1:1A:279:C:OP1 | 2.11 | 0.51 |
| 1:1A:2848:G:C8 | 15:1T:97:ALA:HB2 | 2.45 | 0.51 |
| 9:1N:62:VAL:HG11 | 9:1N:66:LYS:HB2 | 1.93 | 0.51 |
| 13:1R:8:ARG:HG3 | 13:1R:43:GLU:OE2 | 2.11 | 0.51 |
| 18:1W:65:LEU:HD12 | 18:1W:68:ARG:HE | 1.76 | 0.51 |
| 1:2A:1203:G:OP2 | 1:2A:1204:A:O2' | 2.20 | 0.51 |
| 1:2A:1906:G:OP2 | 1:2A:1929:G:O2' | 2.29 | 0.51 |
| 1:2A:1920:4OC:HM22 | 1:2A:1921:G:H5' | 1.93 | 0.51 |
| 6:2G:126:ASP:OD2 | 6:2G:130:ASN:ND2 | 2.44 | 0.51 |
| 21:2Z:54:HIS:CD2 | 21:2Z:101:PRO:HG3 | 2.46 | 0.51 |
| 32:2a:539:A:H2' | 32:2a:540:G:C8 | 2.46 | 0.51 |
| 32:2a:545:C:P | 35:2d:65:ARG:HH12 | 2.33 | 0.51 |
| 39:2h:25:ASP:N | 39:2h:25:ASP:OD1 | 2.44 | 0.51 |
| 1:1A:336:C:O2' | 20:1Y:35:TYR:OH | 2.28 | 0.50 |
| 3:1D:12:SER:HB3 | 3:1D:208:LYS:HB3 | 1.93 | 0.50 |
| 31:19:32:HIS:O | 31:19:34:GLN:HG3 | 2.11 | 0.50 |
| 32:1a:176:C:H2' | 32:1a:177:C:C6 | 2.46 | 0.50 |
| 32:1a:1458:G:H5" | 51:1t:31:SER:HB2 | 1.93 | 0.50 |
| 48:1q:6:LEU:HG | 48:1q:23:VAL:HG11 | 1.93 | 0.50 |
| 1:2A:2142:C:H2' | 1:2A:2143:C:O4' | 2.11 | 0.50 |
| 7:2H:35:VAL:HG13 | 7:2H:71:LEU:HD23 | 1.93 | 0.50 |
| 8:2I:43:ASN:ND2 | 23:21:75:GLU:OE1 | 2.44 | 0.50 |
| 21:2Z:153:SER:HB3 | 21:2Z:167:PRO:HB3 | 1.93 | 0.50 |
| 32:2a:56:U:H2' | 32:2a:57:G:C8 | 2.46 | 0.50 |
| 32:2a:196:A:OP1 | 51:2t:68:LYS:NZ | 2.42 | 0.50 |
| 32:2a:1182:G:H4' | 32:2a:1183:A:H5" | 1.93 | 0.50 |
| 39:2h:21:LYS:O | 39:2h:65:TYR:OH | 2.27 | 0.50 |
| 1:1A:365:C:OP2 | 61:1A:6825:HOH:O | 2.20 | 0.50 |
| 1:1A:1427:A:H4' | 1:1A:1428:C:O4' | 2.11 | 0.50 |
| 1:1A:1448:G:H4' | 1:1A:1542:A:OP1 | 2.11 | 0.50 |
| 5:1F:39:TRP:CZ2 | 5:1F:43:LYS:HE3 | 2.46 | 0.50 |
| 6:1G:3:LEU:O | 6:1G:8:LYS:NZ | 2.40 | 0.50 |
| 15:1T:24:PRO:HD3 | 15:1T:52:ILE:HD12 | 1.93 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 18:1W:78:GLU:OE2 | 18:1W:99:ARG:NH1 | 2.40 | 0.50 |
| 54:1w:23:A:H3' | 54:1w:24:G:C8 | 2.45 | 0.50 |
| 1:2A:652(B):A:N6 | 1:2A:655:A:H1' | 2.26 | 0.50 |
| 1:2A:1514:U:H2' | 1:2A:1515:G:C8 | 2.44 | 0.50 |
| 32:2a:660:G:H1 | 32:2a:745:C:H42 | 1.58 | 0.50 |
| 32:2a:673:G:H5" | 37:2f:87:ARG:CZ | 2.41 | 0.50 |
| 32:2a:1001:A:H2' | 32:2a:1001(A):G:C8 | 2.45 | 0.50 |
| 32:2a:1082:G:N7 | 61:2a:3305:HOH:O | 2.35 | 0.50 |
| 33:2b:195:ASP:OD1 | 33:2b:195:ASP:N | 2.44 | 0.50 |
| 1:1A:1498:C:OP1 | 61:1A:7295:HOH:O | 2.19 | 0.50 |
| 20:1Y:98:VAL:HG12 | 20:1Y:105:ALA:HA | 1.93 | 0.50 |
| 1:2A:144:C:H5' | 19:2X:2:LYS:HZ2 | 1.76 | 0.50 |
| 1:2A:1316:U:H2' | 1:2A:1317:A:C8 | 2.46 | 0.50 |
| 1:2A:2198:A:OP1 | 8:2I:33:ARG:NH2 | 2.44 | 0.50 |
| 12:2Q:17:LEU:HB3 | 12:2Q:39:PRO:HB2 | 1.92 | 0.50 |
| 32:2a:359:U:H2' | 32:2a:360:A:C8 | 2.46 | 0.50 |
| 32:2a:770:C:O2' | 32:2a:899:C:N3 | 2.37 | 0.50 |
| 32:2a:1001:A:H2' | 32:2a:1001(A):G:H8 | 1.76 | 0.50 |
| 45:2n:48:ALA:HB2 | 45:2n:53:LEU:HD12 | 1.93 | 0.50 |
| 1:1A:55:G:O2' | 1:1A:127:A:N1 | 2.42 | 0.50 |
| 1:1A:1210:A:H5" | 1:1A:1212:G:O4' | 2.11 | 0.50 |
| 21:1Z:125:LEU:HB3 | 21:1Z:165:VAL:HG13 | 1.94 | 0.50 |
| 31:19:16:VAL:HG22 | 31:19:25:VAL:HG22 | 1.93 | 0.50 |
| 1:2A:301:G:OP2 | 20:2Y:84:ARG:NH2 | 2.42 | 0.50 |
| 1:2A:659:C:H2' | 1:2A:660:G:H8 | 1.75 | 0.50 |
| 1:2A:2404:C:O3' | 11:2P:77:ARG:NH2 | 2.44 | 0.50 |
| 8:2I:72:LEU:HD21 | 8:2I:107:VAL:HG11 | 1.94 | 0.50 |
| 10:2O:86:ILE:HG22 | 10:2O:94:ARG:HD3 | 1.93 | 0.50 |
| 32:2a:284:G:H2' | 32:2a:285:G:C8 | 2.47 | 0.50 |
| 32:2a:736:C:H2' | 32:2a:737:A:C8 | 2.46 | 0.50 |
| 34:2c:55:VAL:HG22 | 34:2c:68:VAL:HG22 | 1.93 | 0.50 |
| 37:2f:62:TRP:CH2 | 37:2f:64:GLN:HB2 | 2.47 | 0.50 |
| 48:2q:67:LYS:O | 48:2q:68:ARG:HB3 | 2.12 | 0.50 |
| 1:1A:184:C:H2' | 1:1A:185:U:C6 | 2.46 | 0.50 |
| 1:1A:880:G:H2' | 1:1A:881:G:C8 | 2.38 | 0.50 |
| 1:1A:1045:A:H1' | 1:1A:1047:G:N3 | 2.26 | 0.50 |
| 1:1A:2273:A:H2' | 1:1A:2274:A:C8 | 2.46 | 0.50 |
| 9:1N:4:TYR:CD2 | 16:1U:100:VAL:HG11 | 2.47 | 0.50 |
| 32:1a:983:A:H5' | 32:1a:984:C:OP2 | 2.11 | 0.50 |
| 1:2A:818:G:OP2 | 61:2A:4377:HOH:O | 2.19 | 0.50 |
| 1:2A:1415:U:O2' | 1:2A:1417:C:OP1 | 2.26 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:2A:2206:G:H5" | 1:2A:2207:G:N7 | 2.26 | 0.50 |
| 1:2A:2785:C:OP1 | 4:2E:41:LYS:NZ | 2.41 | 0.50 |
| 15:2T:6:LEU:O | 15:2T:10:VAL:HG23 | 2.12 | 0.50 |
| 32:2a:20:U:H2' | 32:2a:21:G:O4' | 2.11 | 0.50 |
| 32:2a:707:C:H2' | 32:2a:708:C:C6 | 2.46 | 0.50 |
| 32:2a:975:A:N1 | 41:2j:48:THR:HB | 2.26 | 0.50 |
| 46:2o:54:ARG:HG2 | 46:2o:58:MET:HE2 | 1.93 | 0.50 |
| 1:1A:831:G:N2 | 11:1P:53:GLY:O | 2.44 | 0.50 |
| 1:1A:1999:C:H4' | 1:1A:2723:C:O2 | 2.11 | 0.50 |
| 1:1A:2611:U:C4 | 27:15:3:LYS:HG2 | 2.46 | 0.50 |
| 5:1F:135:LYS:HB2 | 5:1F:138:GLU:CD | 2.37 | 0.50 |
| 14:1S:8:GLU:HA | 14:1S:11:LYS:HB2 | 1.92 | 0.50 |
| 14:1S:65:VAL:O | 14:1S:69:VAL:HG12 | 2.12 | 0.50 |
| 29:17:5:TRP:NE1 | 29:17:7:PRO:HG3 | 2.26 | 0.50 |
| 32:1a:370:C:O2 | 32:1a:482:A:O2' | 2.26 | 0.50 |
| 32:1a:509:A:H2' | 32:1a:510:A:C8 | 2.46 | 0.50 |
| 32:1a:584:G:O6 | 61:1a:2029:HOH:O | 2.15 | 0.50 |
| 33:1b:59:GLU:HG2 | 33:1b:63:MET:HE2 | 1.93 | 0.50 |
| 36:1e:152:ARG:O | 39:1h:64:LYS:NZ | 2.36 | 0.50 |
| 44:1m:3:ARG:NH2 | 44:1m:9:ILE:O | 2.43 | 0.50 |
| 46:1o:26:GLU:OE1 | 46:1o:77:ARG:NH2 | 2.45 | 0.50 |
| 48:1q:32:TYR:O | 48:1q:34:LYS:N | 2.42 | 0.50 |
| 1:2A:407:G:H2' | 1:2A:408:G:H8 | 1.77 | 0.50 |
| 6:2G:32:PRO:HB3 | 6:2G:163:ALA:HB2 | 1.91 | 0.50 |
| 10:2O:87:ILE:HD12 | 10:2O:91:LEU:HA | 1.92 | 0.50 |
| 12:2Q:7:MET:HE3 | 12:2Q:10:ARG:HA | 1.92 | 0.50 |
| 18:2W:64:MET:HE2 | 18:2W:109:GLU:HG3 | 1.93 | 0.50 |
| 32:2a:936:C:H2' | 32:2a:937:A:O4' | 2.12 | 0.50 |
| 32:2a:1272:G:C4 | 32:2a:1273:G:H1' | 2.47 | 0.50 |
| 48:2q:61:GLU:HA | 48:2q:71:PHE:CD1 | 2.47 | 0.50 |
| 1:1A:768:G:O2' | 1:1A:1379:A:N1 | 2.41 | 0.50 |
| 1:1A:1053:C:N4 | 1:1A:1106:G:H1 | 2.07 | 0.50 |
| 1:1A:2128:C:H2' | 1:1A:2129:C:O4' | 2.11 | 0.50 |
| 30:18:33:ASN:HA | 30:18:36:LYS:HD2 | 1.93 | 0.50 |
| 32:1a:1126:U:O2 | 32:1a:1280:A:H2' | 2.10 | 0.50 |
| 35:1d:18:LYS:NZ | 35:1d:33:MET:HB3 | 2.27 | 0.50 |
| 1:2A:854:G:H2' | 1:2A:855:G:C8 | 2.43 | 0.50 |
| 1:2A:1300:U:H4' | 1:2A:1301:A:H5" | 1.92 | 0.50 |
| 1:2A:2334:G:H5' | 14:2S:9:ARG:HG2 | 1.93 | 0.50 |
| 1:2A:2504:U:OP2 | 61:2A:4814:HOH:O | 2.20 | 0.50 |
| 10:2O:21:CYS:HB2 | 10:2O:39:ILE:HD12 | 1.94 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 28:26:6:ARG:HH11 | 28:26:26:ASN:HB2 | 1.75 | 0.50 |
| 32:2a:35:G:O2' | 43:2l:118:SER:O | 2.29 | 0.50 |
| 32:2a:737:A:H2' | 32:2a:738:C:C6 | 2.47 | 0.50 |
| 32:2a:946:A:O2' | 32:2a:1333:A:N3 | 2.32 | 0.50 |
| 1:1A:1066:U:H2' | 1:1A:1068:G:OP2 | 2.12 | 0.50 |
| 1:1A:1174:A:H1' | 1:1A:1175:U:O5' | 2.12 | 0.50 |
| 1:1A:1439:A:OP1 | 61:1A:6792:HOH:O | 2.19 | 0.50 |
| 4:1E:56:PRO:HG3 | 4:1E:74:PRO:HG2 | 1.93 | 0.50 |
| 5:1F:123:LEU:HD13 | 5:1F:192:LEU:HB3 | 1.94 | 0.50 |
| 17:1V:43:GLU:OE1 | 17:1V:43:GLU:N | 2.43 | 0.50 |
| 20:1Y:35:TYR:CE2 | 20:1Y:69:ALA:HB3 | 2.47 | 0.50 |
| 32:1a:123:C:OP1 | 32:1a:311:C:O2' | 2.24 | 0.50 |
| 1:2A:27:G:N2 | 1:2A:512:G:H1' | 2.27 | 0.50 |
| 8:2I:116:LEU:HD11 | 8:2I:120:ILE:HG13 | 1.93 | 0.50 |
| 11:2P:99:LEU:HD23 | 11:2P:102:ARG:HH21 | 1.76 | 0.50 |
| 25:23:6:VAL:HG22 | 25:23:56:VAL:HG22 | 1.94 | 0.50 |
| 32:2a:78:G:N1 | 32:2a:91:C:O2 | 2.38 | 0.50 |
| 32:2a:1191:A:H5" | 34:2c:4:LYS:HE3 | 1.93 | 0.50 |
| 33:2b:149:LEU:HA | 33:2b:152:PHE:HB3 | 1.94 | 0.50 |
| 54:2y:51:U:H3 | 54:2y:63:G:H1 | 1.59 | 0.50 |
| 1:1A:249:C:O2' | 11:1P:64:LYS:NZ | 2.31 | 0.50 |
| 1:1A:2110:G:OP1 | 1:1A:2118:U:N3 | 2.38 | 0.50 |
| 2:1B:91:C:H5' | 12:1Q:18:LYS:HA | 1.92 | 0.50 |
| 32:1a:17:U:H2' | 32:1a:18:C:C6 | 2.47 | 0.50 |
| 35:1d:119:GLN:HG2 | 35:1d:123:HIS:CD2 | 2.47 | 0.50 |
| 37:1f:33:TYR:HB2 | 37:1f:75:LEU:HD12 | 1.94 | 0.50 |
| 38:1g:89:MET:SD | 38:1g:155:ARG:HB2 | 2.52 | 0.50 |
| 39:1h:19:VAL:HG23 | 39:1h:21:LYS:HG2 | 1.94 | 0.50 |
| 43:1l:53:ARG:HB3 | 43:1l:69:TYR:HE1 | 1.77 | 0.50 |
| 1:2A:288:C:H2' | 1:2A:289:A:H8 | 1.76 | 0.50 |
| 1:2A:743:G:OP1 | 4:2E:130:GLY:HA2 | 2.11 | 0.50 |
| 1:2A:2870:C:H5" | 13:2R:65:LEU:HD21 | 1.94 | 0.50 |
| 4:2E:77:ILE:HG12 | 4:2E:195:LEU:HD12 | 1.93 | 0.50 |
| 10:2O:36:GLY:HA2 | 10:2O:106:LEU:HD23 | 1.94 | 0.50 |
| 15:2T:51:ARG:HB2 | 15:2T:98:LYS:HD2 | 1.93 | 0.50 |
| 32:2a:1187:G:H4' | 40:2i:111:ARG:HH11 | 1.75 | 0.50 |
| 41:2j:49:VAL:HG12 | 41:2j:61:GLU:O | 2.12 | 0.50 |
| 54:2y:9:A:H8 | 54:2y:11:C:H41 | 1.60 | 0.50 |
| 1:1A:191:A:H2' | 1:1A:192:C:C6 | 2.47 | 0.49 |
| 1:1A:524:U:H2' | 1:1A:525:U:C6 | 2.47 | 0.49 |
| 1:1A:769:G:N7 | 61:1A:7107:HOH:O | 2.34 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1A:862:G:H2' | 1:1A:863:A:O4' | 2.12 | 0.49 |
| 1:1A:1108:U:H2' | 1:1A:1109:C:O4' | 2.11 | 0.49 |
| 1:1A:1996:C:H4' | 1:1A:1997:G:OP1 | 2.12 | 0.49 |
| 1:1A:2185:C:H2' | 1:1A:2186:G:H8 | 1.77 | 0.49 |
| 1:1A:2336:A:H61 | 22:10:43:THR:HG21 | 1.77 | 0.49 |
| 1:1A:2552:2MU:O5' | 1:1A:2552:2MU:H6 | 2.12 | 0.49 |
| 5:1F:110:LEU:HD11 | 5:1F:181:LEU:HG | 1.94 | 0.49 |
| 9:1N:75:TYR:CE2 | 9:1N:77:GLY:HA2 | 2.47 | 0.49 |
| 18:1W:80:PRO:O | 18:1W:100:THR:OG1 | 2.29 | 0.49 |
| 32:1a:146:G:H2' | 32:1a:147:G:O4' | 2.12 | 0.49 |
| 51:1t:10:LEU:HB3 | 51:1t:12:ALA:H | 1.75 | 0.49 |
| 1:2A:657:U:H2' | 1:2A:658:C:C6 | 2.46 | 0.49 |
| 1:2A:879:G:H5' | 1:2A:880:G:OP2 | 2.12 | 0.49 |
| 1:2A:1899:G:O2' | 1:2A:1900:A:OP2 | 2.28 | 0.49 |
| 1:2A:2030:A:H4' | 1:2A:2031:A:C8 | 2.47 | 0.49 |
| 1:2A:2070:G:H2' | 1:2A:2071:A:C8 | 2.47 | 0.49 |
| 1:2A:2218:U:N3 | 23:21:55:GLY:O | 2.45 | 0.49 |
| 1:2A:2360:A:H2' | 1:2A:2361:A:O4' | 2.12 | 0.49 |
| 1:2A:2473:U:O2 | 1:2A:2473:U:H2' | 2.12 | 0.49 |
| 1:2A:2507:C:H4' | 54:2w:75:C:O2' | 2.11 | 0.49 |
| 1:2A:2564:A:OP1 | 1:2A:2648:C:H4' | 2.11 | 0.49 |
| 4:2E:48:GLN:HA | 4:2E:80:GLU:HA | 1.93 | 0.49 |
| 32:2a:107:G:H2' | 32:2a:108:G:O4' | 2.12 | 0.49 |
| 32:2a:794:A:OP2 | 61:2a:3641:HOH:O | 2.20 | 0.49 |
| 42:2k:48:ILE:O | 42:2k:50:TYR:N | 2.45 | 0.49 |
| 44:2m:85:GLY:HA2 | 44:2m:93:ARG:HH21 | 1.77 | 0.49 |
| 1:1A:1047:G:O2' | 1:1A:1048:A:H8 | 1.95 | 0.49 |
| 32:1a:401:C:H2' | 32:1a:402:G:C8 | 2.47 | 0.49 |
| 32:1a:601:C:H2' | 32:1a:602:A:H8 | 1.78 | 0.49 |
| 35:1d:105:VAL:HG13 | 35:1d:110:PHE:HB2 | 1.94 | 0.49 |
| 48:1q:53:LEU:HD23 | 48:1q:82:MET:HE1 | 1.93 | 0.49 |
| 50:1s:48:THR:HG22 | 50:1s:61:TYR:HD1 | 1.76 | 0.49 |
| 1:2A:1292:U:H2' | 1:2A:1293:C:C6 | 2.47 | 0.49 |
| 1:2A:1593:G:H2' | 1:2A:1594:G:C8 | 2.47 | 0.49 |
| 1:2A:2033:A:O2' | 1:2A:2035:G:OP2 | 2.25 | 0.49 |
| 1:2A:2498:C:OP1 | 61:2A:4156:HOH:O | 2.20 | 0.49 |
| 1:2A:2641:G:H5" | 9:2N:76:SER:HB3 | 1.93 | 0.49 |
| 4:2E:167:VAL:HG22 | 4:2E:170:LEU:HD11 | 1.94 | 0.49 |
| 6:2G:97:ASP:N | 6:2G:97:ASP:OD1 | 2.43 | 0.49 |
| 7:2H:3:ARG:HH11 | 7:2H:4:ILE:H | 1.58 | 0.49 |
| 9:2N:97:ARG:HA | 9:2N:100:GLU:HB2 | 1.94 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 32:2a:6:G:H4' | 32:2a:298:A:H4' | 1.94 | 0.49 |
| 32:2a:411:A:H2' | 32:2a:412:A:H4' | 1.94 | 0.49 |
| 32:2a:448:A:P | 32:2a:485:G:H22 | 2.34 | 0.49 |
| 32:2a:728:A:H2' | 32:2a:729:A:C8 | 2.47 | 0.49 |
| 32:2a:1328:C:H3' | 52:2u:7:ARG:HH22 | 1.76 | 0.49 |
| 33:2b:98:LEU:HD12 | 33:2b:101:MET:HE3 | 1.94 | 0.49 |
| 41:2j:78:ASN:O | 41:2j:80:LYS:N | 2.46 | 0.49 |
| 1:1A:1082:U:C4 | 1:1A:1086:A:N1 | 2.75 | 0.49 |
| 32:1a:765:G:N1 | 32:1a:812:C:O2' | 2.37 | 0.49 |
| 36:1e:99:GLY:N | 36:1e:117:ASP:OD1 | 2.38 | 0.49 |
| 39:1h:11:THR:HG22 | 39:1h:15:ASN:ND2 | 2.27 | 0.49 |
| 46:1o:55:GLY:HA2 | 46:1o:58:MET:HE3 | 1.92 | 0.49 |
| 49:1r:58:LEU:HB3 | 49:1r:62:GLU:HB2 | 1.94 | 0.49 |
| 1:2A:184:C:H2' | 1:2A:185:U:C6 | 2.47 | 0.49 |
| 1:2A:236:C:H2' | 1:2A:237:C:H6 | 1.77 | 0.49 |
| 1:2A:484:C:H2' | 1:2A:485:C:C6 | 2.47 | 0.49 |
| 1:2A:1507:A:O2' | 1:2A:1508:A:O4' | 2.29 | 0.49 |
| 2:2B:40:U:O2' | 2:2B:43:C:OP2 | 2.24 | 0.49 |
| 2:2B:105:A:H5' | 2:2B:106:G:OP2 | 2.12 | 0.49 |
| 7:2H:56:SER:HB3 | 7:2H:61:HIS:ND1 | 2.27 | 0.49 |
| 32:2a:34:C:H2' | 32:2a:35:G:H8 | 1.77 | 0.49 |
| 32:2a:570:G:H1' | 32:2a:820:U:C4 | 2.47 | 0.49 |
| 32:2a:576:G:O6 | 32:2a:880:C:O2' | 2.23 | 0.49 |
| 32:2a:955:U:H2' | 32:2a:956:U:O4' | 2.11 | 0.49 |
| 32:2a:1299:A:H2' | 32:2a:1299:A:N3 | 2.27 | 0.49 |
| 32:2a:1305:G:H22 | 32:2a:1331:G:H1' | 1.76 | 0.49 |
| 36:2e:53:LEU:HA | 36:2e:56:GLN:HG2 | 1.93 | 0.49 |
| 1:1A:438:G:H2' | 1:1A:440:G:C8 | 2.47 | 0.49 |
| 1:1A:657:U:H2' | 1:1A:658:C:C6 | 2.47 | 0.49 |
| 1:1A:1268:A:H2' | 1:1A:1269:A:O4' | 2.12 | 0.49 |
| 1:1A:2310:A:N1 | 6:1G:79:ASN:ND2 | 2.60 | 0.49 |
| 8:1I:129:THR:HG22 | 8:1I:139:GLN:HE22 | 1.78 | 0.49 |
| 11:1P:106:LEU:HD22 | 11:1P:112:LEU:HD13 | 1.94 | 0.49 |
| 13:1R:36:THR:HG22 | 13:1R:37:THR:H | 1.77 | 0.49 |
| 15:1T:29:ARG:HG3 | 15:1T:46:GLU:HB2 | 1.94 | 0.49 |
| 33:1b:21:ARG:HB3 | 33:1b:39:ILE:HG13 | 1.95 | 0.49 |
| 37:1f:97:PHE:CD2 | 49:1r:31:LEU:HD11 | 2.47 | 0.49 |
| 1:2A:890:A:H2' | 1:2A:892:G:H8 | 1.77 | 0.49 |
| 1:2A:1019:U:H3 | 1:2A:1142(A):A:H62 | 1.60 | 0.49 |
| 1:2A:1913:A:N6 | 54:2w:37:MIA:O2' | 2.44 | 0.49 |
| 2:2B:50:G:OP1 | 14:2S:63:THR:N | 2.40 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:2G:11:TYR:OH | 6:2G:16:ARG:NH1 | 2.46 | 0.49 |
| 19:2X:26:TYR:HB3 | 19:2X:92:LEU:HD22 | 1.94 | 0.49 |
| 32:2a:673:G:H2' | 32:2a:674:G:H8 | 1.75 | 0.49 |
| 46:2o:3:ILE:HG12 | 46:2o:38:ARG:HE | 1.77 | 0.49 |
| 1:1A:740:U:H2' | 1:1A:741:G:C8 | 2.47 | 0.49 |
| 1:1A:848:G:H2' | 1:1A:849:A:C8 | 2.48 | 0.49 |
| 1:1A:1593:G:H2' | 1:1A:1594:G:C8 | 2.48 | 0.49 |
| 1:1A:2350:C:OP2 | 61:1A:6676:HOH:O | 2.18 | 0.49 |
| 32:1a:486:U:H2' | 32:1a:487:A:C8 | 2.46 | 0.49 |
| 32:1a:1030:C:O2' | 32:1a:1030(D):A:N6 | 2.46 | 0.49 |
| 41:1j:13:HIS:HA | 41:1j:16:LEU:HB3 | 1.95 | 0.49 |
| 41:1j:16:LEU:HD22 | 41:1j:68:HIS:HB2 | 1.93 | 0.49 |
| 43:1l:24:VAL:HB | 43:1l:27:LEU:HD22 | 1.94 | 0.49 |
| 54:1y:36:A:H2' | 54:1y:37:MIA:O4' | 2.12 | 0.49 |
| 1:2A:65:C:O2' | 1:2A:456:C:N3 | 2.36 | 0.49 |
| 1:2A:897:C:H1' | 54:2w:56:C:C5 | 2.41 | 0.49 |
| 1:2A:2127:G:H2' | 1:2A:2128:C:C6 | 2.47 | 0.49 |
| 32:2a:977:A:O2' | 32:2a:979:C:OP2 | 2.24 | 0.49 |
| 33:2b:98:LEU:HB2 | 33:2b:101:MET:HG3 | 1.95 | 0.49 |
| 36:2e:78:HIS:HE1 | 36:2e:143:ARG:H | 1.60 | 0.49 |
| 46:2o:33:THR:HG21 | 46:2o:85:LEU:HD22 | 1.94 | 0.49 |
| 54:2w:6:G:N1 | 54:2w:67:C:O2 | 2.39 | 0.49 |
| 1:1A:64:A:O3' | 19:1X:71:GLY:HA3 | 2.12 | 0.49 |
| 1:1A:286:C:H2' | 1:1A:287:C:C6 | 2.48 | 0.49 |
| 1:1A:1418:G:OP2 | 61:1A:5574:HOH:O | 2.20 | 0.49 |
| 1:1A:1508:A:O2' | 1:1A:1509:C:H5" | 2.12 | 0.49 |
| 32:1a:909:A:H2' | 32:1a:910:C:O4' | 2.13 | 0.49 |
| 45:1n:4:LYS:HA | 45:1n:7:ILE:HG22 | 1.94 | 0.49 |
| 1:2A:852:G:H2' | 1:2A:853:G:C8 | 2.47 | 0.49 |
| 19:2X:4:ALA:HB1 | 19:2X:42:ALA:HA | 1.94 | 0.49 |
| 32:2a:824:C:H2' | 32:2a:825:G:C8 | 2.46 | 0.49 |
| 32:2a:954:G:H2' | 32:2a:955:U:O4' | 2.12 | 0.49 |
| 40:2i:50:LEU:HD13 | 40:2i:56:LEU:HA | 1.94 | 0.49 |
| 44:2m:15:VAL:HG11 | 44:2m:48:LEU:HD11 | 1.95 | 0.49 |
| 47:2p:22:THR:HA | 47:2p:33:ILE:HG13 | 1.94 | 0.49 |
| 54:2y:67:C:H2' | 54:2y:68:C:H6 | 1.78 | 0.49 |
| 4:1E:24:THR:HG23 | 4:1E:184:VAL:HG12 | 1.94 | 0.49 |
| 15:1T:74:ARG:HG2 | 15:1T:76:PHE:CZ | 2.47 | 0.49 |
| 21:1Z:153:SER:HA | 21:1Z:167:PRO:HB3 | 1.95 | 0.49 |
| 32:1a:316:G:OP2 | 32:1a:351:G:O2' | 2.28 | 0.49 |
| 32:1a:1142:G:H2' | 32:1a:1143:G:O4' | 2.12 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 34:1c:116:VAL:HG21 | 34:1c:202:ILE:HD11 | 1.93 | 0.49 |
| 36:1e:78:HIS:HE1 | 36:1e:142:LEU:HA | 1.77 | 0.49 |
| 44:1m:80:ARG:HH22 | 50:1s:69:HIS:CE1 | 2.31 | 0.49 |
| 1:2A:524:U:H2' | 1:2A:525:U:C6 | 2.48 | 0.49 |
| 1:2A:912:C:OP1 | 12:2Q:8:LYS:NZ | 2.38 | 0.49 |
| 1:2A:974:G:OP1 | 1:2A:1187:G:O2' | 2.19 | 0.49 |
| 1:2A:1670:C:OP1 | 61:2A:6087:HOH:O | 2.19 | 0.49 |
| 1:2A:2327:A:H2' | 1:2A:2328:A:C8 | 2.48 | 0.49 |
| 1:2A:2781:A:H5" | 1:2A:2782:G:H5' | 1.95 | 0.49 |
| 9:2N:103:VAL:HG11 | 9:2N:120:LEU:HD22 | 1.95 | 0.49 |
| 14:2S:34:HIS:O | 14:2S:97:ARG:NH2 | 2.45 | 0.49 |
| 23:21:2:SER:HB3 | 23:21:46:LEU:HD12 | 1.94 | 0.49 |
| 32:2a:790:A:H61 | 32:2a:1498:UR3:P | 2.35 | 0.49 |
| 32:2a:833:U:H2' | 32:2a:834:C:C6 | 2.47 | 0.49 |
| 1:1A:2127:G:H1 | 1:1A:2161:C:H42 | 1.60 | 0.49 |
| 1:1A:2176:A:H2' | 1:1A:2177:C:C6 | 2.46 | 0.49 |
| 32:1a:1531:A:H8 | 32:1a:1531:A:O5' | 1.95 | 0.49 |
| 44:1m:11:ARG:C | 44:1m:13:LYS:H | 2.21 | 0.49 |
| 1:2A:1022:G:H22 | 1:2A:1142(A):A:H2 | 1.60 | 0.49 |
| 1:2A:1412:A:H2' | 1:2A:1413:G:C8 | 2.47 | 0.49 |
| 1:2A:1794:U:H2' | 1:2A:1795:C:C6 | 2.48 | 0.49 |
| 6:2G:122:PRO:HB3 | 6:2G:170:ARG:NH1 | 2.28 | 0.49 |
| 15:2T:74:ARG:HG2 | 15:2T:76:PHE:CZ | 2.48 | 0.49 |
| 32:2a:1320:C:H1' | 50:2s:73:GLU:HG2 | 1.94 | 0.49 |
| 47:2p:52:ASP:O | 47:2p:54:GLU:N | 2.42 | 0.49 |
| 1:1A:639:U:H2' | 1:1A:640:C:C6 | 2.47 | 0.49 |
| 1:1A:1364:G:N7 | 23:11:3:LYS:HD2 | 2.27 | 0.49 |
| 1:1A:1756:G:H4' | 1:1A:1758:G:O4' | 2.12 | 0.49 |
| 1:1A:2705:A:N3 | 61:1R:301:HOH:O | 2.35 | 0.49 |
| 2:1B:21:G:N7 | 61:1B:302:HOH:O | 2.35 | 0.49 |
| 10:1O:64:ARG:HD3 | 10:1O:79:PHE:CD1 | 2.48 | 0.49 |
| 32:1a:165:C:H2' | 32:1a:166:G:H8 | 1.78 | 0.49 |
| 32:1a:184:G:H2' | 32:1a:185:A:C8 | 2.44 | 0.49 |
| 32:1a:194:C:H2' | 32:1a:195:A:H5" | 1.95 | 0.49 |
| 50:1s:11:VAL:HG12 | 50:1s:13:ASP:H | 1.78 | 0.49 |
| 1:2A:93:G:H2' | 1:2A:94:C:H6 | 1.78 | 0.49 |
| 1:2A:2130:U:O2 | 1:2A:2134:A:O2' | 2.22 | 0.49 |
| 1:2A:2343:C:O3' | 1:2A:2373:G:H4' | 2.12 | 0.49 |
| 1:2A:2590:A:H5" | 3:2D:239:ARG:HG3 | 1.94 | 0.49 |
| 25:23:12:PRO:HB2 | 25:23:20:LYS:HG2 | 1.94 | 0.49 |
| 32:2a:742:G:OP2 | 46:2o:35:ARG:NH2 | 2.45 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 32:2a:1369:C:OP2 | 40:2i:112:LYS:N | 2.37 | 0.49 |
| 39:2h:10:LEU:HD22 | 39:2h:83:ILE:HD11 | 1.95 | 0.49 |
| 55:2x:44:A:H2' | 55:2x:45:G:C8 | 2.47 | 0.49 |
| 1:1A:414:C:H2' | 1:1A:415:A:C8 | 2.47 | 0.49 |
| 1:1A:2506:U:O2' | 54:1w:76:A:H4' | 2.12 | 0.49 |
| 1:1A:2849:U:H4' | 1:1A:2868:A:C2 | 2.48 | 0.49 |
| 15:1T:65:LYS:HE3 | 15:1T:67:SER:HB2 | 1.95 | 0.49 |
| 32:1a:636:U:H2' | 32:1a:637:G:C8 | 2.47 | 0.49 |
| 34:1c:22:TRP:CE2 | 45:1n:54:PRO:HG2 | 2.47 | 0.49 |
| 41:1j:32:ALA:HB3 | 41:1j:76:ASN:H | 1.76 | 0.49 |
| 46:1o:56:LEU:O | 46:1o:60:VAL:HG23 | 2.13 | 0.49 |
| 1:2A:275:G:H2' | 1:2A:276:A:O4' | 2.13 | 0.49 |
| 1:2A:848:G:N3 | 1:2A:933:A:H1' | 2.28 | 0.49 |
| 1:2A:1751:C:O2' | 1:2A:2861:G:O2' | 2.28 | 0.49 |
| 1:2A:1798:U:H5' | 3:2D:259:THR:CG2 | 2.42 | 0.49 |
| 6:2G:173:LEU:HB3 | 6:2G:178:PHE:CD2 | 2.48 | 0.49 |
| 32:2a:590:C:H2' | 32:2a:591:U:C6 | 2.48 | 0.49 |
| 32:2a:1118:C:H1' | 32:2a:1179:A:C5 | 2.48 | 0.49 |
| 33:2b:12:GLU:O | 33:2b:15:VAL:HG22 | 2.13 | 0.49 |
| 49:2r:53:ARG:HG2 | 49:2r:63:GLN:HE21 | 1.77 | 0.49 |
| 49:2r:58:LEU:HD11 | 49:2r:66:LEU:HD13 | 1.95 | 0.49 |
| 61:1A:6898:HOH:O | 16:1U:16:LYS:HD3 | 2.13 | 0.48 |
| 6:1G:64:THR:HB | 6:1G:94:LEU:HD21 | 1.94 | 0.48 |
| 18:1W:58:ALA:HB1 | 18:1W:64:MET:HB2 | 1.95 | 0.48 |
| 19:1X:43:VAL:HG21 | 19:1X:81:VAL:HG11 | 1.96 | 0.48 |
| 32:1a:509:A:H5" | 35:1d:55:ALA:HB2 | 1.95 | 0.48 |
| 32:1a:1391:U:H2' | 32:1a:1392:G:C8 | 2.48 | 0.48 |
| 33:1b:230:VAL:HG22 | 33:1b:232:PRO:HD2 | 1.95 | 0.48 |
| 1:2A:249:C:O2 | 30:28:12:LYS:NZ | 2.38 | 0.48 |
| 1:2A:531:C:H4' | 1:2A:532:A:H5" | 1.95 | 0.48 |
| 1:2A:1023:U:O2' | 1:2A:1122:G:H5' | 2.14 | 0.48 |
| 1:2A:2110:G:H3' | 1:2A:2111:C:H5' | 1.95 | 0.48 |
| 1:2A:2526:G:O3' | 31:29:33:LYS:NZ | 2.46 | 0.48 |
| 3:2D:242:ARG:HH11 | 3:2D:242:ARG:HG3 | 1.79 | 0.48 |
| 4:2E:5:LEU:HD21 | 4:2E:79:ARG:HB2 | 1.94 | 0.48 |
| 5:2F:179:GLU:OE1 | 5:2F:179:GLU:N | 2.45 | 0.48 |
| 8:2I:117:GLU:HG3 | 8:2I:118:LYS:H | 1.77 | 0.48 |
| 9:2N:58:ASP:OD1 | 9:2N:58:ASP:N | 2.41 | 0.48 |
| 11:2P:63:PRO:HG2 | 30:28:25:MET:HB2 | 1.94 | 0.48 |
| 21:2Z:74:VAL:HG22 | 21:2Z:86:VAL:HG12 | 1.95 | 0.48 |
| 32:2a:316:G:OP2 | 32:2a:351:G:O2' | 2.28 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 32:2a:920:U:H2' | 32:2a:921:U:C6 | 2.48 | 0.48 |
| 32:2a:952:U:H2' | 32:2a:953:G:H8 | 1.77 | 0.48 |
| 33:2b:93:VAL:HG21 | 33:2b:97:TRP:HD1 | 1.77 | 0.48 |
| 1:1A:1230:C:H2' | 1:1A:1231:G:C8 | 2.49 | 0.48 |
| 1:1A:2096:U:H3 | 1:1A:2193:G:H1 | 1.61 | 0.48 |
| 1:1A:2804:C:H2' | 1:1A:2805:G:O4' | 2.12 | 0.48 |
| 12:1Q:31:ASP:OD1 | 12:1Q:134:ARG:NH1 | 2.43 | 0.48 |
| 32:1a:271:C:H2' | 32:1a:272:C:C6 | 2.48 | 0.48 |
| 32:1a:330:C:O2 | 61:1a:2121:HOH:O | 2.17 | 0.48 |
| 32:1a:1249:C:O2' | 40:1i:73:GLN:NE2 | 2.46 | 0.48 |
| 33:1b:24:TRP:CZ3 | 33:1b:26:PRO:HA | 2.48 | 0.48 |
| 50:1s:11:VAL:HG11 | 50:1s:16:LEU:HB2 | 1.95 | 0.48 |
| 1:2A:661:C:H2' | 1:2A:662:G:H8 | 1.78 | 0.48 |
| 1:2A:1496:A:O2' | 1:2A:1497:U:O2 | 2.25 | 0.48 |
| 1:2A:1711:C:H2' | 1:2A:1712:C:C6 | 2.48 | 0.48 |
| 1:2A:1816:G:O6 | 3:2D:35:LYS:NZ | 2.44 | 0.48 |
| 1:2A:2102:U:H2' | 1:2A:2103:C:C6 | 2.47 | 0.48 |
| 2:2B:14:U:OP2 | 2:2B:70:C:O2' | 2.25 | 0.48 |
| 2:2B:40:U:H2' | 26:24:2:LYS:HE3 | 1.95 | 0.48 |
| 27:25:41:PRO:O | 27:25:44:THR:OG1 | 2.23 | 0.48 |
| 29:27:12:ARG:NH2 | 29:27:44:PRO:HB3 | 2.27 | 0.48 |
| 30:28:30:ARG:HB3 | 30:28:31:HIS:HD2 | 1.78 | 0.48 |
| 32:2a:340:U:H2' | 32:2a:341:C:C6 | 2.49 | 0.48 |
| 32:2a:560:U:H4' | 32:2a:561:U:O5' | 2.13 | 0.48 |
| 32:2a:596:C:OP2 | 61:2a:3425:HOH:O | 2.20 | 0.48 |
| 33:2b:18:GLY:HA3 | 33:2b:42:ILE:H | 1.77 | 0.48 |
| 1:1A:18:C:O2' | 1:1A:554:U:OP1 | 2.29 | 0.48 |
| 2:1B:2:C:H2' | 2:1B:3:C:C6 | 2.48 | 0.48 |
| 21:1Z:130:PRO:HA | 21:1Z:133:ILE:HG13 | 1.96 | 0.48 |
| 32:1a:19:C:H2' | 32:1a:20:U:C6 | 2.48 | 0.48 |
| 33:1b:178:ARG:HH22 | 39:1h:74:PRO:HB3 | 1.79 | 0.48 |
| 21:2Z:156:LYS:HE3 | 21:2Z:158:PRO:HD3 | 1.95 | 0.48 |
| 26:24:58:ARG:HG3 | 50:2s:68:GLY:H | 1.77 | 0.48 |
| 32:2a:148:G:H2' | 32:2a:149:A:H8 | 1.77 | 0.48 |
| 32:2a:181:G:H4' | 32:2a:182:U:H5' | 1.95 | 0.48 |
| 32:2a:442:C:H42 | 32:2a:492:G:H1 | 1.61 | 0.48 |
| 1:1A:1085:A:O2' | 1:1A:1104:C:O2' | 2.19 | 0.48 |
| 1:1A:1670:C:O2 | 4:1E:129:HIS:NE2 | 2.39 | 0.48 |
| 1:1A:2206:G:H5" | 1:1A:2207:G:C5 | 2.48 | 0.48 |
| 1:1A:2364:C:H2' | 1:1A:2365:G:O4' | 2.14 | 0.48 |
| 2:1B:12:C:H2' | 22:10:73:GLY:HA3 | 1.96 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:1B:31:C:H4' | 6:1G:29:TRP:CH2 | 2.48 | 0.48 |
| 4:1E:12:THR:HG22 | 4:1E:13:ARG:H | 1.77 | 0.48 |
| 32:1a:128:G:O2' | 48:1q:3:LYS:NZ | 2.46 | 0.48 |
| 32:1a:452:A:H4' | 47:1p:72:ARG:NH1 | 2.28 | 0.48 |
| 44:1m:50:GLU:HA | 44:1m:53:VAL:HB | 1.95 | 0.48 |
| 44:1m:87:TYR:CE2 | 44:1m:91:ARG:HD2 | 2.47 | 0.48 |
| 54:1y:38:A:H2' | 54:1y:39:PSU:O4' | 2.13 | 0.48 |
| 1:2A:140:G:N2 | 1:2A:1596:A:H4' | 2.28 | 0.48 |
| 1:2A:251:A:C5 | 1:2A:252:G:H1' | 2.48 | 0.48 |
| 1:2A:887:A:H4' | 1:2A:888:C:C5 | 2.49 | 0.48 |
| 1:2A:1016:G:O6 | 1:2A:1147:C:N4 | 2.46 | 0.48 |
| 1:2A:1023:U:OP2 | 61:2A:5647:HOH:O | 2.20 | 0.48 |
| 1:2A:1916:A:H2' | 1:2A:1917:PSU:O4' | 2.12 | 0.48 |
| 6:2G:97:ASP:HA | 6:2G:100:TRP:HD1 | 1.79 | 0.48 |
| 21:2Z:28:MET:HE1 | 21:2Z:61:LEU:HD21 | 1.95 | 0.48 |
| 32:2a:109:A:C6 | 32:2a:326:G:C6 | 3.02 | 0.48 |
| 32:2a:324:G:N1 | 32:2a:327:A:OP2 | 2.47 | 0.48 |
| 32:2a:1016:A:C5 | 32:2a:1017:G:H1' | 2.48 | 0.48 |
| 32:2a:1176:A:H2' | 32:2a:1177:G:C8 | 2.49 | 0.48 |
| 32:2a:1306:A:H1' | 32:2a:1332:A:C2 | 2.48 | 0.48 |
| 34:2c:47:LEU:HB2 | 34:2c:52:LEU:HD22 | 1.94 | 0.48 |
| 11:1P:98:GLU:O | 11:1P:101:VAL:HG12 | 2.14 | 0.48 |
| 16:1U:49:HIS:HA | 16:1U:52:ARG:HB3 | 1.94 | 0.48 |
| 18:1W:12:ILE:HD13 | 18:1W:17:VAL:HG13 | 1.95 | 0.48 |
| 19:1X:26:TYR:HB3 | 19:1X:92:LEU:HD22 | 1.95 | 0.48 |
| 32:1a:501:C:H2' | 32:1a:502:G:H8 | 1.78 | 0.48 |
| 32:1a:659:U:H2' | 32:1a:660:G:H8 | 1.78 | 0.48 |
| 32:1a:1260:C:O5' | 32:1a:1284:C:H4' | 2.13 | 0.48 |
| 33:1b:16:HIS:HB2 | 33:1b:204:ASN:HB3 | 1.96 | 0.48 |
| 36:1e:110:LEU:HD13 | 36:1e:118:ILE:HG21 | 1.95 | 0.48 |
| 1:2A:271(H):G:H2' | 1:2A:271(I):G:C8 | 2.44 | 0.48 |
| 1:2A:2161:C:H2' | 1:2A:2162:G:O4' | 2.14 | 0.48 |
| 11:2P:120:ALA:HB2 | 11:2P:137:LYS:HB3 | 1.94 | 0.48 |
| 32:2a:228:A:H2' | 32:2a:229:U:O4' | 2.12 | 0.48 |
| 32:2a:429:U:H1' | 32:2a:430:A:H5" | 1.94 | 0.48 |
| 32:2a:1103:C:H5" | 33:2b:98:LEU:HD22 | 1.95 | 0.48 |
| 32:2a:1264:C:N4 | 32:2a:1271:G:N1 | 2.39 | 0.48 |
| 34:2c:138:VAL:HG11 | 34:2c:169:ALA:HA | 1.95 | 0.48 |
| 40:2i:26:VAL:HG13 | 40:2i:61:ALA:HB3 | 1.94 | 0.48 |
| 1:1A:301:G:OP2 | 20:1Y:84:ARG:NH2 | 2.46 | 0.48 |
| 1:1A:528:A:O2' | 1:1A:529:A:H5' | 2.14 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1A:796:C:H2' | 1:1A:797:C:C6 | 2.48 | 0.48 |
| 32:1a:848:C:H2' | 32:1a:849:C:C6 | 2.49 | 0.48 |
| 32:1a:1202:G:O4' | 45:1n:29:ARG:NH1 | 2.45 | 0.48 |
| 33:1b:95:GLN:OE1 | 33:1b:147:LYS:HG2 | 2.13 | 0.48 |
| 36:1e:77:PRO:HD2 | 36:1e:142:LEU:HD13 | 1.94 | 0.48 |
| 45:1n:23:ARG:HD2 | 45:1n:28:GLY:O | 2.14 | 0.48 |
| 51:1t:47:GLY:HA2 | 51:1t:48:LYS:C | 2.38 | 0.48 |
| 1:2A:172:C:H2' | 1:2A:173:G:H8 | 1.78 | 0.48 |
| 1:2A:855:G:O2' | 22:20:27:GLU:OE2 | 2.31 | 0.48 |
| 11:2P:50:ARG:HD3 | 30:28:7:HIS:CD2 | 2.48 | 0.48 |
| 32:2a:235:C:N4 | 61:2a:3351:HOH:O | 2.46 | 0.48 |
| 32:2a:1019:C:H2' | 32:2a:1020:U:H4' | 1.96 | 0.48 |
| 32:2a:1250:A:H4' | 40:2i:68:GLY:N | 2.29 | 0.48 |
| 32:2a:1423:G:H2' | 32:2a:1424:C:H6 | 1.79 | 0.48 |
| 39:2h:51:VAL:HG11 | 39:2h:60:ARG:NH1 | 2.28 | 0.48 |
| 41:2j:16:LEU:HD21 | 41:2j:70:ARG:HG2 | 1.95 | 0.48 |
| 51:2t:18:GLN:O | 51:2t:22:ARG:HG3 | 2.13 | 0.48 |
| 1:1A:883:G:H22 | 1:1A:893:C:N4 | 2.12 | 0.48 |
| 1:1A:2790:A:H5' | 1:1A:2893:G:H21 | 1.78 | 0.48 |
| 2:1B:66:A:H61 | 2:1B:109:C:H5' | 1.77 | 0.48 |
| 32:1a:848:C:H2' | 32:1a:849:C:H6 | 1.79 | 0.48 |
| 32:1a:974:A:H8 | 32:1a:974:A:OP1 | 1.96 | 0.48 |
| 33:1b:74:LYS:HD2 | 33:1b:166:ASP:HB2 | 1.95 | 0.48 |
| 34:1c:5:ILE:HG12 | 34:1c:6:HIS:H | 1.78 | 0.48 |
| 1:2A:118:A:N3 | 1:2A:178:G:H1' | 2.28 | 0.48 |
| 1:2A:208:C:H2' | 1:2A:209:C:C6 | 2.48 | 0.48 |
| 1:2A:582:G:H2' | 1:2A:583:G:C8 | 2.49 | 0.48 |
| 1:2A:878:A:N6 | 1:2A:899:A:O2' | 2.46 | 0.48 |
| 2:2B:90:A:C5 | 2:2B:91:C:H1' | 2.48 | 0.48 |
| 3:2D:206:LEU:HA | 3:2D:211:ARG:HE | 1.79 | 0.48 |
| 7:2H:4:ILE:O | 7:2H:69:ARG:HD2 | 2.14 | 0.48 |
| 32:2a:37:U:O2' | 32:2a:500:G:H4' | 2.14 | 0.48 |
| 32:2a:839:U:H3' | 32:2a:840:C:H6 | 1.79 | 0.48 |
| 37:2f:69:GLU:CD | 37:2f:69:GLU:H | 2.21 | 0.48 |
| 32:1a:719:C:O2' | 49:1r:49:LYS:HB3 | 2.13 | 0.48 |
| 32:1a:1317:C:O2 | 50:1s:37:ARG:NH2 | 2.46 | 0.48 |
| 54:1y:19:G:O4' | 54:1y:57:G:N1 | 2.47 | 0.48 |
| 1:2A:645:C:H5" | 1:2A:646:A:OP2 | 2.14 | 0.48 |
| 1:2A:832:G:H5' | 11:2P:45:LEU:HD21 | 1.95 | 0.48 |
| 1:2A:1470:G:O2' | 1:2A:1520:G:O6 | 2.31 | 0.48 |
| 1:2A:2849:U:H4' | 1:2A:2868:A:C2 | 2.49 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 11:2P:59:LEU:HD22 | 11:2P:60:MET:HE2 | 1.95 | 0.48 |
| 30:28:31:HIS:ND1 | 30:28:32:LEU:HD13 | 2.28 | 0.48 |
| 32:2a:1060:C:H5" | 41:2j:51:ARG:HG2 | 1.94 | 0.48 |
| 32:2a:1245:A:H2' | 32:2a:1246:C:O4' | 2.13 | 0.48 |
| 32:2a:1359:C:OP1 | 45:2n:22:THR:OG1 | 2.29 | 0.48 |
| 32:2a:1442:G:H2' | 32:2a:1442:G:N3 | 2.27 | 0.48 |
| 32:2a:1518:MA6:N6 | 32:2a:1519:MA6:H103 | 2.29 | 0.48 |
| 34:2c:16:ARG:HH21 | 34:2c:54:ARG:NH1 | 2.12 | 0.48 |
| 36:2e:101:ILE:HG13 | 36:2e:119:LEU:HD23 | 1.96 | 0.48 |
| 37:2f:97:PHE:CE2 | 49:2r:62:GLU:HG2 | 2.46 | 0.48 |
| 1:1A:218:A:C2 | 1:1A:235:U:H4' | 2.49 | 0.48 |
| 1:1A:297:C:OP1 | 20:1Y:87:LYS:NZ | 2.42 | 0.48 |
| 1:1A:881:G:H3' | 1:1A:882:G:H8 | 1.78 | 0.48 |
| 1:1A:1045:A:OP1 | 1:1A:1045:A:H4' | 2.14 | 0.48 |
| 1:1A:1223:G:N2 | 1:1A:1226:A:OP2 | 2.37 | 0.48 |
| 1:1A:1300:U:H4' | 1:1A:1301:A:H5" | 1.95 | 0.48 |
| 1:1A:1766:U:H2' | 1:1A:1767:C:H6 | 1.79 | 0.48 |
| 1:1A:2478:A:H5' | 31:19:31:LYS:HD3 | 1.96 | 0.48 |
| 23:11:82:LEU:HD13 | 23:11:90:ILE:HG23 | 1.94 | 0.48 |
| 32:1a:769:G:H4' | 32:1a:1513:A:H4' | 1.94 | 0.48 |
| 32:1a:929:G:H1 | 32:1a:1388:C:N4 | 2.12 | 0.48 |
| 44:1m:80:ARG:HH22 | 50:1s:69:HIS:HE1 | 1.61 | 0.48 |
| 1:2A:857:C:H1' | 22:20:26:TYR:CE1 | 2.49 | 0.48 |
| 1:2A:1747:G:H2' | 1:2A:1747(A):G:H8 | 1.79 | 0.48 |
| 1:2A:2032:G:OP2 | 1:2A:2454:G:O2' | 2.23 | 0.48 |
| 4:2E:181:LEU:HD11 | 15:2T:6:LEU:HD23 | 1.95 | 0.48 |
| 18:2W:18:ARG:HG2 | 18:2W:76:VAL:HB | 1.96 | 0.48 |
| 20:2Y:9:LYS:HA | 20:2Y:10:GLY:HA2 | 1.51 | 0.48 |
| 20:2Y:38:ILE:HD11 | 20:2Y:66:PRO:HG3 | 1.96 | 0.48 |
| 20:2Y:102:CYS:SG | 20:2Y:103:GLY:N | 2.87 | 0.48 |
| 30:28:26:LYS:HB2 | 30:28:44:LYS:O | 2.14 | 0.48 |
| 32:2a:1029:C:C2 | 32:2a:1032:G:N2 | 2.78 | 0.48 |
| 33:2b:219:VAL:HG22 | 33:2b:222:ILE:HD12 | 1.96 | 0.48 |
| 38:2g:26:PHE:CE2 | 38:2g:30:ILE:HD11 | 2.48 | 0.48 |
| 1:1A:839:U:H2' | 1:1A:840:C:C6 | 2.49 | 0.48 |
| 7:1H:56:SER:HB3 | 7:1H:61:HIS:ND1 | 2.28 | 0.48 |
| 35:1d:26:CYS:CB | 60:1d:302:SF4:S1 | 3.01 | 0.48 |
| 39:1h:11:THR:HG23 | 39:1h:14:ARG:HH21 | 1.79 | 0.48 |
| 54:1w:5:G:H2' | 54:1w:6:G:C8 | 2.49 | 0.48 |
| 1:2A:902:C:H2' | 1:2A:903:C:C6 | 2.49 | 0.48 |
| 1:2A:2547:U:O2 | 10:2O:23:ARG:NH2 | 2.46 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:2A:2889:C:H2' | 1:2A:2891:G:O4' | 2.14 | 0.48 |
| 5:2F:187:VAL:HG12 | 11:2P:3:LEU:HD12 | 1.95 | 0.48 |
| 26:24:40:HIS:CD2 | 26:24:41:PRO:HD2 | 2.49 | 0.48 |
| 32:2a:237:C:H5" | 48:2q:25:ARG:CZ | 2.43 | 0.48 |
| 32:2a:1026:G:O6 | 32:2a:1036:G:N2 | 2.47 | 0.48 |
| 32:2a:1272:G:N3 | 32:2a:1273:G:H1' | 2.29 | 0.48 |
| 38:2g:47:CYS:HA | 38:2g:50:ILE:HG22 | 1.96 | 0.48 |
| 1:1A:324:A:N6 | 1:1A:338:G:O2' | 2.47 | 0.47 |
| 1:1A:540:C:H2' | 1:1A:541:C:C6 | 2.49 | 0.47 |
| 1:1A:1717:G:H2' | 1:1A:1718:G:H8 | 1.79 | 0.47 |
| 1:1A:2137:C:H2' | 1:1A:2138:C:C6 | 2.49 | 0.47 |
| 1:1A:2409:G:O2' | 61:1A:6964:HOH:O | 2.20 | 0.47 |
| 32:1a:319:G:H2' | 32:1a:320:C:O4' | 2.14 | 0.47 |
| 32:1a:736:C:H2' | 32:1a:737:A:C8 | 2.49 | 0.47 |
| 45:1n:48:ALA:HB2 | 45:1n:53:LEU:HD12 | 1.95 | 0.47 |
| 50:1s:63:THR:OG1 | 50:1s:65:ASN:OD1 | 2.30 | 0.47 |
| 55:1x:13:C:H2' | 55:1x:14:A:H5" | 1.95 | 0.47 |
| 1:2A:947:G:H2' | 1:2A:948:G:C8 | 2.49 | 0.47 |
| 1:2A:1973:G:OP2 | 61:2A:4871:HOH:O | 2.19 | 0.47 |
| 1:2A:2062:A:H2' | 1:2A:2062:A:N3 | 2.29 | 0.47 |
| 1:2A:2127:G:N3 | 1:2A:2161:C:N3 | 2.61 | 0.47 |
| 1:2A:2345:G:H1' | 1:2A:2382:G:H5' | 1.96 | 0.47 |
| 1:2A:2364:C:H2' | 1:2A:2365:G:O4' | 2.14 | 0.47 |
| 22:20:27:GLU:HG3 | 22:20:68:GLU:HA | 1.96 | 0.47 |
| 28:26:9:LEU:HD13 | 28:26:51:GLU:HB2 | 1.95 | 0.47 |
| 32:2a:46:G:O2' | 32:2a:365:U:H1' | 2.14 | 0.47 |
| 32:2a:336:C:H2' | 32:2a:337:C:C6 | 2.49 | 0.47 |
| 32:2a:434:U:H2' | 32:2a:435:C:C6 | 2.48 | 0.47 |
| 33:2b:162:ILE:O | 33:2b:185:ILE:HG12 | 2.14 | 0.47 |
| 1:1A:1057:A:N6 | 1:1A:1087:G:OP2 | 2.47 | 0.47 |
| 1:1A:1420:U:O2' | 1:1A:1421:G:H8 | 1.97 | 0.47 |
| 1:1A:2228:G:OP1 | 3:1D:263:ARG:NH2 | 2.42 | 0.47 |
| 1:1A:2595:G:N2 | 1:1A:2598:A:OP2 | 2.45 | 0.47 |
| 19:1X:94:GLY:H | 19:1X:95:LEU:HB2 | 1.79 | 0.47 |
| 32:1a:558:G:OP1 | 61:1a:2088:HOH:O | 2.20 | 0.47 |
| 32:1a:741:G:H2' | 32:1a:742:G:O4' | 2.15 | 0.47 |
| 32:1a:1035:A:N3 | 32:1a:1036:G:N2 | 2.62 | 0.47 |
| 32:1a:1103:C:H2' | 32:1a:1104:G:O4' | 2.14 | 0.47 |
| 32:1a:1367:C:H2' | 32:1a:1368:G:O4' | 2.14 | 0.47 |
| 41:1j:5:ARG:O | 41:1j:99:LYS:N | 2.46 | 0.47 |
| 1:2A:196:A:N3 | 1:2A:196:A:H2' | 2.29 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:2A:893:C:H2' | 1:2A:894:C:C5 | 2.49 | 0.47 |
| 1:2A:1237:A:OP2 | 61:2A:5390:HOH:O | 2.20 | 0.47 |
| 1:2A:2658:C:P | 7:2H:160:LYS:HZ1 | 2.35 | 0.47 |
| 5:2F:28:ILE:HG12 | 5:2F:112:MET:HG2 | 1.95 | 0.47 |
| 8:2I:5:LEU:HD11 | 8:2I:19:VAL:HG22 | 1.96 | 0.47 |
| 32:2a:137:C:H2' | 32:2a:138:G:H8 | 1.77 | 0.47 |
| 33:2b:60:ASP:O | 33:2b:64:ARG:HG2 | 2.14 | 0.47 |
| 35:2d:19:LEU:HG | 35:2d:67:ILE:HG12 | 1.96 | 0.47 |
| 35:2d:57:ARG:NH2 | 36:2e:107:ARG:HD3 | 2.29 | 0.47 |
| 42:2k:48:ILE:C | 42:2k:50:TYR:H | 2.22 | 0.47 |
| 51:2t:10:LEU:HB3 | 51:2t:12:ALA:H | 1.78 | 0.47 |
| 1:1A:747:U:H1' | 18:1W:92:ARG:HH12 | 1.79 | 0.47 |
| 1:1A:1028:A:N6 | 1:1A:1125:G:H2' | 2.29 | 0.47 |
| 1:1A:1062:G:P | 1:1A:1070:A:H1' | 2.54 | 0.47 |
| 1:1A:1372:U:H2' | 1:1A:1373:A:O4' | 2.14 | 0.47 |
| 1:1A:2532:G:O2' | 1:1A:2657:A:N1 | 2.45 | 0.47 |
| 23:11:8:SER:HB3 | 23:11:66:HIS:CD2 | 2.49 | 0.47 |
| 32:1a:193:C:H2' | 32:1a:194:C:C6 | 2.49 | 0.47 |
| 32:1a:789:U:O2' | 32:1a:791:G:N7 | 2.40 | 0.47 |
| 32:1a:814:A:H2' | 32:1a:816:A:H5" | 1.97 | 0.47 |
| 32:1a:1038:C:O2' | 32:1a:1039:C:H5' | 2.13 | 0.47 |
| 32:1a:1497:G:N7 | 61:1a:2420:HOH:O | 2.35 | 0.47 |
| 34:1c:22:TRP:CZ2 | 45:1n:54:PRO:HG2 | 2.50 | 0.47 |
| 37:1f:67:MET:HE1 | 37:1f:75:LEU:HD22 | 1.96 | 0.47 |
| 55:1x:75:C:H5" | 55:1x:76:A:OP2 | 2.14 | 0.47 |
| 1:2A:93:G:H2' | 1:2A:94:C:C6 | 2.49 | 0.47 |
| 1:2A:383:U:H2' | 1:2A:385:C:H5 | 1.80 | 0.47 |
| 1:2A:629:G:H1' | 1:2A:639:U:O2' | 2.14 | 0.47 |
| 1:2A:827:U:O2' | 1:2A:2068:U:C2 | 2.66 | 0.47 |
| 1:2A:1509(B):A:H2' | 1:2A:1510:G:H8 | 1.79 | 0.47 |
| 1:2A:2822:G:O2' | 1:2A:2824:C:OP2 | 2.23 | 0.47 |
| 12:2Q:81:VAL:HB | 22:20:7:LEU:HD21 | 1.96 | 0.47 |
| 17:2V:43:GLU:OE1 | 17:2V:43:GLU:N | 2.31 | 0.47 |
| 28:26:9:LEU:HA | 28:26:54:ILE:HB | 1.95 | 0.47 |
| 31:29:16:VAL:HG22 | 31:29:25:VAL:HG22 | 1.96 | 0.47 |
| 32:2a:974:A:O4' | 45:2n:31:ARG:HD3 | 2.14 | 0.47 |
| 32:2a:1353:G:OP1 | 52:2u:10:ARG:NH1 | 2.46 | 0.47 |
| 33:2b:178:ARG:NH2 | 39:2h:74:PRO:HB3 | 2.29 | 0.47 |
| 34:2c:177:THR:HG22 | 34:2c:180:ALA:H | 1.79 | 0.47 |
| 39:2h:25:ASP:OD2 | 39:2h:60:ARG:NH2 | 2.46 | 0.47 |
| 43:2l:84:LEU:HB2 | 43:2l:105:TYR:CE2 | 2.49 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1A:2250:G:O2' | 1:1A:2496:C:OP1 | 2.29 | 0.47 |
| 11:1P:82:GLY:HA2 | 11:1P:113:LYS:O | 2.15 | 0.47 |
| 22:10:26:TYR:H | 22:10:29:GLN:NE2 | 2.11 | 0.47 |
| 32:1a:78:G:C6 | 32:1a:91:C:N4 | 2.81 | 0.47 |
| 32:1a:1106:G:H2' | 32:1a:1107:C:C6 | 2.49 | 0.47 |
| 45:1n:21:TYR:OH | 45:1n:23:ARG:NH2 | 2.45 | 0.47 |
| 54:1w:4:C:H2' | 54:1w:5:G:H8 | 1.78 | 0.47 |
| 1:2A:218:A:C2 | 1:2A:235:U:H4' | 2.49 | 0.47 |
| 1:2A:479:A:N3 | 1:2A:481:G:H5" | 2.29 | 0.47 |
| 1:2A:778:G:H5" | 3:2D:48:ARG:HD2 | 1.96 | 0.47 |
| 1:2A:2680:C:H5' | 4:2E:189:PRO:HA | 1.96 | 0.47 |
| 2:2B:95:C:H2' | 2:2B:96:U:C6 | 2.49 | 0.47 |
| 32:2a:1172:C:N4 | 32:2a:1173:G:O6 | 2.48 | 0.47 |
| 32:2a:1191:A:OP2 | 34:2c:3:ASN:ND2 | 2.48 | 0.47 |
| 35:2d:172:PRO:HD2 | 35:2d:173:TRP:CZ3 | 2.50 | 0.47 |
| 41:2j:9:ARG:NE | 41:2j:69:ASN:OD1 | 2.46 | 0.47 |
| 50:2s:40:ILE:HB | 50:2s:67:VAL:O | 2.15 | 0.47 |
| 54:2w:7:A:N1 | 54:2w:66:U:O4 | 2.48 | 0.47 |
| 1:1A:2134:A:H4' | 1:1A:2135:A:OP1 | 2.15 | 0.47 |
| 13:1R:59:ASP:OD1 | 13:1R:59:ASP:N | 2.47 | 0.47 |
| 32:1a:266:G:O3' | 48:1q:67:LYS:HB2 | 2.14 | 0.47 |
| 32:1a:625:G:H4' | 47:1p:16:HIS:CD2 | 2.50 | 0.47 |
| 55:1x:8:4SU:O2 | 55:1x:21:A:H2 | 1.97 | 0.47 |
| 1:2A:866:A:H2 | 1:2A:867:C:C4 | 2.31 | 0.47 |
| 1:2A:1496:A:N3 | 1:2A:1577:C:O2' | 2.46 | 0.47 |
| 1:2A:2498:C:H3' | 61:2A:5660:HOH:O | 2.14 | 0.47 |
| 7:2H:154:PRO:HB3 | 7:2H:163:TYR:CE1 | 2.50 | 0.47 |
| 8:2I:65:ALA:O | 8:2I:69:LYS:N | 2.45 | 0.47 |
| 9:2N:67:LEU:HA | 9:2N:87:LEU:HD22 | 1.95 | 0.47 |
| 35:2d:64:LEU:HB2 | 35:2d:198:VAL:HG11 | 1.95 | 0.47 |
| 1:1A:1014:U:OP2 | 61:1A:6533:HOH:O | 2.20 | 0.47 |
| 26:14:24:THR:OG1 | 26:14:25:TYR:N | 2.48 | 0.47 |
| 32:1a:191:G:N2 | 51:1t:102:GLY:O | 2.43 | 0.47 |
| 32:1a:234:C:H2' | 32:1a:235:C:C6 | 2.50 | 0.47 |
| 33:1b:142:LEU:HA | 33:1b:145:LEU:HD12 | 1.95 | 0.47 |
| 39:1h:91:ARG:HD3 | 48:1q:32:TYR:O | 2.14 | 0.47 |
| 1:2A:322:A:OP1 | 5:2F:168:ARG:HD2 | 2.14 | 0.47 |
| 1:2A:526:A:N3 | 1:2A:2044:C:H1' | 2.30 | 0.47 |
| 1:2A:1161:C:H2' | 1:2A:1162:G:H8 | 1.78 | 0.47 |
| 2:2B:24:G:N3 | 2:2B:26:A:N6 | 2.62 | 0.47 |
| 21:2Z:48:PHE:CE1 | 21:2Z:52:SER:HA | 2.49 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 54:2w:43:C:H2' | 54:2w:44:G:C8 | 2.49 | 0.47 |
| 54:2y:10:G:H1 | 54:2y:25:C:H42 | 1.62 | 0.47 |
| 1:1A:34:C:H5" | 1:1A:35:G:OP2 | 2.15 | 0.47 |
| 1:1A:247:G:H4' | 1:1A:386:G:C5 | 2.49 | 0.47 |
| 1:1A:643:A:N1 | 1:1A:2369:A:O2' | 2.43 | 0.47 |
| 1:1A:853:G:C2' | 1:1A:854:G:H5' | 2.44 | 0.47 |
| 1:1A:1075:C:H42 | 1:1A:1077:A:H62 | 1.62 | 0.47 |
| 1:1A:1190:G:OP1 | 11:1P:30:THR:OG1 | 2.28 | 0.47 |
| 1:1A:1641:A:H2' | 1:1A:1642:G:O4' | 2.15 | 0.47 |
| 1:1A:1712:C:H2' | 1:1A:1713:U:O4' | 2.15 | 0.47 |
| 1:1A:1803:A:O2' | 3:1D:259:THR:HG21 | 2.14 | 0.47 |
| 1:1A:2126:A:N3 | 1:1A:2127:G:H1' | 2.30 | 0.47 |
| 1:1A:2127:G:H1 | 1:1A:2161:C:N4 | 2.11 | 0.47 |
| 1:1A:2533:A:H2' | 1:1A:2534:A:O4' | 2.15 | 0.47 |
| 1:1A:2803:C:H2' | 1:1A:2804:C:C6 | 2.49 | 0.47 |
| 32:1a:34:C:H2' | 32:1a:35:G:C8 | 2.50 | 0.47 |
| 32:1a:40:C:H2' | 32:1a:41:G:H8 | 1.78 | 0.47 |
| 32:1a:539:A:H2' | 32:1a:540:G:C8 | 2.49 | 0.47 |
| 32:1a:1129:C:O2' | 32:1a:1139:G:N7 | 2.39 | 0.47 |
| 38:1g:77:SER:HA | 38:1g:85:TYR:O | 2.15 | 0.47 |
| 50:1s:80:TYR:CZ | 50:1s:82:GLY:HA2 | 2.49 | 0.47 |
| 51:1t:9:ASN:O | 51:1t:10:LEU:HB2 | 2.14 | 0.47 |
| 51:1t:47:GLY:N | 51:1t:48:LYS:HB2 | 2.30 | 0.47 |
| 1:2A:484:C:H2' | 1:2A:485:C:H6 | 1.80 | 0.47 |
| 1:2A:848:G:H2' | 1:2A:849:A:C8 | 2.49 | 0.47 |
| 1:2A:2127:G:N2 | 1:2A:2161:C:N1 | 2.63 | 0.47 |
| 1:2A:2291:U:H2' | 1:2A:2292:C:C6 | 2.50 | 0.47 |
| 2:2B:91:C:OP1 | 12:2Q:16:ARG:HG3 | 2.14 | 0.47 |
| 6:2G:17:PRO:HA | 6:2G:20:ILE:HD12 | 1.97 | 0.47 |
| 7:2H:127:GLU:OE1 | 7:2H:130:ARG:NE | 2.46 | 0.47 |
| 7:2H:154:PRO:HB3 | 7:2H:163:TYR:CZ | 2.49 | 0.47 |
| 9:2N:121:LYS:HD3 | 9:2N:130:HIS:CE1 | 2.50 | 0.47 |
| 13:2R:44:LEU:HD23 | 13:2R:44:LEU:HA | 1.81 | 0.47 |
| 15:2T:1:MET:HE2 | 15:2T:3:ARG:HG2 | 1.97 | 0.47 |
| 19:2X:94:GLY:N | 19:2X:95:LEU:HA | 2.30 | 0.47 |
| 20:2Y:35:TYR:CE2 | 20:2Y:69:ALA:HB3 | 2.50 | 0.47 |
| 32:2a:76:C:H42 | 32:2a:93:G:H1 | 1.62 | 0.47 |
| 32:2a:909:A:N3 | 32:2a:1413:A:O2' | 2.37 | 0.47 |
| 32:2a:942:G:H21 | 40:2i:124:GLN:NE2 | 2.12 | 0.47 |
| 32:2a:983:A:O2' | 32:2a:1050:G:OP2 | 2.28 | 0.47 |
| 32:2a:1368:G:H5' | 40:2i:112:LYS:HB3 | 1.97 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 32:2a:1376:U:H2' | 32:2a:1377:A:H8 | 1.78 | 0.47 |
| 32:2a:1423:G:H2' | 32:2a:1424:C:C6 | 2.49 | 0.47 |
| 32:2a:1479:C:H2' | 32:2a:1480:G:C8 | 2.49 | 0.47 |
| 34:2c:58:GLU:O | 34:2c:65:ALA:N | 2.46 | 0.47 |
| 34:2c:77:ILE:HG13 | 34:2c:78:GLY:N | 2.30 | 0.47 |
| 34:2c:117:ALA:HB2 | 34:2c:200:ALA:HB2 | 1.97 | 0.47 |
| 34:2c:142:MET:HG3 | 34:2c:170:GLN:HB3 | 1.95 | 0.47 |
| 38:2g:65:ALA:HB1 | 38:2g:127:ALA:HB3 | 1.96 | 0.47 |
| 40:2i:8:GLY:HA3 | 40:2i:76:ALA:O | 2.14 | 0.47 |
| 42:2k:81:ASP:OD1 | 42:2k:107:SER:OG | 2.30 | 0.47 |
| 48:2q:45:HIS:CD2 | 48:2q:47:PRO:HD3 | 2.50 | 0.47 |
| 48:2q:67:LYS:HA | 48:2q:70:ARG:HH12 | 1.79 | 0.47 |
| 50:2s:64:GLU:CD | 50:2s:64:GLU:H | 2.22 | 0.47 |
| 50:2s:66:MET:HB2 | 50:2s:74:PHE:CZ | 2.49 | 0.47 |
| 1:1A:56:A:H2' | 1:1A:57:C:O4' | 2.15 | 0.47 |
| 1:1A:614(C):A:C4 | 5:1F:180:GLY:HA2 | 2.50 | 0.47 |
| 1:1A:684:G:OP1 | 29:17:16:HIS:ND1 | 2.45 | 0.47 |
| 1:1A:1364:G:P | 23:11:3:LYS:HG3 | 2.55 | 0.47 |
| 1:1A:1936:A:OP1 | 1:1A:1937:A:H5' | 2.15 | 0.47 |
| 1:1A:2052:G:O2' | 61:1A:4204:HOH:O | 2.16 | 0.47 |
| 1:1A:2134:A:O2' | 1:1A:2135:A:O5' | 2.31 | 0.47 |
| 1:1A:2693:A:H2' | 1:1A:2694:G:C8 | 2.50 | 0.47 |
| 3:1D:211:ARG:HG3 | 3:1D:214:TRP:CE3 | 2.50 | 0.47 |
| 5:1F:156:LEU:HD21 | 5:1F:163:VAL:HG12 | 1.97 | 0.47 |
| 32:1a:381:C:H2' | 32:1a:382:A:O4' | 2.14 | 0.47 |
| 32:1a:1035:A:C4 | 32:1a:1036:G:N2 | 2.82 | 0.47 |
| 49:1r:38:GLU:HA | 49:1r:41:LYS:HE2 | 1.97 | 0.47 |
| 1:2A:888:C:H2' | 1:2A:889:C:C4 | 2.50 | 0.47 |
| 1:2A:1932:A:H2' | 1:2A:1933:G:O4' | 2.15 | 0.47 |
| 6:2G:124:SER:HB2 | 6:2G:131:TYR:CE1 | 2.50 | 0.47 |
| 10:2O:68:GLU:OE1 | 10:2O:78:ARG:NH1 | 2.47 | 0.47 |
| 14:2S:7:TYR:CZ | 14:2S:91:PRO:HG3 | 2.50 | 0.47 |
| 32:2a:417:C:H2' | 32:2a:418:C:H6 | 1.80 | 0.47 |
| 32:2a:629:G:H2' | 32:2a:630:G:O4' | 2.14 | 0.47 |
| 32:2a:750:G:N3 | 46:2o:23:GLY:HA3 | 2.29 | 0.47 |
| 32:2a:977:A:N6 | 32:2a:1224:G:O5' | 2.48 | 0.47 |
| 32:2a:1318:A:OP1 | 50:2s:3:ARG:NH1 | 2.29 | 0.47 |
| 34:2c:150:LYS:HG3 | 34:2c:169:ALA:HB2 | 1.96 | 0.47 |
| 40:2i:127:LYS:O | 40:2i:128:ARG:HG2 | 2.15 | 0.47 |
| 1:1A:579:G:H2' | 1:1A:580:C:C6 | 2.50 | 0.47 |
| 1:1A:1252:G:O4' | 16:1U:33:ARG:HD2 | 2.15 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 20:1Y:13:VAL:HB | 20:1Y:72:VAL:HG22 | 1.96 | 0.47 |
| 24:12:32:LEU:HD11 | 24:12:54:LYS:HG2 | 1.97 | 0.47 |
| 25:13:10:LYS:HB3 | 25:13:53:LEU:HA | 1.97 | 0.47 |
| 32:1a:35:G:O2' | 43:1l:118:SER:O | 2.29 | 0.47 |
| 32:1a:51:A:N7 | 32:1a:114:U:O2' | 2.42 | 0.47 |
| 33:1b:17:PHE:HB3 | 33:1b:44:LEU:HD11 | 1.97 | 0.47 |
| 34:1c:124:ILE:HG22 | 34:1c:130:VAL:HG22 | 1.95 | 0.47 |
| 39:1h:81:HIS:HB2 | 39:1h:138:TRP:CD1 | 2.50 | 0.47 |
| 1:2A:839:U:H2' | 1:2A:840:C:C6 | 2.50 | 0.47 |
| 1:2A:903:C:H2' | 1:2A:904:C:C6 | 2.49 | 0.47 |
| 1:2A:2723:C:OP1 | 13:2R:3:HIS:ND1 | 2.38 | 0.47 |
| 1:2A:2751:G:H5' | 7:2H:2:SER:HA | 1.96 | 0.47 |
| 2:2B:24:G:N7 | 2:2B:56:G:H2' | 2.29 | 0.47 |
| 7:2H:86:GLU:OE2 | 7:2H:132:ARG:NH2 | 2.47 | 0.47 |
| 8:2I:93:THR:HG22 | 8:2I:119:PRO:HB3 | 1.95 | 0.47 |
| 32:2a:646:U:H2' | 32:2a:647:C:H6 | 1.79 | 0.47 |
| 32:2a:1370:G:C8 | 40:2i:109:VAL:HG11 | 2.50 | 0.47 |
| 39:2h:30:ARG:O | 39:2h:34:GLU:HG2 | 2.15 | 0.47 |
| 41:2j:8:LEU:HB2 | 41:2j:70:ARG:HB2 | 1.97 | 0.47 |
| 1:1A:586:A:N1 | 1:1A:809:G:O2' | 2.44 | 0.47 |
| 1:1A:625:G:O6 | 11:1P:107:LYS:NZ | 2.44 | 0.47 |
| 1:1A:918:A:H5" | 2:1B:98:G:O2' | 2.15 | 0.47 |
| 1:1A:1091:G:C6 | 1:1A:1101:U:C2 | 3.03 | 0.47 |
| 1:1A:1432:C:H2' | 1:1A:1433:U:O4' | 2.15 | 0.47 |
| 1:1A:2108:C:H2' | 1:1A:2109:U:C6 | 2.50 | 0.47 |
| 6:1G:56:ALA:O | 6:1G:59:GLU:HG2 | 2.15 | 0.47 |
| 22:10:38:VAL:HB | 22:10:59:LEU:HB2 | 1.96 | 0.47 |
| 32:1a:895:G:H2' | 32:1a:896:C:C6 | 2.50 | 0.47 |
| 32:1a:1343:G:H1' | 40:1i:121:ARG:NH1 | 2.29 | 0.47 |
| 36:1e:11:ILE:HG23 | 36:1e:105:VAL:HG22 | 1.97 | 0.47 |
| 36:1e:78:HIS:CE1 | 36:1e:142:LEU:HA | 2.50 | 0.47 |
| 42:1k:18:ARG:HB2 | 42:1k:33:THR:OG1 | 2.15 | 0.47 |
| 44:1m:3:ARG:HH21 | 44:1m:9:ILE:HG13 | 1.80 | 0.47 |
| 1:2A:658:C:H2' | 1:2A:659:C:C6 | 2.50 | 0.47 |
| 1:2A:1246:A:OP1 | 5:2F:38:ARG:NH2 | 2.39 | 0.47 |
| 1:2A:1509(B):A:H2' | 1:2A:1510:G:C8 | 2.50 | 0.47 |
| 1:2A:2483:C:N3 | 12:2Q:124:LYS:HE3 | 2.30 | 0.47 |
| 1:2A:2705:A:O2' | 1:2A:2852:G:OP1 | 2.20 | 0.47 |
| 7:2H:64:LEU:O | 7:2H:68:THR:OG1 | 2.24 | 0.47 |
| 7:2H:137:ASP:HB3 | 7:2H:140:LYS:HB3 | 1.97 | 0.47 |
| 17:2V:62:LEU:HD21 | 17:2V:95:LEU:HB2 | 1.97 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 32:2a:70:G:H1 | 32:2a:99:U:H3 | 1.62 | 0.47 |
| 32:2a:1301:U:O2' | 32:2a:1302:U:H5' | 2.15 | 0.47 |
| 40:2i:42:ARG:HE | 40:2i:42:ARG:HB3 | 1.42 | 0.47 |
| 53:2v:22:U:H2' | 53:2v:23:A:H8 | 1.80 | 0.47 |
| 55:2x:14:A:N6 | 55:2x:21:A:H2 | 2.11 | 0.47 |
| 1:1A:264:C:O2' | 1:1A:265:A:H2' | 2.15 | 0.46 |
| 1:1A:1092:C:H2' | 1:1A:1093:G:O4' | 2.15 | 0.46 |
| 1:1A:1266:G:O2' | 1:1A:2012:G:O6 | 2.26 | 0.46 |
| 16:1U:76:TYR:CZ | 16:1U:80:ILE:HG13 | 2.50 | 0.46 |
| 17:1V:14:VAL:HB | 17:1V:96:ILE:HG13 | 1.96 | 0.46 |
| 21:1Z:98:MET:O | 21:1Z:125:LEU:HD12 | 2.15 | 0.46 |
| 32:1a:977:A:H1' | 32:1a:982:U:O4 | 2.15 | 0.46 |
| 32:1a:1499:A:H3' | 61:1a:2345:HOH:O | 2.13 | 0.46 |
| 33:1b:93:VAL:HG21 | 33:1b:97:TRP:CD1 | 2.50 | 0.46 |
| 35:1d:31:CYS:SG | 60:1d:302:SF4:S2 | 3.14 | 0.46 |
| 55:1x:8:4SU:O5' | 55:1x:8:4SU:H6 | 2.16 | 0.46 |
| 1:2A:597:U:H2' | 1:2A:598:G:C8 | 2.51 | 0.46 |
| 1:2A:968:G:H2' | 1:2A:969:U:C6 | 2.49 | 0.46 |
| 1:2A:979:G:H5" | 1:2A:980:A:C5' | 2.46 | 0.46 |
| 6:2G:122:PRO:HG3 | 6:2G:182:LYS:H | 1.80 | 0.46 |
| 7:2H:156:ALA:O | 7:2H:172:LYS:HG2 | 2.15 | 0.46 |
| 22:20:53:MET:HG2 | 22:20:57:PHE:HA | 1.95 | 0.46 |
| 29:27:34:ARG:NH2 | 29:27:39:ARG:HG2 | 2.30 | 0.46 |
| 32:2a:359:U:H2' | 32:2a:360:A:H8 | 1.78 | 0.46 |
| 32:2a:429:U:H3' | 35:2d:9:CYS:SG | 2.54 | 0.46 |
| 32:2a:564:C:C4 | 48:2q:31:LEU:HD11 | 2.49 | 0.46 |
| 32:2a:1003:G:H2' | 32:2a:1004:A:O4' | 2.15 | 0.46 |
| 32:2a:1011:G:N2 | 32:2a:1018:C:C2 | 2.80 | 0.46 |
| 35:2d:175:SER:HB3 | 35:2d:184:LYS:HB3 | 1.97 | 0.46 |
| 38:2g:32:ARG:HH21 | 38:2g:109:ASN:ND2 | 2.13 | 0.46 |
| 41:2j:46:ARG:HG2 | 41:2j:64:GLU:HB3 | 1.97 | 0.46 |
| 43:2l:113:ARG:HD2 | 43:2l:114:LYS:H | 1.80 | 0.46 |
| 51:2t:42:GLN:HE21 | 51:2t:46:GLU:HG3 | 1.80 | 0.46 |
| 1:1A:2066:C:H5" | 61:1A:5237:HOH:O | 2.15 | 0.46 |
| 1:1A:2252:G:N7 | 22:10:4:LYS:NZ | 2.63 | 0.46 |
| 5:1F:33:LEU:HD13 | 5:1F:112:MET:HE3 | 1.96 | 0.46 |
| 16:1U:55:ARG:O | 16:1U:59:ARG:HG3 | 2.15 | 0.46 |
| 32:1a:1118:C:H2' | 32:1a:1119:C:C6 | 2.50 | 0.46 |
| 1:2A:1351:C:O3' | 1:2A:1571:A:O2' | 2.33 | 0.46 |
| 1:2A:1711:C:H2' | 1:2A:1712:C:H6 | 1.80 | 0.46 |
| 32:2a:598:U:H4' | 39:2h:94:TYR:CG | 2.49 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 34:2c:22:TRP:CG | 34:2c:59:ARG:HG3 | 2.50 | 0.46 |
| 39:2h:6:ILE:O | 39:2h:10:LEU:HG | 2.15 | 0.46 |
| 40:2i:6:GLY:HA3 | 40:2i:80:GLY:O | 2.15 | 0.46 |
| 1:1A:784:A:O4' | 3:1D:227:ASN:ND2 | 2.48 | 0.46 |
| 1:1A:1052:C:H2' | 1:1A:1053:C:C6 | 2.50 | 0.46 |
| 1:1A:1792:G:O2' | 1:1A:1830:C:OP1 | 2.32 | 0.46 |
| 1:1A:2687:U:H2' | 1:1A:2688:U:O4' | 2.16 | 0.46 |
| 1:1A:2785:C:OP1 | 4:1E:41:LYS:NZ | 2.46 | 0.46 |
| 6:1G:18:GLU:HG3 | 6:1G:22:ARG:HD2 | 1.96 | 0.46 |
| 28:16:19:ARG:HD3 | 61:16:201:HOH:O | 2.14 | 0.46 |
| 32:1a:921:U:O2 | 36:1e:19:MET:HB2 | 2.14 | 0.46 |
| 37:1f:100:ASN:HB2 | 49:1r:28:GLU:HA | 1.97 | 0.46 |
| 41:1j:40:LEU:HB2 | 41:1j:69:ASN:HB2 | 1.97 | 0.46 |
| 46:1o:60:VAL:O | 46:1o:64:ARG:HB2 | 2.15 | 0.46 |
| 1:2A:921:G:H4' | 1:2A:2269:A:C5 | 2.49 | 0.46 |
| 1:2A:1275:A:N1 | 1:2A:1295:C:O2' | 2.45 | 0.46 |
| 1:2A:1358:G:O2' | 1:2A:1373:A:N6 | 2.45 | 0.46 |
| 1:2A:1578:U:C2' | 1:2A:1579:A:H5' | 2.46 | 0.46 |
| 1:2A:2061:G:H5" | 1:2A:2503:2MA:C2 | 2.45 | 0.46 |
| 1:2A:2314:C:H2' | 1:2A:2315:G:C8 | 2.50 | 0.46 |
| 4:2E:76:ARG:HB2 | 4:2E:77:ILE:HD12 | 1.97 | 0.46 |
| 5:2F:11:VAL:HG22 | 5:2F:125:LEU:HB2 | 1.97 | 0.46 |
| 6:2G:114:ILE:HB | 6:2G:117:PHE:HD1 | 1.80 | 0.46 |
| 15:2T:94:ALA:HB1 | 15:2T:99:LEU:HD21 | 1.96 | 0.46 |
| 32:2a:108:G:N1 | 51:2t:15:ARG:HG2 | 2.31 | 0.46 |
| 32:2a:547:A:H4' | 32:2a:548:G:O5' | 2.14 | 0.46 |
| 32:2a:1129:C:H5' | 32:2a:1130:A:OP1 | 2.15 | 0.46 |
| 35:2d:11:LEU:HG | 35:2d:66:ARG:HD3 | 1.97 | 0.46 |
| 35:2d:38:TYR:OH | 35:2d:45:GLN:NE2 | 2.48 | 0.46 |
| 36:2e:9:LYS:HD2 | 36:2e:9:LYS:HA | 1.63 | 0.46 |
| 54:2w:12:U:H3' | 54:2w:13:C:C5' | 2.44 | 0.46 |
| 3:1D:69:ARG:HE | 3:1D:130:ALA:HB2 | 1.81 | 0.46 |
| 6:1G:101:ILE:O | 6:1G:105:LYS:NZ | 2.49 | 0.46 |
| 11:1P:97:PRO:HD3 | 11:1P:126:VAL:O | 2.15 | 0.46 |
| 26:14:58:ARG:N | 26:14:58:ARG:HD2 | 2.29 | 0.46 |
| 32:1a:108:G:H1 | 51:1t:15:ARG:HG2 | 1.81 | 0.46 |
| 32:1a:1305:G:H22 | 32:1a:1331:G:H1' | 1.79 | 0.46 |
| 34:1c:71:ALA:HB2 | 34:1c:115:LEU:HD21 | 1.98 | 0.46 |
| 41:1j:11:PHE:HE1 | 41:1j:67:THR:HG22 | 1.79 | 0.46 |
| 1:2A:289:A:H2' | 1:2A:290:G:O4' | 2.16 | 0.46 |
| 1:2A:900:A:HO2' | 1:2A:901:A:P | 2.37 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:2A:1264:G:H2' | 1:2A:2014:A:N6 | 2.31 | 0.46 |
| 1:2A:1608:A:H1' | 1:2A:1610:A:OP2 | 2.16 | 0.46 |
| 1:2A:2061:G:O6 | 57:2A:3888:CLM:H3 | 2.14 | 0.46 |
| 1:2A:2238:G:H2' | 1:2A:2238:G:N3 | 2.29 | 0.46 |
| 1:2A:2398:U:H2' | 1:2A:2399:G:H8 | 1.80 | 0.46 |
| 2:2B:75:G:H22 | 21:2Z:73:GLN:NE2 | 2.13 | 0.46 |
| 4:2E:174:ASP:OD1 | 4:2E:175:VAL:N | 2.47 | 0.46 |
| 5:2F:102:PRO:HB2 | 5:2F:105:VAL:HG23 | 1.98 | 0.46 |
| 14:2S:35:ILE:HG23 | 14:2S:69:VAL:HG11 | 1.97 | 0.46 |
| 15:2T:60:THR:HG22 | 15:2T:77:PRO:HA | 1.96 | 0.46 |
| 32:2a:1201:A:H4' | 32:2a:1202:G:O5' | 2.15 | 0.46 |
| 32:2a:1371:G:O3' | 40:2i:69:GLY:HA3 | 2.15 | 0.46 |
| 33:2b:24:TRP:CD1 | 33:2b:24:TRP:H | 2.34 | 0.46 |
| 36:2e:65:ASN:HD21 | 36:2e:140:ARG:NH2 | 2.13 | 0.46 |
| 1:1A:747:U:O2 | 1:1A:2014:A:H1' | 2.16 | 0.46 |
| 1:1A:841:A:H2' | 1:1A:842:G:C8 | 2.50 | 0.46 |
| 1:1A:1818:U:H2' | 3:1D:157:ARG:HG3 | 1.98 | 0.46 |
| 1:1A:2090:G:N2 | 23:11:45:ASN:OD1 | 2.32 | 0.46 |
| 1:1A:2564:A:C2 | 1:1A:2647:U:H4' | 2.50 | 0.46 |
| 1:1A:2689:U:OP2 | 1:1A:2719:G:N2 | 2.33 | 0.46 |
| 6:1G:11:TYR:HA | 6:1G:15:VAL:HB | 1.97 | 0.46 |
| 32:1a:824:C:H2' | 32:1a:825:G:C8 | 2.51 | 0.46 |
| 32:1a:1038:C:H2' | 32:1a:1039:C:H6 | 1.81 | 0.46 |
| 33:1b:18:GLY:HA3 | 33:1b:42:ILE:HG13 | 1.97 | 0.46 |
| 40:1i:5:TYR:HH | 40:1i:7:THR:HG1 | 1.62 | 0.46 |
| 50:1s:27:GLU:HG2 | 50:1s:28:LYS:HD2 | 1.97 | 0.46 |
| 50:1s:64:GLU:HA | 50:1s:67:VAL:HG23 | 1.98 | 0.46 |
| 1:2A:1031:G:H5" | 31:29:8:LYS:HE3 | 1.98 | 0.46 |
| 1:2A:1156:A:O4' | 16:2U:51:LYS:NZ | 2.49 | 0.46 |
| 2:2B:25:A:H2' | 2:2B:26:A:C8 | 2.51 | 0.46 |
| 2:2B:32:C:H42 | 2:2B:50:G:H1 | 1.61 | 0.46 |
| 3:2D:18:VAL:HG12 | 3:2D:211:ARG:HH12 | 1.80 | 0.46 |
| 3:2D:85:ASP:OD2 | 3:2D:88:ARG:NH1 | 2.42 | 0.46 |
| 4:2E:48:GLN:HE21 | 4:2E:78:LEU:HD23 | 1.78 | 0.46 |
| 9:2N:108:PRO:O | 9:2N:113:GLY:HA3 | 2.15 | 0.46 |
| 16:2U:28:ARG:NH1 | 16:2U:38:THR:OG1 | 2.45 | 0.46 |
| 32:2a:34:C:H2' | 32:2a:35:G:C8 | 2.51 | 0.46 |
| 32:2a:401:C:O2' | 32:2a:621:A:N3 | 2.40 | 0.46 |
| 32:2a:1247:U:H1' | 32:2a:1291:G:N2 | 2.30 | 0.46 |
| 32:2a:1250:A:OP1 | 40:2i:67:GLY:N | 2.41 | 0.46 |
| 32:2a:1347:G:C8 | 40:2i:107:ARG:HB2 | 2.50 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 34:2c:24:ALA:HB3 | 34:2c:29:TYR:HD1 | 1.81 | 0.46 |
| 44:2m:65:LYS:O | 44:2m:70:LEU:HD12 | 2.14 | 0.46 |
| 49:2r:47:THR:O | 49:2r:47:THR:OG1 | 2.26 | 0.46 |
| 1:1A:97:C:OP1 | 24:12:2:LYS:HE2 | 2.16 | 0.46 |
| 1:1A:1035:U:H2' | 1:1A:1036:G:C8 | 2.51 | 0.46 |
| 1:1A:1803:A:H4' | 3:1D:259:THR:HG23 | 1.97 | 0.46 |
| 1:1A:1939:5MU:OP1 | 1:1A:2604:U:O2' | 2.34 | 0.46 |
| 1:1A:2771:C:H2' | 1:1A:2772:C:C6 | 2.50 | 0.46 |
| 11:1P:138:LEU:HD23 | 11:1P:145:PRO:HB3 | 1.98 | 0.46 |
| 16:1U:17:ILE:HG23 | 16:1U:39:LEU:HD12 | 1.98 | 0.46 |
| 20:1Y:13:VAL:HG12 | 20:1Y:74:PRO:HA | 1.97 | 0.46 |
| 32:1a:542:G:H5' | 35:1d:41:GLY:HA3 | 1.96 | 0.46 |
| 32:1a:1273:G:H3' | 32:1a:1274:G:H8 | 1.80 | 0.46 |
| 38:1g:74:GLU:O | 38:1g:88:PRO:HA | 2.15 | 0.46 |
| 43:1l:7:ILE:HD13 | 43:1l:10:LEU:HD12 | 1.97 | 0.46 |
| 1:2A:191:A:H2' | 1:2A:192:C:C6 | 2.50 | 0.46 |
| 1:2A:884:C:H3' | 1:2A:885:C:C6 | 2.50 | 0.46 |
| 1:2A:1005:C:H2' | 1:2A:1006:C:C6 | 2.51 | 0.46 |
| 1:2A:1818:U:H2' | 3:2D:157:ARG:HG3 | 1.97 | 0.46 |
| 1:2A:2137:C:O2' | 1:2A:2138:C:OP2 | 2.31 | 0.46 |
| 3:2D:134:ARG:HD2 | 3:2D:135:PHE:CZ | 2.50 | 0.46 |
| 4:2E:1:MET:O | 4:2E:84:PHE:HB2 | 2.15 | 0.46 |
| 12:2Q:36:ALA:HB2 | 12:2Q:103:MET:SD | 2.56 | 0.46 |
| 32:2a:403:C:O2' | 35:2d:122:ARG:NH2 | 2.48 | 0.46 |
| 32:2a:984:C:H2' | 32:2a:985:C:C6 | 2.50 | 0.46 |
| 55:2x:21:A:H62 | 55:2x:46:G:C2' | 2.29 | 0.46 |
| 1:1A:119:A:H4' | 1:1A:120:U:OP1 | 2.15 | 0.46 |
| 1:1A:286:C:H2' | 1:1A:287:C:H6 | 1.81 | 0.46 |
| 1:1A:784:A:N6 | 3:1D:229:VAL:HG11 | 2.31 | 0.46 |
| 1:1A:2086:U:H2' | 1:1A:2087:G:C8 | 2.50 | 0.46 |
| 1:1A:2291:U:H2' | 1:1A:2292:C:C6 | 2.51 | 0.46 |
| 1:1A:2507:C:H4' | 54:1w:75:C:O2' | 2.16 | 0.46 |
| 1:1A:2508:G:H5' | 54:1w:74:C:H42 | 1.79 | 0.46 |
| 3:1D:8:PRO:HB3 | 3:1D:14:ARG:HG2 | 1.97 | 0.46 |
| 5:1F:178:PRO:HB2 | 5:1F:201:VAL:CG2 | 2.46 | 0.46 |
| 7:1H:154:PRO:HB3 | 7:1H:163:TYR:CZ | 2.51 | 0.46 |
| 28:16:9:LEU:HD13 | 28:16:51:GLU:HB2 | 1.98 | 0.46 |
| 32:1a:44:G:C2 | 32:1a:45:U:H1' | 2.51 | 0.46 |
| 32:1a:392:G:OP1 | 47:1p:8:ARG:NH2 | 2.49 | 0.46 |
| 32:1a:555:C:H2' | 32:1a:556:C:C6 | 2.50 | 0.46 |
| 32:1a:1127:G:H5' | 32:1a:1280:A:O2' | 2.15 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 32:1a:1233:G:H2' | 32:1a:1234:C:C6 | 2.50 | 0.46 |
| 33:1b:112:VAL:O | 33:1b:116:GLU:N | 2.31 | 0.46 |
| 34:1c:180:ALA:HA | 34:1c:206:GLU:HA | 1.97 | 0.46 |
| 47:1p:50:LYS:HD2 | 47:1p:50:LYS:HA | 1.74 | 0.46 |
| 49:1r:31:LEU:HD13 | 49:1r:65:ILE:HB | 1.96 | 0.46 |
| 54:1w:5:G:H2' | 54:1w:6:G:H8 | 1.81 | 0.46 |
| 54:1y:61:C:H2' | 54:1y:62:C:C6 | 2.51 | 0.46 |
| 1:2A:774:A:H2' | 1:2A:774:A:N3 | 2.31 | 0.46 |
| 1:2A:848:G:C2 | 1:2A:933:A:H1' | 2.50 | 0.46 |
| 1:2A:1796:U:H2' | 1:2A:1797:C:H6 | 1.81 | 0.46 |
| 1:2A:2019:A:OP2 | 27:25:9:LYS:NZ | 2.39 | 0.46 |
| 1:2A:2683:C:OP1 | 15:2T:53:ARG:NH2 | 2.47 | 0.46 |
| 7:2H:3:ARG:HH21 | 7:2H:54:ARG:NH1 | 2.14 | 0.46 |
| 32:2a:407:G:H2' | 32:2a:408:A:C8 | 2.51 | 0.46 |
| 32:2a:765:G:N1 | 32:2a:812:C:O2' | 2.36 | 0.46 |
| 32:2a:834:C:H2' | 32:2a:835:U:C6 | 2.49 | 0.46 |
| 32:2a:1179:A:H2' | 32:2a:1180:A:O4' | 2.16 | 0.46 |
| 37:2f:23:LYS:NZ | 37:2f:42:GLU:OE1 | 2.34 | 0.46 |
| 50:2s:27:GLU:HB2 | 50:2s:28:LYS:HA | 1.98 | 0.46 |
| 1:1A:458:G:O2' | 1:1A:469:G:O6 | 2.30 | 0.46 |
| 1:1A:1047:G:O2' | 1:1A:1048:A:O5' | 2.33 | 0.46 |
| 1:1A:1930:G:O2' | 1:1A:1968:G:O6 | 2.28 | 0.46 |
| 1:1A:2142:C:O2 | 1:1A:2149:G:N1 | 2.40 | 0.46 |
| 1:1A:2497:A:O2' | 61:1A:5717:HOH:O | 2.16 | 0.46 |
| 5:1F:13:SER:OG | 5:1F:16:GLY:O | 2.30 | 0.46 |
| 14:1S:10:ARG:O | 14:1S:14:VAL:HG13 | 2.16 | 0.46 |
| 15:1T:39:ARG:HH21 | 32:1a:345:C:H5" | 1.81 | 0.46 |
| 21:1Z:6:LYS:HE3 | 21:1Z:8:TYR:OH | 2.15 | 0.46 |
| 32:1a:96:U:H2' | 32:1a:97:G:C8 | 2.51 | 0.46 |
| 32:1a:431:A:H2' | 32:1a:432:A:O4' | 2.15 | 0.46 |
| 32:1a:859:A:H2' | 32:1a:860:A:O4' | 2.16 | 0.46 |
| 32:1a:1314:C:H2' | 32:1a:1315:U:C6 | 2.51 | 0.46 |
| 1:2A:248:G:C2 | 1:2A:2431:U:H4' | 2.50 | 0.46 |
| 1:2A:320:A:H4' | 1:2A:322:A:C8 | 2.51 | 0.46 |
| 1:2A:350:U:H2' | 1:2A:351:G:O4' | 2.16 | 0.46 |
| 1:2A:1803:A:H4' | 3:2D:259:THR:HG23 | 1.97 | 0.46 |
| 1:2A:2394:C:P | 30:28:30:ARG:HH21 | 2.39 | 0.46 |
| 2:2B:28:C:H2' | 2:2B:29:A:O4' | 2.15 | 0.46 |
| 2:2B:107:G:H2' | 2:2B:108:U:H5" | 1.98 | 0.46 |
| 5:2F:164:ARG:O | 5:2F:168:ARG:HB2 | 2.16 | 0.46 |
| 21:2Z:101:PRO:HA | 21:2Z:123:ASP:HA | 1.97 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 28:26:40:CYS:O | 28:26:44:ARG:N | 2.49 | 0.46 |
| 32:2a:160:A:H61 | 32:2a:347:G:H1' | 1.81 | 0.46 |
| 32:2a:811:C:O2' | 32:2a:901:A:N1 | 2.47 | 0.46 |
| 32:2a:1183:A:O2' | 32:2a:1185:G:OP2 | 2.34 | 0.46 |
| 32:2a:1481:U:H2' | 32:2a:1482:G:C8 | 2.51 | 0.46 |
| 34:2c:50:ALA:HB1 | 34:2c:70:VAL:HG11 | 1.98 | 0.46 |
| 43:2l:53:ARG:HB3 | 43:2l:69:TYR:HE1 | 1.81 | 0.46 |
| 1:1A:335:C:H4' | 20:1Y:73:ARG:HD2 | 1.98 | 0.46 |
| 32:1a:1239:A:H62 | 32:1a:1299:A:N6 | 2.14 | 0.46 |
| 34:1c:52:LEU:HA | 34:1c:70:VAL:HG22 | 1.97 | 0.46 |
| 36:1e:106:PRO:O | 36:1e:110:LEU:HG | 2.15 | 0.46 |
| 1:2A:359:A:H3' | 1:2A:360:G:H8 | 1.80 | 0.46 |
| 1:2A:613:G:O2' | 1:2A:614(C):A:N1 | 2.43 | 0.46 |
| 1:2A:1195:G:N7 | 11:2P:15:ARG:NH2 | 2.61 | 0.46 |
| 1:2A:1592:C:H2' | 1:2A:1593:G:C8 | 2.50 | 0.46 |
| 1:2A:1919:A:O3' | 32:2a:1517:G:H1' | 2.16 | 0.46 |
| 1:2A:2432:A:C8 | 23:21:33:LYS:HD2 | 2.51 | 0.46 |
| 32:2a:554:C:O2' | 61:2a:3302:HOH:O | 2.21 | 0.46 |
| 32:2a:1030:C:N4 | 32:2a:1031:G:N1 | 2.62 | 0.46 |
| 32:2a:1057:G:H2' | 32:2a:1058:G:O4' | 2.16 | 0.46 |
| 32:2a:1107:C:O2 | 32:2a:1191:A:O2' | 2.34 | 0.46 |
| 49:2r:26:LEU:HD21 | 49:2r:42:ARG:HE | 1.80 | 0.46 |
| 51:2t:87:LYS:O | 51:2t:91:LEU:HG | 2.15 | 0.46 |
| 1:1A:330:A:H8 | 1:1A:1210:A:C4 | 2.34 | 0.46 |
| 1:1A:897:C:H4' | 54:1w:55:PSU:O3' | 2.15 | 0.46 |
| 1:1A:2111:C:N3 | 1:1A:2145:C:O2' | 2.48 | 0.46 |
| 1:1A:2319:G:H22 | 14:1S:3:ARG:NH1 | 2.14 | 0.46 |
| 1:1A:2751:G:H4' | 7:1H:4:ILE:HD11 | 1.97 | 0.46 |
| 8:1I:12:LEU:HD23 | 8:1I:12:LEU:HA | 1.73 | 0.46 |
| 14:1S:14:VAL:O | 14:1S:18:ILE:HG12 | 2.16 | 0.46 |
| 21:1Z:1:MET:HA | 21:1Z:2:GLU:HA | 1.53 | 0.46 |
| 21:1Z:24:LEU:HB2 | 21:1Z:41:LEU:HD12 | 1.98 | 0.46 |
| 21:1Z:123:ASP:OD1 | 21:1Z:123:ASP:N | 2.47 | 0.46 |
| 32:1a:339:C:H2' | 32:1a:340:U:C6 | 2.51 | 0.46 |
| 32:1a:604:G:H2' | 32:1a:605:U:C6 | 2.51 | 0.46 |
| 32:1a:1218:C:H2' | 32:1a:1219:U:C6 | 2.51 | 0.46 |
| 32:1a:1302:U:C6 | 44:1m:17:VAL:HG11 | 2.50 | 0.46 |
| 33:1b:71:VAL:HA | 33:1b:93:VAL:HG23 | 1.98 | 0.46 |
| 39:1h:51:VAL:HG12 | 39:1h:52:ASP:H | 1.81 | 0.46 |
| 44:1m:17:VAL:O | 44:1m:20:THR:OG1 | 2.29 | 0.46 |
| 47:1p:14:ASN:HA | 47:1p:42:ARG:NH2 | 2.31 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:2A:380:U:H2' | 1:2A:381:G:H8 | 1.81 | 0.46 |
| 1:2A:646:A:H2' | 1:2A:647:G:O4' | 2.16 | 0.46 |
| 1:2A:1845:G:OP1 | 3:2D:258:LYS:NZ | 2.45 | 0.46 |
| 8:2I:92:VAL:HG13 | 8:2I:120:ILE:HB | 1.97 | 0.46 |
| 32:2a:201:C:H42 | 32:2a:216:G:H1 | 1.64 | 0.46 |
| 32:2a:1218:C:H2' | 32:2a:1219:U:C6 | 2.51 | 0.46 |
| 32:2a:1244:C:H42 | 32:2a:1293:G:H1 | 1.63 | 0.46 |
| 33:2b:157:ARG:NH2 | 33:2b:160:ASP:OD1 | 2.49 | 0.46 |
| 34:2c:135:LYS:NZ | 36:2e:52:PRO:HG2 | 2.31 | 0.46 |
| 38:2g:26:PHE:HB2 | 38:2g:101:LEU:HD22 | 1.97 | 0.46 |
| 41:2j:44:VAL:HG22 | 41:2j:66:ARG:HG2 | 1.98 | 0.46 |
| 55:2x:43:A:H2' | 55:2x:44:A:C8 | 2.50 | 0.46 |
| 1:1A:1354:A:H2' | 1:1A:1355:G:O4' | 2.17 | 0.45 |
| 1:1A:2790:A:H3' | 1:1A:2790:A:N3 | 2.31 | 0.45 |
| 5:1F:32:LEU:HB3 | 5:1F:112:MET:HE1 | 1.97 | 0.45 |
| 5:1F:89:VAL:HG12 | 5:1F:90:PHE:CD2 | 2.51 | 0.45 |
| 8:1I:79:ILE:HG22 | 8:1I:81:VAL:HG13 | 1.98 | 0.45 |
| 12:1Q:54:MET:HG2 | 12:1Q:117:ALA:HB1 | 1.98 | 0.45 |
| 18:1W:92:ARG:NH1 | 61:1W:302:HOH:O | 2.38 | 0.45 |
| 32:1a:186:C:H2' | 32:1a:187:C:H6 | 1.81 | 0.45 |
| 32:1a:189(K):U:H2' | 32:1a:189(L):G:C8 | 2.51 | 0.45 |
| 32:1a:606:G:N2 | 32:1a:631:G:N7 | 2.64 | 0.45 |
| 32:1a:755:G:OP2 | 46:1o:65:ARG:HD3 | 2.16 | 0.45 |
| 32:1a:1323:G:H2' | 32:1a:1324:A:C8 | 2.51 | 0.45 |
| 32:1a:1348:U:H4' | 40:1i:120:ARG:HD2 | 1.98 | 0.45 |
| 33:1b:52:GLU:O | 33:1b:56:ARG:NH1 | 2.49 | 0.45 |
| 34:1c:56:ASP:O | 34:1c:66:VAL:HA | 2.16 | 0.45 |
| 43:1l:60:LEU:HD11 | 43:1l:85:ILE:HD13 | 1.97 | 0.45 |
| 54:1y:15:G:N2 | 54:1y:48:C:H42 | 2.14 | 0.45 |
| 1:2A:143:G:H2' | 1:2A:143(A):C:C6 | 2.51 | 0.45 |
| 1:2A:185:U:H4' | 1:2A:218:A:H4' | 1.97 | 0.45 |
| 1:2A:299:A:H5" | 20:2Y:86:ARG:NH2 | 2.30 | 0.45 |
| 1:2A:458:G:O2' | 29:27:39:ARG:HD2 | 2.16 | 0.45 |
| 1:2A:1025:G:C4 | 1:2A:1135:C:H1' | 2.51 | 0.45 |
| 1:2A:1456:G:N7 | 61:2A:5365:HOH:O | 2.36 | 0.45 |
| 1:2A:1790:C:H5" | 1:2A:1791:A:OP1 | 2.15 | 0.45 |
| 1:2A:1814:G:H4' | 3:2D:51:VAL:HG21 | 1.98 | 0.45 |
| 1:2A:1853:A:N1 | 1:2A:2087:G:H1' | 2.31 | 0.45 |
| 1:2A:1910:G:H22 | 1:2A:1920:4OC:C2 | 2.28 | 0.45 |
| 1:2A:2001:A:H2' | 1:2A:2002:G:C8 | 2.51 | 0.45 |
| 1:2A:2110:G:OP2 | 1:2A:2149:G:O2' | 2.27 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:2A:2744:G:N2 | 7:2H:143:GLN:OE1 | 2.48 | 0.45 |
| 5:2F:109:GLY:HA2 | 5:2F:112:MET:HE3 | 1.98 | 0.45 |
| 16:2U:76:TYR:OH | 16:2U:92:ARG:NE | 2.39 | 0.45 |
| 32:2a:229:U:H5" | 47:2p:33:ILE:HD13 | 1.98 | 0.45 |
| 32:2a:1390:U:H2' | 32:2a:1391:U:C6 | 2.51 | 0.45 |
| 33:2b:101:MET:HA | 33:2b:108:ILE:HG21 | 1.98 | 0.45 |
| 1:1A:27:G:N2 | 1:1A:512:G:H1' | 2.31 | 0.45 |
| 1:1A:1876:A:H2' | 1:1A:1877:A:C8 | 2.51 | 0.45 |
| 5:1F:25:PRO:HD2 | 5:1F:115:ALA:HB2 | 1.97 | 0.45 |
| 5:1F:192:LEU:HD13 | 5:1F:194:MET:HE2 | 1.96 | 0.45 |
| 29:17:12:ARG:HH21 | 29:17:44:PRO:HB3 | 1.81 | 0.45 |
| 32:1a:407:G:H5" | 35:1d:115:ARG:CG | 2.46 | 0.45 |
| 32:1a:667:G:H4' | 46:1o:51:HIS:ND1 | 2.31 | 0.45 |
| 32:1a:1048:G:O6 | 32:1a:1210:C:N4 | 2.50 | 0.45 |
| 35:1d:170:VAL:HG22 | 35:1d:171:GLY:H | 1.81 | 0.45 |
| 35:1d:175:SER:HB3 | 35:1d:184:LYS:HB3 | 1.98 | 0.45 |
| 1:2A:1316:U:H2' | 1:2A:1317:A:H8 | 1.80 | 0.45 |
| 1:2A:1814:G:OP1 | 3:2D:40:THR:OG1 | 2.33 | 0.45 |
| 1:2A:2307:G:H8 | 1:2A:2307:G:OP1 | 1.99 | 0.45 |
| 1:2A:2786:U:H2' | 1:2A:2787:C:C6 | 2.51 | 0.45 |
| 4:2E:9:VAL:HG22 | 4:2E:25:VAL:HB | 1.98 | 0.45 |
| 9:2N:15:LEU:HD23 | 9:2N:137:LYS:HG3 | 1.99 | 0.45 |
| 32:2a:130:A:H1' | 32:2a:263:A:O2' | 2.17 | 0.45 |
| 32:2a:524:G:H2' | 32:2a:525:C:C6 | 2.50 | 0.45 |
| 32:2a:627:G:H2' | 32:2a:628:G:C8 | 2.51 | 0.45 |
| 32:2a:828:A:H2' | 32:2a:829:G:O4' | 2.16 | 0.45 |
| 32:2a:1121:U:C2' | 32:2a:1122:U:H5' | 2.47 | 0.45 |
| 32:2a:1312:G:H1 | 32:2a:1325:C:N4 | 2.10 | 0.45 |
| 33:2b:52:GLU:O | 33:2b:56:ARG:NH1 | 2.49 | 0.45 |
| 36:2e:57:LYS:HG2 | 36:2e:61:TYR:CE2 | 2.51 | 0.45 |
| 38:2g:144:MET:HE2 | 38:2g:144:MET:HB3 | 1.79 | 0.45 |
| 1:1A:323:G:H1' | 1:1A:1205:U:O2 | 2.16 | 0.45 |
| 1:1A:825:C:O2' | 11:1P:55:ARG:HD3 | 2.16 | 0.45 |
| 3:1D:145:VAL:HG11 | 3:1D:175:LEU:HD11 | 1.98 | 0.45 |
| 32:1a:216:G:H2' | 32:1a:217:C:C6 | 2.51 | 0.45 |
| 32:1a:279:A:C5 | 48:1q:98:LEU:HD23 | 2.52 | 0.45 |
| 32:1a:976:G:OP2 | 32:1a:1358:U:O2' | 2.32 | 0.45 |
| 35:1d:81:GLU:CD | 35:1d:139:ARG:HH22 | 2.24 | 0.45 |
| 39:1h:25:ASP:N | 39:1h:25:ASP:OD1 | 2.50 | 0.45 |
| 45:1n:23:ARG:NH1 | 45:1n:30:ALA:HB2 | 2.30 | 0.45 |
| 1:2A:971:C:H2' | 1:2A:972:G:O4' | 2.16 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:2A:1288:U:O2' | 1:2A:1647:G:N2 | 2.50 | 0.45 |
| 7:2H:107:VAL:HG11 | 7:2H:162:ILE:HD11 | 1.98 | 0.45 |
| 13:2R:87:TYR:HD1 | 13:2R:90:ARG:HD2 | 1.82 | 0.45 |
| 16:2U:66:ASN:HD21 | 16:2U:70:ARG:HH21 | 1.64 | 0.45 |
| 21:2Z:75:ASN:O | 21:2Z:84:GLU:N | 2.37 | 0.45 |
| 32:2a:558:G:OP1 | 61:2a:3416:HOH:O | 2.20 | 0.45 |
| 32:2a:1226:C:H6 | 44:2m:103:THR:HB | 1.81 | 0.45 |
| 32:2a:1272:G:C2 | 32:2a:1273:G:H1' | 2.52 | 0.45 |
| 32:2a:1323:G:N2 | 32:2a:1361:G:O2' | 2.45 | 0.45 |
| 34:2c:131:ARG:NH2 | 34:2c:135:LYS:HE3 | 2.31 | 0.45 |
| 49:2r:76:LEU:HD12 | 49:2r:76:LEU:HA | 1.83 | 0.45 |
| 55:2x:16:C:H5' | 55:2x:59:A:N1 | 2.31 | 0.45 |
| 1:1A:570:G:H2' | 1:1A:2030:A:N7 | 2.32 | 0.45 |
| 1:1A:952:G:OP1 | 12:1Q:16:ARG:NH2 | 2.45 | 0.45 |
| 1:1A:1044:G:H5' | 1:1A:1045:A:OP2 | 2.16 | 0.45 |
| 1:1A:2155:G:H3' | 1:1A:2156:G:C8 | 2.50 | 0.45 |
| 5:1F:161:GLU:HG2 | 5:1F:164:ARG:NH2 | 2.30 | 0.45 |
| 7:1H:83:TYR:CE2 | 7:1H:138:LYS:HB2 | 2.52 | 0.45 |
| 18:1W:73:ALA:HB3 | 18:1W:106:ILE:HB | 1.98 | 0.45 |
| 21:1Z:91:LEU:HD12 | 21:1Z:91:LEU:HA | 1.75 | 0.45 |
| 26:14:61:ARG:HH12 | 50:1s:9:VAL:HG11 | 1.81 | 0.45 |
| 32:1a:435:C:H2' | 32:1a:436:C:H6 | 1.81 | 0.45 |
| 32:1a:598:U:H2' | 32:1a:599:C:C6 | 2.51 | 0.45 |
| 32:1a:1060:C:OP1 | 45:1n:45:ARG:NH2 | 2.42 | 0.45 |
| 33:1b:16:HIS:CD2 | 33:1b:204:ASN:H | 2.34 | 0.45 |
| 33:1b:163:PHE:CD1 | 33:1b:185:ILE:HG13 | 2.51 | 0.45 |
| 34:1c:18:TRP:O | 34:1c:54:ARG:NH2 | 2.49 | 0.45 |
| 40:1i:11:LYS:C | 40:1i:13:ALA:H | 2.24 | 0.45 |
| 1:2A:839:U:H1' | 1:2A:1191:G:H1' | 1.98 | 0.45 |
| 1:2A:879:G:H3' | 1:2A:880:G:C8 | 2.52 | 0.45 |
| 1:2A:2495:G:H5" | 12:2Q:82:ARG:HG2 | 1.98 | 0.45 |
| 1:2A:2702:U:H4' | 1:2A:2703:C:OP1 | 2.17 | 0.45 |
| 1:2A:2705:A:H2' | 1:2A:2706:G:O4' | 2.17 | 0.45 |
| 3:2D:68:LYS:C | 3:2D:70:TRP:H | 2.24 | 0.45 |
| 10:2O:26:LYS:O | 10:2O:30:ALA:HB2 | 2.16 | 0.45 |
| 13:2R:57:ARG:HH22 | 13:2R:61:HIS:CD2 | 2.35 | 0.45 |
| 13:2R:63:ARG:O | 13:2R:67:LEU:HB2 | 2.17 | 0.45 |
| 14:2S:87:PHE:CZ | 14:2S:102:ALA:HB2 | 2.51 | 0.45 |
| 26:24:62:ARG:HD3 | 26:24:62:ARG:HA | 1.72 | 0.45 |
| 28:26:15:GLU:OE1 | 28:26:45:LYS:NZ | 2.50 | 0.45 |
| 30:28:14:VAL:HG22 | 30:28:24:ALA:HB2 | 1.98 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 32:2a:129(A):G:C6 | 32:2a:189(E):U:H4' | 2.51 | 0.45 |
| 32:2a:986:A:H2' | 32:2a:987:G:O4' | 2.17 | 0.45 |
| 32:2a:1122:U:H3 | 32:2a:1151:A:H61 | 1.63 | 0.45 |
| 32:2a:1242:C:H2' | 32:2a:1243:C:O4' | 2.16 | 0.45 |
| 32:2a:1372:U:H2' | 32:2a:1373:G:O4' | 2.15 | 0.45 |
| 32:2a:1509:C:H2' | 32:2a:1510:U:O4' | 2.16 | 0.45 |
| 34:2c:119:ARG:HE | 34:2c:140:ARG:CZ | 2.30 | 0.45 |
| 42:2k:79:SER:HA | 42:2k:104:GLN:HB3 | 1.98 | 0.45 |
| 45:2n:45:ARG:O | 45:2n:49:HIS:HD2 | 2.00 | 0.45 |
| 55:2x:15:G:H2' | 55:2x:59:A:N1 | 2.31 | 0.45 |
| 1:1A:363(A):A:H2' | 1:1A:363(B):G:C8 | 2.51 | 0.45 |
| 1:1A:2649:U:H2' | 1:1A:2650:U:C6 | 2.52 | 0.45 |
| 1:1A:2693:A:H2' | 1:1A:2694:G:H8 | 1.81 | 0.45 |
| 8:1I:93:THR:H | 8:1I:96:ASP:HB2 | 1.81 | 0.45 |
| 13:1R:22:ARG:HG2 | 13:1R:69:ASP:HB3 | 1.97 | 0.45 |
| 32:1a:202:U:H3' | 32:1a:203:U:C5 | 2.52 | 0.45 |
| 32:1a:401:C:OP2 | 35:1d:73:ARG:NH2 | 2.49 | 0.45 |
| 32:1a:1289:A:N1 | 32:1a:1371:G:O2' | 2.48 | 0.45 |
| 38:1g:57:GLU:O | 38:1g:61:VAL:HG23 | 2.16 | 0.45 |
| 54:1w:2:C:N4 | 54:1w:71:G:H1 | 2.15 | 0.45 |
| 54:1y:19:G:N1 | 54:1y:56:C:N4 | 2.62 | 0.45 |
| 1:2A:892:G:H3' | 1:2A:893:C:H5" | 1.99 | 0.45 |
| 1:2A:2638:G:P | 4:2E:82:ARG:HH12 | 2.39 | 0.45 |
| 3:2D:142:VAL:HG23 | 3:2D:193:VAL:HA | 1.98 | 0.45 |
| 6:2G:129:GLY:O | 6:2G:161:THR:OG1 | 2.29 | 0.45 |
| 31:29:7:VAL:HG12 | 31:29:34:GLN:HB3 | 1.99 | 0.45 |
| 32:2a:685:G:C2 | 32:2a:686:U:C4 | 3.05 | 0.45 |
| 32:2a:1075:C:OP1 | 33:2b:179:LYS:NZ | 2.44 | 0.45 |
| 32:2a:1128:C:O2' | 32:2a:1129:C:OP1 | 2.35 | 0.45 |
| 32:2a:1176:A:H2' | 32:2a:1177:G:H8 | 1.82 | 0.45 |
| 32:2a:1288:A:H1' | 32:2a:1353:G:H4' | 1.99 | 0.45 |
| 37:2f:72:VAL:HG23 | 37:2f:90:VAL:HG11 | 1.99 | 0.45 |
| 1:1A:222:A:H5" | 1:1A:421:U:OP1 | 2.15 | 0.45 |
| 1:1A:1174:A:H4' | 1:1A:1175:U:OP1 | 2.16 | 0.45 |
| 1:1A:2864:G:OP1 | 15:1T:119:LYS:HD2 | 2.17 | 0.45 |
| 4:1E:12:THR:HG21 | 15:1T:11:GLU:HG2 | 1.98 | 0.45 |
| 8:1I:92:VAL:HG11 | 8:1I:144:VAL:HG11 | 1.98 | 0.45 |
| 13:1R:2:ARG:NH1 | 13:1R:5:LYS:O | 2.50 | 0.45 |
| 16:1U:52:ARG:NH1 | 16:1U:55:ARG:HH21 | 2.14 | 0.45 |
| 32:1a:119:A:H4' | 32:1a:120:A:C8 | 2.51 | 0.45 |
| 32:1a:219:C:H2' | 32:1a:220:G:O4' | 2.17 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 37:1f:21:LEU:O | 37:1f:25:ILE:HG13 | 2.17 | 0.45 |
| 40:1i:110:GLU:HG2 | 40:1i:113:LYS:HZ1 | 1.81 | 0.45 |
| 1:2A:274:G:H2' | 1:2A:275:G:C8 | 2.52 | 0.45 |
| 1:2A:1651:G:H2' | 1:2A:1652:A:O4' | 2.17 | 0.45 |
| 1:2A:2014:A:H4' | 18:2W:92:ARG:HH11 | 1.81 | 0.45 |
| 1:2A:2261:C:OP1 | 22:20:19:LYS:NZ | 2.46 | 0.45 |
| 1:2A:2507:C:H5" | 1:2A:2573:C:N4 | 2.30 | 0.45 |
| 1:2A:2717:G:H2' | 1:2A:2718:G:O4' | 2.17 | 0.45 |
| 61:2A:3999:HOH:O | 23:21:3:LYS:HE2 | 2.17 | 0.45 |
| 15:2T:16:ARG:NH2 | 15:2T:18:ASP:OD2 | 2.37 | 0.45 |
| 24:22:1:MET:SD | 24:22:56:GLN:NE2 | 2.89 | 0.45 |
| 32:2a:441:A:H5' | 32:2a:442:C:OP2 | 2.16 | 0.45 |
| 32:2a:822:C:H2' | 32:2a:823:G:C8 | 2.52 | 0.45 |
| 32:2a:1329:A:OP2 | 52:2u:7:ARG:NH1 | 2.50 | 0.45 |
| 33:2b:95:GLN:HB2 | 33:2b:148:TYR:HD1 | 1.81 | 0.45 |
| 1:1A:715:G:C2 | 46:1o:56:LEU:HD21 | 2.51 | 0.45 |
| 1:1A:1826:G:H4' | 3:1D:242:ARG:NH1 | 2.32 | 0.45 |
| 1:1A:2855:C:H2' | 1:1A:2856:C:C6 | 2.52 | 0.45 |
| 5:1F:28:ILE:O | 5:1F:30:PRO:HD3 | 2.16 | 0.45 |
| 6:1G:53:LEU:HD11 | 6:1G:87:PRO:HB2 | 1.98 | 0.45 |
| 9:1N:67:LEU:O | 9:1N:88:GLU:HG3 | 2.16 | 0.45 |
| 32:1a:196:A:OP1 | 51:1t:68:LYS:NZ | 2.46 | 0.45 |
| 32:1a:620:C:H2' | 32:1a:621:A:O4' | 2.17 | 0.45 |
| 32:1a:863:U:OP1 | 61:1a:2189:HOH:O | 2.21 | 0.45 |
| 32:1a:1118:C:H1' | 32:1a:1179:A:C4 | 2.52 | 0.45 |
| 44:1m:19:LEU:HD12 | 44:1m:19:LEU:HA | 1.74 | 0.45 |
| 51:1t:74:LYS:HA | 51:1t:74:LYS:HD2 | 1.71 | 0.45 |
| 1:2A:721:C:H2' | 1:2A:722:A:C8 | 2.52 | 0.45 |
| 1:2A:2590:A:O3' | 3:2D:239:ARG:NH2 | 2.50 | 0.45 |
| 12:2Q:37:LEU:HD21 | 12:2Q:130:LYS:HE2 | 1.99 | 0.45 |
| 21:2Z:93:ASP:HB3 | 21:2Z:131:ARG:HH22 | 1.81 | 0.45 |
| 32:2a:1050:G:H1' | 32:2a:1214:C:O2 | 2.17 | 0.45 |
| 35:2d:114:ARG:HA | 35:2d:117:ALA:HB3 | 1.99 | 0.45 |
| 39:2h:34:GLU:O | 39:2h:38:ILE:HG12 | 2.16 | 0.45 |
| 40:2i:11:LYS:HA | 40:2i:108:VAL:HG12 | 1.97 | 0.45 |
| 54:2w:11:C:N3 | 54:2w:24:G:N2 | 2.64 | 0.45 |
| 1:1A:2183:C:O2' | 1:1A:2184:G:OP1 | 2.33 | 0.45 |
| 1:1A:2319:G:H22 | 14:1S:3:ARG:HA | 1.82 | 0.45 |
| 1:1A:2334:G:H5' | 14:1S:9:ARG:HG2 | 1.99 | 0.45 |
| 1:1A:2591:C:H2' | 1:1A:2592:G:C8 | 2.51 | 0.45 |
| 1:1A:2630:G:H2' | 1:1A:2631:G:C8 | 2.52 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:1D:142:VAL:HG23 | 3:1D:193:VAL:HA | 1.98 | 0.45 |
| 7:1H:127:GLU:H | 7:1H:127:GLU:HG3 | 1.60 | 0.45 |
| 20:1Y:6:HIS:H | 20:1Y:6:HIS:CD2 | 2.35 | 0.45 |
| 27:15:42:PRO:HB2 | 27:15:43:HIS:ND1 | 2.30 | 0.45 |
| 32:1a:1005:A:OP2 | 32:1a:1006:C:N4 | 2.49 | 0.45 |
| 32:1a:1109:C:H2' | 32:1a:1110:A:O4' | 2.17 | 0.45 |
| 35:1d:156:GLU:OE1 | 35:1d:156:GLU:N | 2.39 | 0.45 |
| 40:1i:9:ARG:HD3 | 40:1i:14:VAL:HG12 | 1.98 | 0.45 |
| 44:1m:3:ARG:HG3 | 44:1m:4:ILE:N | 2.31 | 0.45 |
| 54:1y:9:A:O3' | 54:1y:45:U:O2' | 2.32 | 0.45 |
| 1:2A:30:G:O2' | 1:2A:1214:A:N3 | 2.46 | 0.45 |
| 1:2A:335:C:H4' | 20:2Y:73:ARG:HD2 | 1.97 | 0.45 |
| 1:2A:1410:G:H2' | 1:2A:1411:C:C6 | 2.52 | 0.45 |
| 1:2A:1592:C:H2' | 1:2A:1593:G:H8 | 1.82 | 0.45 |
| 1:2A:1903:G:OP1 | 3:2D:241:PRO:HB2 | 2.17 | 0.45 |
| 1:2A:2271:G:OP1 | 22:20:18:ALA:HB1 | 2.17 | 0.45 |
| 1:2A:2507:C:O2' | 54:2w:75:C:O2 | 2.32 | 0.45 |
| 4:2E:52:LEU:HB3 | 4:2E:76:ARG:HD3 | 1.98 | 0.45 |
| 9:2N:73:THR:HG23 | 9:2N:82:LEU:HD11 | 1.98 | 0.45 |
| 18:2W:33:ARG:NH2 | 18:2W:52:GLU:OE1 | 2.40 | 0.45 |
| 32:2a:966:M2G:HM23 | 32:2a:967:5MC:H1' | 1.98 | 0.45 |
| 32:2a:980:C:H1' | 45:2n:19:ARG:HA | 1.99 | 0.45 |
| 32:2a:1406:U:C6 | 32:2a:1407:5MC:HM52 | 2.52 | 0.45 |
| 33:2b:16:HIS:HB2 | 33:2b:204:ASN:CB | 2.40 | 0.45 |
| 34:2c:131:ARG:HH21 | 34:2c:135:LYS:HE3 | 1.82 | 0.45 |
| 47:2p:58:TYR:O | 47:2p:61:SER:OG | 2.23 | 0.45 |
| 51:2t:35:THR:O | 51:2t:39:LYS:N | 2.39 | 0.45 |
| 1:1A:2126:A:N6 | 1:1A:2162:G:O2' | 2.50 | 0.45 |
| 3:1D:232:PRO:HB3 | 3:1D:244:ARG:CZ | 2.46 | 0.45 |
| 7:1H:3:ARG:HH11 | 7:1H:4:ILE:H | 1.65 | 0.45 |
| 10:1O:64:ARG:NH2 | 10:1O:99:PHE:O | 2.50 | 0.45 |
| 32:1a:839:U:H3' | 32:1a:840:C:H5' | 1.99 | 0.45 |
| 32:1a:1499:A:OP2 | 61:1a:2345:HOH:O | 2.21 | 0.45 |
| 49:1r:40:LEU:HD13 | 49:1r:79:LEU:HD11 | 1.98 | 0.45 |
| 1:2A:614(B):G:N3 | 5:2F:44:ARG:HG2 | 2.32 | 0.45 |
| 1:2A:1449:A:O2' | 1:2A:1529:G:N2 | 2.24 | 0.45 |
| 1:2A:1821:A:H2' | 1:2A:1822:G:C8 | 2.52 | 0.45 |
| 1:2A:1913:A:H4' | 1:2A:1914:C:C5' | 2.47 | 0.45 |
| 1:2A:2884:U:OP2 | 61:2A:4777:HOH:O | 2.21 | 0.45 |
| 4:2E:7:VAL:HG12 | 4:2E:27:LEU:HB3 | 1.99 | 0.45 |
| 5:2F:185:ASP:HA | 5:2F:188:ARG:HD3 | 1.98 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 11:2P:52:GLU:HB3 | 11:2P:55:ARG:CZ | 2.46 | 0.45 |
| 20:2Y:28:LYS:N | 20:2Y:38:ILE:O | 2.50 | 0.45 |
| 29:27:47:ARG:HD3 | 29:27:47:ARG:HA | 1.61 | 0.45 |
| 32:2a:1057:G:O3' | 34:2c:197:GLY:HA3 | 2.16 | 0.45 |
| 32:2a:1327:C:H2' | 32:2a:1328:C:C6 | 2.52 | 0.45 |
| 34:2c:12:LEU:HD11 | 45:2n:51:GLY:HA2 | 1.99 | 0.45 |
| 39:2h:20:TYR:HA | 39:2h:65:TYR:CZ | 2.52 | 0.45 |
| 43:2l:24:VAL:HB | 43:2l:27:LEU:HD22 | 1.98 | 0.45 |
| 1:1A:515:A:H1' | 1:1A:581:C:H1' | 1.99 | 0.45 |
| 1:1A:861:A:N3 | 2:1B:79:C:O2' | 2.50 | 0.45 |
| 1:1A:1310:G:H1' | 1:1A:1611:C:H5' | 1.99 | 0.45 |
| 1:1A:1636:C:H2' | 1:1A:1637:A:C8 | 2.52 | 0.45 |
| 4:1E:1:MET:HE3 | 4:1E:199:ARG:HB3 | 1.98 | 0.45 |
| 23:11:59:THR:O | 23:11:91:LYS:NZ | 2.50 | 0.45 |
| 28:16:13:CYS:SG | 28:16:47:THR:HG21 | 2.57 | 0.45 |
| 32:1a:501:C:H2' | 32:1a:502:G:C8 | 2.51 | 0.45 |
| 35:1d:60:GLU:HG2 | 35:1d:202:LEU:HB2 | 1.99 | 0.45 |
| 45:1n:33:VAL:HA | 45:1n:40:CYS:HA | 1.99 | 0.45 |
| 1:2A:445:C:OP1 | 16:2U:2:PRO:HA | 2.17 | 0.45 |
| 1:2A:747:U:O2 | 1:2A:2014:A:H1' | 2.17 | 0.45 |
| 1:2A:813:U:H2' | 1:2A:814:C:C6 | 2.53 | 0.45 |
| 1:2A:1037:G:H1 | 1:2A:1118:C:H42 | 1.63 | 0.45 |
| 1:2A:1248:G:C5 | 16:2U:3:ARG:HB2 | 2.52 | 0.45 |
| 1:2A:1448:G:H4' | 1:2A:1542:A:OP1 | 2.17 | 0.45 |
| 1:2A:1607:C:H5" | 1:2A:1608:A:H5' | 1.99 | 0.45 |
| 1:2A:1889:A:H2' | 1:2A:1890:A:C8 | 2.52 | 0.45 |
| 1:2A:2630:G:H2' | 1:2A:2631:G:H8 | 1.80 | 0.45 |
| 3:2D:75:ILE:HG21 | 3:2D:99:ASP:HB2 | 1.99 | 0.45 |
| 7:2H:164:TYR:HB2 | 7:2H:167:GLU:HB2 | 1.99 | 0.45 |
| 11:2P:95:VAL:HG13 | 11:2P:125:VAL:HA | 1.98 | 0.45 |
| 16:2U:49:HIS:HA | 16:2U:52:ARG:HB3 | 1.98 | 0.45 |
| 32:2a:743:U:H2' | 32:2a:744:C:C6 | 2.52 | 0.45 |
| 32:2a:868:C:H2' | 32:2a:869:G:O4' | 2.16 | 0.45 |
| 32:2a:875:C:O2' | 39:2h:15:ASN:ND2 | 2.47 | 0.45 |
| 32:2a:1002:G:H5' | 32:2a:1003:G:OP2 | 2.16 | 0.45 |
| 32:2a:1137:C:H4' | 32:2a:1138:G:O5' | 2.17 | 0.45 |
| 32:2a:1456:G:N1 | 51:2t:51:GLU:OE2 | 2.45 | 0.45 |
| 37:2f:14:LEU:HD22 | 37:2f:18:GLN:HB3 | 1.99 | 0.45 |
| 50:2s:15:LEU:HD12 | 50:2s:18:LYS:HD2 | 1.98 | 0.45 |
| 54:2w:72:C:H2' | 54:2w:73:A:H8 | 1.81 | 0.45 |
| 55:2x:25:C:H2' | 55:2x:26:G:O4' | 2.17 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1A:8:A:H2' | 1:1A:9:U:C6 | 2.53 | 0.44 |
| 1:1A:944:G:N7 | 61:1A:4211:HOH:O | 2.36 | 0.44 |
| 1:1A:1032:A:H2 | 1:1A:1122:G:H22 | 1.65 | 0.44 |
| 1:1A:1052:C:H2' | 1:1A:1053:C:H6 | 1.82 | 0.44 |
| 1:1A:1218:C:H42 | 1:1A:1231:G:H1 | 1.66 | 0.44 |
| 1:1A:1935:G:H1' | 1:1A:1964:G:N2 | 2.32 | 0.44 |
| 1:1A:1972:A:H2' | 1:1A:1973:G:H8 | 1.81 | 0.44 |
| 1:1A:2155:G:H3' | 1:1A:2156:G:H8 | 1.82 | 0.44 |
| 1:1A:2870:C:H2' | 1:1A:2871:C:O4' | 2.16 | 0.44 |
| 21:1Z:99:TYR:HA | 21:1Z:124:ILE:O | 2.16 | 0.44 |
| 32:1a:1317:C:OP2 | 45:1n:17:LYS:HE2 | 2.17 | 0.44 |
| 32:1a:1518:MA6:H93 | 32:1a:1519:MA6:H92 | 1.99 | 0.44 |
| 33:1b:28:PHE:CD2 | 33:1b:190:THR:HA | 2.52 | 0.44 |
| 50:1s:31:ILE:HD12 | 50:1s:49:ILE:HG12 | 1.98 | 0.44 |
| 1:2A:581:C:H2' | 1:2A:582:G:H8 | 1.82 | 0.44 |
| 1:2A:705:A:C2 | 1:2A:727:A:H1' | 2.52 | 0.44 |
| 1:2A:820:A:N3 | 1:2A:943:U:H4' | 2.32 | 0.44 |
| 1:2A:1579:A:H2' | 1:2A:1580:A:C8 | 2.52 | 0.44 |
| 1:2A:1636:C:H2' | 1:2A:1637:A:C8 | 2.52 | 0.44 |
| 32:2a:189(F):U:H3 | 48:2q:72:ARG:HH22 | 1.65 | 0.44 |
| 32:2a:997:U:O2 | 32:2a:1044:A:N1 | 2.50 | 0.44 |
| 33:2b:97:TRP:HZ3 | 33:2b:172:ILE:HG22 | 1.81 | 0.44 |
| 1:1A:271(A):A:N1 | 1:1A:272(D):G:O2' | 2.42 | 0.44 |
| 1:1A:774:A:N3 | 1:1A:774:A:H2' | 2.32 | 0.44 |
| 1:1A:1790:C:H5" | 1:1A:1791:A:OP1 | 2.16 | 0.44 |
| 1:1A:2181:G:O2' | 1:1A:2182:G:OP1 | 2.31 | 0.44 |
| 1:1A:2418:A:H2' | 1:1A:2419:U:C6 | 2.52 | 0.44 |
| 1:1A:2712:U:O2' | 1:1A:2713:A:H5' | 2.17 | 0.44 |
| 3:1D:37:LEU:HB2 | 3:1D:62:TYR:HB2 | 1.99 | 0.44 |
| 14:1S:34:HIS:O | 14:1S:97:ARG:NH2 | 2.50 | 0.44 |
| 15:1T:118:ARG:HG2 | 32:1a:1442(A):G:C8 | 2.52 | 0.44 |
| 32:1a:189(C):C:H2' | 32:1a:189(D):C:O4' | 2.17 | 0.44 |
| 32:1a:339:C:H2' | 32:1a:340:U:H6 | 1.82 | 0.44 |
| 33:1b:55:PHE:HD1 | 33:1b:221:LEU:HD22 | 1.82 | 0.44 |
| 50:1s:20:LEU:HD21 | 50:1s:43:GLU:HG2 | 1.99 | 0.44 |
| 1:2A:71:A:H5" | 1:2A:73:A:C8 | 2.52 | 0.44 |
| 1:2A:1843:C:H5' | 3:2D:253:GLN:OE1 | 2.18 | 0.44 |
| 1:2A:2232:U:P | 23:21:40:ARG:HH12 | 2.40 | 0.44 |
| 1:2A:2845:G:H2' | 1:2A:2846:G:C8 | 2.52 | 0.44 |
| 7:2H:74:ASN:O | 7:2H:78:GLY:N | 2.50 | 0.44 |
| 9:2N:49:GLY:O | 9:2N:119:ARG:NH1 | 2.50 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 17:2V:72:VAL:HG13 | 17:2V:85:LYS:HB3 | 1.99 | 0.44 |
| 32:2a:711:G:H2' | 32:2a:712:A:H8 | 1.83 | 0.44 |
| 32:2a:1104:G:H4' | 33:2b:111:ARG:HE | 1.81 | 0.44 |
| 32:2a:1260:C:P | 32:2a:1284:C:H4' | 2.57 | 0.44 |
| 33:2b:16:HIS:CD2 | 33:2b:204:ASN:H | 2.35 | 0.44 |
| 35:2d:116:GLN:HE22 | 35:2d:161:ASN:HD21 | 1.63 | 0.44 |
| 40:2i:128:ARG:HH21 | 55:2x:32:5MC:P | 2.40 | 0.44 |
| 46:2o:5:LYS:HE2 | 46:2o:5:LYS:HB2 | 1.89 | 0.44 |
| 55:2x:66:C:H2' | 55:2x:67:C:O4' | 2.18 | 0.44 |
| 1:1A:272:G:N7 | 1:1A:421:U:H2' | 2.33 | 0.44 |
| 1:1A:1364:G:C8 | 23:11:3:LYS:HD2 | 2.53 | 0.44 |
| 1:1A:2334:G:O6 | 22:10:74:ARG:NH1 | 2.44 | 0.44 |
| 1:1A:2557:G:H2' | 1:1A:2558:C:C6 | 2.53 | 0.44 |
| 2:1B:66:A:H61 | 2:1B:108:U:H2' | 1.82 | 0.44 |
| 6:1G:114:ILE:HG12 | 6:1G:140:ILE:HG12 | 1.99 | 0.44 |
| 24:12:14:ARG:O | 24:12:67:LYS:NZ | 2.49 | 0.44 |
| 32:1a:642:A:N3 | 39:1h:113:SER:OG | 2.42 | 0.44 |
| 32:1a:1518:MA6:O5' | 32:1a:1518:MA6:H8 | 2.17 | 0.44 |
| 33:1b:155:LEU:HD11 | 33:1b:159:PRO:HG3 | 1.99 | 0.44 |
| 35:1d:78:LEU:HD23 | 35:1d:97:LEU:HD23 | 2.00 | 0.44 |
| 1:2A:1116:C:H2' | 1:2A:1117:G:C8 | 2.52 | 0.44 |
| 1:2A:1946:U:H2' | 1:2A:1947:C:C6 | 2.52 | 0.44 |
| 1:2A:1952:A:N3 | 1:2A:2560:C:O2' | 2.43 | 0.44 |
| 1:2A:2062:A:OP1 | 61:2A:4300:HOH:O | 2.21 | 0.44 |
| 1:2A:2152:G:C2 | 1:2A:2153:G:H1' | 2.52 | 0.44 |
| 1:2A:2390:U:P | 30:28:35:GLN:HE22 | 2.39 | 0.44 |
| 2:2B:42:C:C4 | 2:2B:43:C:C4 | 3.06 | 0.44 |
| 3:2D:148:GLU:HB2 | 3:2D:151:LYS:HD2 | 1.98 | 0.44 |
| 5:2F:36:VAL:O | 5:2F:40:GLN:HG3 | 2.17 | 0.44 |
| 7:2H:3:ARG:NH1 | 7:2H:4:ILE:H | 2.15 | 0.44 |
| 12:2Q:2:LEU:HD12 | 12:2Q:69:PHE:HE1 | 1.82 | 0.44 |
| 15:2T:65:LYS:HE2 | 15:2T:65:LYS:HB3 | 1.78 | 0.44 |
| 32:2a:448:A:O5' | 32:2a:485:G:N2 | 2.45 | 0.44 |
| 32:2a:1251:A:N6 | 32:2a:1285:A:N1 | 2.65 | 0.44 |
| 32:2a:1298:C:OP2 | 38:2g:114:ARG:NH2 | 2.50 | 0.44 |
| 38:2g:37:ASN:HD21 | 40:2i:40:LEU:HD23 | 1.82 | 0.44 |
| 40:2i:128:ARG:NH2 | 55:2x:33:U:OP2 | 2.47 | 0.44 |
| 1:1A:24:G:O2' | 18:1W:78:GLU:O | 2.26 | 0.44 |
| 2:1B:88:C:H2' | 2:1B:89:G:O4' | 2.18 | 0.44 |
| 4:1E:181:LEU:HD12 | 4:1E:181:LEU:HA | 1.72 | 0.44 |
| 6:1G:170:ARG:NH2 | 6:1G:182:LYS:O | 2.48 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:1H:113:VAL:HG11 | 7:1H:151:ILE:HG21 | 1.98 | 0.44 |
| 28:16:14:THR:HG21 | 28:16:48:VAL:HG13 | 1.99 | 0.44 |
| 32:1a:835:U:OP1 | 49:1r:64:ARG:NH2 | 2.33 | 0.44 |
| 32:1a:881:G:P | 43:1l:12:ARG:HH22 | 2.39 | 0.44 |
| 54:1y:58:A:HO2' | 54:1y:59:U:P | 2.37 | 0.44 |
| 1:2A:94(A):G:H2' | 1:2A:95:G:O4' | 2.17 | 0.44 |
| 1:2A:521:G:H2' | 1:2A:522:G:H8 | 1.83 | 0.44 |
| 1:2A:607:U:OP1 | 5:2F:102:PRO:HA | 2.18 | 0.44 |
| 1:2A:882:G:H1 | 1:2A:894:C:N4 | 2.14 | 0.44 |
| 1:2A:927:G:H2' | 1:2A:928:G:O4' | 2.16 | 0.44 |
| 1:2A:1657:C:H2' | 1:2A:1658:C:C6 | 2.53 | 0.44 |
| 1:2A:2312:U:H5' | 6:2G:88:ILE:HD11 | 1.98 | 0.44 |
| 3:2D:18:VAL:HG12 | 3:2D:211:ARG:NH1 | 2.32 | 0.44 |
| 9:2N:138:LEU:HD23 | 9:2N:138:LEU:HA | 1.85 | 0.44 |
| 32:2a:671:G:H2' | 32:2a:672:U:O4' | 2.18 | 0.44 |
| 32:2a:876:G:OP1 | 39:2h:14:ARG:NH1 | 2.50 | 0.44 |
| 32:2a:1189:C:H2' | 34:2c:176:HIS:CE1 | 2.53 | 0.44 |
| 38:2g:79:ARG:HH21 | 38:2g:80:VAL:H | 1.65 | 0.44 |
| 54:2y:54:5MU:C4 | 54:2y:55:PSU:C2 | 3.05 | 0.44 |
| 1:1A:1401:G:H2' | 1:1A:1402:C:O4' | 2.17 | 0.44 |
| 1:1A:1406:U:H2' | 1:1A:1407:C:H6 | 1.79 | 0.44 |
| 1:1A:1823:G:P | 3:1D:54:ARG:HH21 | 2.40 | 0.44 |
| 1:1A:2102:U:H3 | 1:1A:2187:G:H1 | 1.65 | 0.44 |
| 1:1A:2336:A:H61 | 22:10:43:THR:HG22 | 1.82 | 0.44 |
| 3:1D:101:GLU:OE2 | 3:1D:103:ARG:NE | 2.42 | 0.44 |
| 6:1G:43:LEU:HD12 | 6:1G:43:LEU:HA | 1.81 | 0.44 |
| 12:1Q:134:ARG:NH1 | 21:1Z:122:ARG:HH21 | 2.15 | 0.44 |
| 26:14:49:PHE:HB3 | 26:14:50:VAL:H | 1.51 | 0.44 |
| 32:1a:883:C:N4 | 32:1a:884:U:O4 | 2.51 | 0.44 |
| 32:1a:1223:C:P | 50:1s:78:ARG:HH21 | 2.41 | 0.44 |
| 32:1a:1376:U:H2' | 32:1a:1377:A:C8 | 2.52 | 0.44 |
| 38:1g:144:MET:HB3 | 38:1g:144:MET:HE2 | 1.66 | 0.44 |
| 40:1i:50:LEU:HD23 | 40:1i:81:ILE:HD11 | 2.00 | 0.44 |
| 1:2A:250:G:OP1 | 30:28:13:ARG:NH2 | 2.50 | 0.44 |
| 1:2A:571:A:O2' | 17:2V:78:LYS:HE2 | 2.18 | 0.44 |
| 1:2A:1231:G:H2' | 1:2A:1232:G:H8 | 1.82 | 0.44 |
| 1:2A:2875:C:H2' | 1:2A:2876:G:O4' | 2.18 | 0.44 |
| 9:2N:67:LEU:O | 9:2N:88:GLU:HG3 | 2.17 | 0.44 |
| 17:2V:58:VAL:HB | 17:2V:98:GLU:HG3 | 2.00 | 0.44 |
| 30:28:62:LEU:HB3 | 30:28:65:GLU:HG2 | 1.99 | 0.44 |
| 32:2a:19:C:H5" | 36:2e:86:ALA:HB3 | 2.00 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 32:2a:1107:C:OP1 | 34:2c:173:VAL:N | 2.50 | 0.44 |
| 32:2a:1228:C:H5" | 44:2m:108:ARG:HH22 | 1.82 | 0.44 |
| 34:2c:112:SER:HB3 | 34:2c:115:LEU:HD22 | 1.99 | 0.44 |
| 35:2d:65:ARG:HG3 | 35:2d:75:PHE:CG | 2.53 | 0.44 |
| 51:2t:47:GLY:HA2 | 51:2t:48:LYS:C | 2.42 | 0.44 |
| 54:2w:27:G:N2 | 54:2w:43:C:N3 | 2.65 | 0.44 |
| 1:1A:551:G:O2' | 1:1A:1220:A:N3 | 2.48 | 0.44 |
| 1:1A:614(B):G:N2 | 5:1F:44:ARG:O | 2.46 | 0.44 |
| 1:1A:2121:G:H2' | 1:1A:2122:U:C6 | 2.53 | 0.44 |
| 1:1A:2181:G:HO2' | 1:1A:2182:G:P | 2.39 | 0.44 |
| 20:1Y:9:LYS:HA | 20:1Y:10:GLY:HA2 | 1.54 | 0.44 |
| 21:1Z:99:TYR:HB3 | 21:1Z:123:ASP:OD2 | 2.18 | 0.44 |
| 32:1a:11:G:O2' | 32:1a:506:G:N2 | 2.49 | 0.44 |
| 32:1a:120:A:OP1 | 61:1a:1901:HOH:O | 2.21 | 0.44 |
| 32:1a:405:U:O4 | 35:1d:2:GLY:N | 2.51 | 0.44 |
| 33:1b:174:VAL:O | 33:1b:178:ARG:HG3 | 2.18 | 0.44 |
| 40:1i:81:ILE:O | 40:1i:85:LEU:HG | 2.18 | 0.44 |
| 54:1y:20:U:O2' | 54:1y:21:A:H4' | 2.17 | 0.44 |
| 54:1y:28:G:H2' | 54:1y:29:G:C8 | 2.52 | 0.44 |
| 1:2A:1155:A:H5" | 16:2U:55:ARG:NE | 2.32 | 0.44 |
| 1:2A:1637:A:H5' | 1:2A:1760:A:O2' | 2.18 | 0.44 |
| 1:2A:2516:G:C6 | 1:2A:2517:C:C4 | 3.06 | 0.44 |
| 1:2A:2689:U:P | 1:2A:2719:G:H22 | 2.41 | 0.44 |
| 2:2B:34:U:O4 | 2:2B:44:G:O2' | 2.33 | 0.44 |
| 12:2Q:50:ALA:HB1 | 12:2Q:121:ALA:HB1 | 1.99 | 0.44 |
| 16:2U:76:TYR:CZ | 16:2U:80:ILE:HG13 | 2.52 | 0.44 |
| 32:2a:173:U:H5" | 32:2a:197:A:O4' | 2.17 | 0.44 |
| 32:2a:551:U:H2' | 32:2a:552:U:C6 | 2.53 | 0.44 |
| 32:2a:858:G:O6 | 32:2a:869:G:H3' | 2.17 | 0.44 |
| 32:2a:1025:U:N3 | 32:2a:1036:G:N1 | 2.50 | 0.44 |
| 55:2x:28:C:H2' | 55:2x:29:G:C8 | 2.48 | 0.44 |
| 1:1A:234:C:H2' | 1:1A:235:U:H6 | 1.82 | 0.44 |
| 1:1A:1566:A:OP1 | 3:1D:211:ARG:NH1 | 2.49 | 0.44 |
| 1:1A:2590:A:H2' | 1:1A:2591:C:H6 | 1.82 | 0.44 |
| 1:1A:2887:U:H2' | 1:1A:2888:C:C6 | 2.52 | 0.44 |
| 19:1X:35:THR:HG22 | 19:1X:37:THR:H | 1.83 | 0.44 |
| 32:1a:40:C:H2' | 32:1a:41:G:C8 | 2.53 | 0.44 |
| 32:1a:93:G:H2' | 32:1a:96:U:O4' | 2.16 | 0.44 |
| 32:1a:186:C:H2' | 32:1a:187:C:C6 | 2.52 | 0.44 |
| 32:1a:286:G:N7 | 61:1a:2299:HOH:O | 2.36 | 0.44 |
| 32:1a:540:G:H2' | 32:1a:541:G:O4' | 2.17 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 33:1b:47:THR:O | 33:1b:51:LEU:HG | 2.18 | 0.44 |
| 46:1o:18:PHE:O | 46:1o:20:GLY:N | 2.50 | 0.44 |
| 46:1o:29:VAL:HB | 46:1o:81:LEU:HD21 | 2.00 | 0.44 |
| 1:2A:1007:C:P | 9:2N:37:LYS:HZ2 | 2.41 | 0.44 |
| 1:2A:2125:G:N1 | 1:2A:2172:U:OP1 | 2.41 | 0.44 |
| 1:2A:2506:U:O2' | 54:2w:76:A:H4' | 2.18 | 0.44 |
| 3:2D:3:VAL:HG21 | 3:2D:203:ASN:HB2 | 2.00 | 0.44 |
| 3:2D:77:ALA:HA | 3:2D:97:TYR:HA | 2.00 | 0.44 |
| 17:2V:48:GLY:HA2 | 17:2V:52:VAL:HG13 | 1.99 | 0.44 |
| 32:2a:377:G:OP1 | 47:2p:3:LYS:HD3 | 2.17 | 0.44 |
| 32:2a:863:U:O2' | 32:2a:865:A:N7 | 2.47 | 0.44 |
| 32:2a:1401:G:C2 | 32:2a:1402:4OC:H1' | 2.52 | 0.44 |
| 33:2b:189:ASP:OD1 | 33:2b:189:ASP:N | 2.44 | 0.44 |
| 43:2l:7:ILE:O | 43:2l:11:VAL:HG23 | 2.17 | 0.44 |
| 44:2m:68:GLY:HA2 | 44:2m:71:ARG:HB2 | 1.99 | 0.44 |
| 48:2q:9:VAL:HA | 48:2q:55:ASP:O | 2.18 | 0.44 |
| 1:1A:407:G:H2' | 1:1A:408:G:H8 | 1.83 | 0.44 |
| 1:1A:438:G:H2' | 1:1A:440:G:H8 | 1.83 | 0.44 |
| 1:1A:1069:A:H2 | 1:1A:1095:A:O2' | 2.01 | 0.44 |
| 1:1A:1166:C:H2' | 1:1A:1167:U:C6 | 2.53 | 0.44 |
| 1:1A:1275:A:H4' | 61:1A:7623:HOH:O | 2.17 | 0.44 |
| 1:1A:2171:A:HO2' | 1:1A:2172:U:H5" | 1.82 | 0.44 |
| 1:1A:2179:C:H2' | 1:1A:2180:U:C6 | 2.53 | 0.44 |
| 4:1E:143:ASN:HD22 | 4:1E:147:PRO:HD3 | 1.82 | 0.44 |
| 9:1N:36:GLY:HA2 | 9:1N:38:HIS:CE1 | 2.53 | 0.44 |
| 10:1O:64:ARG:HB2 | 10:1O:79:PHE:CD2 | 2.53 | 0.44 |
| 12:1Q:134:ARG:CZ | 21:1Z:122:ARG:HH21 | 2.31 | 0.44 |
| 13:1R:54:LEU:HD12 | 13:1R:54:LEU:HA | 1.83 | 0.44 |
| 16:1U:104:GLN:NE2 | 16:1U:105:VAL:HG23 | 2.33 | 0.44 |
| 28:16:18:ARG:HD2 | 28:16:42:TRP:CD1 | 2.53 | 0.44 |
| 32:1a:659:U:H2' | 32:1a:660:G:C8 | 2.53 | 0.44 |
| 32:1a:1027:C:H5 | 32:1a:1028:C:C4 | 2.36 | 0.44 |
| 32:1a:1048:G:OP1 | 45:1n:3:ARG:HB3 | 2.17 | 0.44 |
| 33:1b:96:ARG:HH11 | 33:1b:98:LEU:HD22 | 1.83 | 0.44 |
| 33:1b:155:LEU:HD12 | 33:1b:155:LEU:HA | 1.87 | 0.44 |
| 41:1j:38:ILE:HD11 | 41:1j:71:LEU:HD23 | 1.99 | 0.44 |
| 1:2A:35:G:H2' | 1:2A:36:G:O4' | 2.17 | 0.44 |
| 1:2A:271(R):G:OP1 | 23:21:76:ARG:NH1 | 2.51 | 0.44 |
| 1:2A:407:G:H2' | 1:2A:408:G:C8 | 2.52 | 0.44 |
| 1:2A:489:G:H2' | 1:2A:491:G:O4' | 2.18 | 0.44 |
| 1:2A:1017:G:N7 | 61:2A:5060:HOH:O | 2.46 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:2A:2364:C:OP1 | 22:20:55:ARG:NH1 | 2.47 | 0.44 |
| 7:2H:80:SER:OG | 7:2H:81:GLU:N | 2.51 | 0.44 |
| 21:2Z:91:LEU:HD12 | 21:2Z:91:LEU:HA | 1.85 | 0.44 |
| 32:2a:423:G:H3' | 32:2a:423:G:N3 | 2.33 | 0.44 |
| 32:2a:545:C:O2' | 32:2a:549:C:OP1 | 2.29 | 0.44 |
| 32:2a:659:U:OP1 | 46:2o:9:GLN:NE2 | 2.50 | 0.44 |
| 32:2a:734:G:H21 | 49:2r:75:ILE:HD11 | 1.81 | 0.44 |
| 39:2h:20:TYR:HA | 39:2h:65:TYR:CE1 | 2.52 | 0.44 |
| 55:2x:15:G:N2 | 55:2x:21:A:N3 | 2.66 | 0.44 |
| 1:1A:185:U:H2' | 1:1A:186:G:H8 | 1.83 | 0.44 |
| 1:1A:911:A:H2' | 12:1Q:9:TYR:OH | 2.18 | 0.44 |
| 1:1A:1065:U:N3 | 1:1A:1070:A:OP1 | 2.42 | 0.44 |
| 1:1A:1420:U:H6 | 1:1A:1420:U:H2' | 1.62 | 0.44 |
| 1:1A:1637:A:OP2 | 61:1A:7206:HOH:O | 2.21 | 0.44 |
| 1:1A:2330:G:H2' | 1:1A:2331:G:O4' | 2.18 | 0.44 |
| 32:1a:50:A:H1' | 32:1a:52:G:C8 | 2.52 | 0.44 |
| 32:1a:72:C:H2' | 32:1a:73:G:C8 | 2.53 | 0.44 |
| 32:1a:160:A:H1' | 32:1a:344:A:C8 | 2.53 | 0.44 |
| 32:1a:193:C:H2' | 32:1a:194:C:H6 | 1.83 | 0.44 |
| 32:1a:674:G:H2' | 32:1a:675:A:C8 | 2.53 | 0.44 |
| 35:1d:173:TRP:CD1 | 35:1d:174:LEU:HG | 2.53 | 0.44 |
| 54:1w:11:C:H42 | 54:1w:24:G:H1 | 1.66 | 0.44 |
| 54:1w:66:U:H2' | 54:1w:67:C:C6 | 2.53 | 0.44 |
| 1:2A:322:A:H5' | 1:2A:340:A:H1' | 1.99 | 0.44 |
| 1:2A:752:A:P | 29:27:3:ARG:HH22 | 2.41 | 0.44 |
| 1:2A:892:G:H3' | 1:2A:893:C:C5' | 2.48 | 0.44 |
| 1:2A:1012:U:O4 | 9:2N:28:THR:HG21 | 2.18 | 0.44 |
| 1:2A:1239:G:H2' | 1:2A:1240:U:O4' | 2.18 | 0.44 |
| 1:2A:2562:U:H4' | 10:2O:25:LEU:HD21 | 2.00 | 0.44 |
| 1:2A:2611:U:C4 | 27:25:3:LYS:HG2 | 2.53 | 0.44 |
| 1:2A:2820:A:OP1 | 13:2R:2:ARG:NH2 | 2.47 | 0.44 |
| 2:2B:41:U:H5 | 6:2G:70:VAL:N | 2.16 | 0.44 |
| 5:2F:178:PRO:HB2 | 5:2F:201:VAL:HG21 | 1.99 | 0.44 |
| 32:2a:355:C:H1' | 32:2a:388:G:H1' | 1.99 | 0.44 |
| 32:2a:643:C:H2' | 32:2a:644:G:C8 | 2.50 | 0.44 |
| 32:2a:973:G:H3' | 32:2a:974:A:H5" | 2.00 | 0.44 |
| 33:2b:16:HIS:HD2 | 33:2b:18:GLY:H | 1.65 | 0.44 |
| 49:2r:73:ALA:HB1 | 49:2r:78:LEU:HB2 | 2.00 | 0.44 |
| 1:1A:242:G:C8 | 30:18:5:LYS:HG2 | 2.53 | 0.43 |
| 1:1A:271(K):U:H4' | 1:1A:271(L):U:OP2 | 2.16 | 0.43 |
| 1:1A:1754:C:N3 | 1:1A:2716:U:O2' | 2.44 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1A:2441:C:OP2 | 1:1A:2586:C:O2' | 2.31 | 0.43 |
| 10:1O:4:PRO:O | 10:1O:5:GLN:HB2 | 2.18 | 0.43 |
| 11:1P:3:LEU:HD12 | 11:1P:3:LEU:HA | 1.90 | 0.43 |
| 11:1P:124:LYS:HA | 11:1P:144:GLU:HB3 | 1.98 | 0.43 |
| 12:1Q:25:ASP:OD1 | 12:1Q:25:ASP:N | 2.50 | 0.43 |
| 20:1Y:5:MET:HE2 | 20:1Y:5:MET:HB2 | 1.81 | 0.43 |
| 32:1a:165:C:H2' | 32:1a:166:G:C8 | 2.53 | 0.43 |
| 32:1a:266:G:H2' | 32:1a:266:G:N3 | 2.32 | 0.43 |
| 32:1a:324:G:N2 | 32:1a:327:A:OP2 | 2.51 | 0.43 |
| 32:1a:580:U:H2' | 32:1a:581:G:O4' | 2.18 | 0.43 |
| 32:1a:1068:G:H8 | 32:1a:1068:G:OP2 | 2.01 | 0.43 |
| 32:1a:1191:A:OP1 | 34:1c:4:LYS:NZ | 2.35 | 0.43 |
| 32:1a:1222:G:OP1 | 50:1s:77:THR:HG21 | 2.18 | 0.43 |
| 32:1a:1355:G:H2' | 32:1a:1356:G:C8 | 2.53 | 0.43 |
| 35:1d:3:ARG:NH1 | 35:1d:5:ILE:HG13 | 2.33 | 0.43 |
| 35:1d:144:ASP:OD1 | 35:1d:144:ASP:N | 2.51 | 0.43 |
| 1:2A:1028:A:H61 | 1:2A:1125:G:H2' | 1.81 | 0.43 |
| 1:2A:1427:A:H4' | 1:2A:1428:C:O5' | 2.18 | 0.43 |
| 1:2A:2127:G:H2' | 1:2A:2128:C:H6 | 1.82 | 0.43 |
| 1:2A:2547:U:H2' | 1:2A:2548:G:C8 | 2.53 | 0.43 |
| 1:2A:2853:C:H2' | 1:2A:2854:G:H8 | 1.82 | 0.43 |
| 2:2B:55:U:H1' | 6:2G:29:TRP:CD1 | 2.53 | 0.43 |
| 5:2F:57:VAL:HG13 | 5:2F:59:TYR:H | 1.83 | 0.43 |
| 8:2I:125:GLU:OE1 | 8:2I:143:SER:HB3 | 2.18 | 0.43 |
| 11:2P:52:GLU:HG3 | 30:28:57:ARG:HH22 | 1.82 | 0.43 |
| 13:2R:13:HIS:CE1 | 13:2R:16:HIS:HB2 | 2.53 | 0.43 |
| 32:2a:142:G:H2' | 32:2a:143:A:C8 | 2.53 | 0.43 |
| 32:2a:1238:A:C2 | 32:2a:1303:C:H4' | 2.53 | 0.43 |
| 32:2a:1500:A:H5" | 32:2a:1508:G:H5" | 1.99 | 0.43 |
| 36:2e:24:ARG:HD2 | 53:2v:24:A:OP2 | 2.18 | 0.43 |
| 38:2g:23:VAL:O | 38:2g:27:ILE:HG13 | 2.18 | 0.43 |
| 42:2k:31:THR:HG22 | 42:2k:42:TRP:HB2 | 1.99 | 0.43 |
| 54:2w:9:A:H8 | 54:2w:11:C:H41 | 1.65 | 0.43 |
| 1:1A:118:A:C8 | 1:1A:119:A:C8 | 3.05 | 0.43 |
| 1:1A:324:A:H2' | 1:1A:325:G:O4' | 2.18 | 0.43 |
| 1:1A:1448:G:H5" | 1:1A:1542:A:OP2 | 2.19 | 0.43 |
| 1:1A:1504:C:H2' | 1:1A:1505:C:C6 | 2.54 | 0.43 |
| 1:1A:1754:C:H5 | 15:1T:96:ARG:NH2 | 2.16 | 0.43 |
| 1:1A:1799:G:O2' | 3:1D:181:GLU:OE2 | 2.29 | 0.43 |
| 2:1B:74:U:H2' | 2:1B:75:G:O4' | 2.18 | 0.43 |
| 5:1F:106:ARG:H | 5:1F:106:ARG:HG2 | 1.56 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:1H:89:ILE:O | 7:1H:129:THR:OG1 | 2.34 | 0.43 |
| 11:1P:3:LEU:HD12 | 11:1P:6:LEU:HD12 | 2.00 | 0.43 |
| 32:1a:58:C:O2' | 32:1a:388:G:N7 | 2.37 | 0.43 |
| 32:1a:860:A:H3' | 32:1a:861:G:H8 | 1.83 | 0.43 |
| 1:2A:362:U:O2' | 1:2A:363:G:H5' | 2.18 | 0.43 |
| 1:2A:567:A:OP2 | 11:2P:29:LYS:NZ | 2.51 | 0.43 |
| 1:2A:625:G:O6 | 11:2P:107:LYS:NZ | 2.46 | 0.43 |
| 1:2A:660:G:H5' | 5:2F:99:TYR:CE1 | 2.53 | 0.43 |
| 1:2A:784:A:C6 | 3:2D:229:VAL:HG11 | 2.53 | 0.43 |
| 1:2A:1576:U:H2' | 1:2A:1577:C:C6 | 2.53 | 0.43 |
| 1:2A:1754:C:N3 | 1:2A:2716:U:O2' | 2.47 | 0.43 |
| 1:2A:2065:C:H4' | 1:2A:2251:OMG:HM22 | 2.00 | 0.43 |
| 1:2A:2251:OMG:OP2 | 1:2A:2251:OMG:H8 | 2.01 | 0.43 |
| 1:2A:2695:C:H2' | 1:2A:2696:U:C6 | 2.53 | 0.43 |
| 11:2P:70:GLN:O | 11:2P:73:GLY:N | 2.36 | 0.43 |
| 21:2Z:53:ILE:HG22 | 21:2Z:71:VAL:O | 2.18 | 0.43 |
| 32:2a:992:U:H6 | 32:2a:992:U:H5' | 1.83 | 0.43 |
| 32:2a:1356:G:H2' | 32:2a:1357:A:C8 | 2.53 | 0.43 |
| 34:2c:120:VAL:HG21 | 34:2c:137:ALA:HB2 | 2.00 | 0.43 |
| 37:2f:100:ASN:ND2 | 49:2r:23:LYS:HE2 | 2.33 | 0.43 |
| 45:2n:23:ARG:NH1 | 45:2n:30:ALA:HB2 | 2.34 | 0.43 |
| 51:2t:10:LEU:HD23 | 51:2t:12:ALA:HB2 | 2.00 | 0.43 |
| 54:2w:50:U:H2' | 54:2w:51:U:C6 | 2.53 | 0.43 |
| 1:1A:121:G:H4' | 1:1A:149:A:H5' | 2.00 | 0.43 |
| 1:1A:602:G:O2' | 1:1A:655:A:N6 | 2.51 | 0.43 |
| 1:1A:1155:A:OP1 | 16:1U:55:ARG:HD2 | 2.19 | 0.43 |
| 1:1A:1692:U:O2' | 1:1A:1693:U:H2' | 2.18 | 0.43 |
| 1:1A:2120:G:C2' | 1:1A:2121:G:H5' | 2.48 | 0.43 |
| 1:1A:2788:C:O2' | 1:1A:2809:A:N3 | 2.41 | 0.43 |
| 5:1F:185:ASP:HA | 5:1F:188:ARG:HD3 | 2.00 | 0.43 |
| 7:1H:13:LYS:HA | 7:1H:14:GLY:HA2 | 1.65 | 0.43 |
| 10:1O:115:VAL:HG13 | 10:1O:121:VAL:HG21 | 1.99 | 0.43 |
| 11:1P:50:ARG:HD3 | 30:18:7:HIS:HD2 | 1.79 | 0.43 |
| 26:14:63:TYR:N | 26:14:63:TYR:CD1 | 2.85 | 0.43 |
| 32:1a:92:C:H2' | 32:1a:93:G:H8 | 1.82 | 0.43 |
| 32:1a:657:G:H2' | 32:1a:658:G:H8 | 1.84 | 0.43 |
| 33:1b:24:TRP:HZ3 | 33:1b:29:ALA:HB2 | 1.82 | 0.43 |
| 1:2A:208:C:H2' | 1:2A:209:C:H6 | 1.83 | 0.43 |
| 1:2A:1364:G:P | 23:21:3:LYS:HG3 | 2.58 | 0.43 |
| 1:2A:1598:C:H2' | 1:2A:1599:C:C6 | 2.53 | 0.43 |
| 1:2A:1651:G:OP1 | 13:2R:37:THR:OG1 | 2.36 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:2A:2086:U:H2' | 1:2A:2087:G:C8 | 2.53 | 0.43 |
| 1:2A:2108:C:H42 | 1:2A:2181:G:H1 | 1.64 | 0.43 |
| 1:2A:2441:C:OP2 | 1:2A:2586:C:O2' | 2.32 | 0.43 |
| 1:2A:2526:G:H5' | 1:2A:2742:C:O2' | 2.18 | 0.43 |
| 2:2B:24:G:H4' | 2:2B:25:A:C8 | 2.54 | 0.43 |
| 3:2D:9:TYR:CD1 | 3:2D:10:THR:HG23 | 2.53 | 0.43 |
| 3:2D:183:ARG:HG3 | 3:2D:270:ILE:HG12 | 2.01 | 0.43 |
| 6:2G:49:ASP:OD1 | 6:2G:49:ASP:N | 2.48 | 0.43 |
| 8:2I:79:ILE:O | 8:2I:144:VAL:HA | 2.18 | 0.43 |
| 12:2Q:38:GLU:OE2 | 12:2Q:128:LYS:N | 2.40 | 0.43 |
| 20:2Y:6:HIS:ND1 | 20:2Y:7:VAL:HG23 | 2.33 | 0.43 |
| 26:24:67:TYR:HD2 | 50:2s:9:VAL:HB | 1.83 | 0.43 |
| 28:26:8:LYS:HD3 | 30:28:34:TRP:CD2 | 2.54 | 0.43 |
| 32:2a:41:G:H2' | 32:2a:42:G:H8 | 1.83 | 0.43 |
| 32:2a:769:G:H4' | 32:2a:1513:A:H4' | 2.00 | 0.43 |
| 32:2a:865:A:H2 | 32:2a:918:A:H4' | 1.83 | 0.43 |
| 32:2a:872:A:O2' | 32:2a:873:A:H3' | 2.18 | 0.43 |
| 44:2m:114:ARG:H | 44:2m:114:ARG:HG2 | 1.62 | 0.43 |
| 48:2q:54:GLY:O | 48:2q:81:ARG:N | 2.32 | 0.43 |
| 1:1A:182:A:N3 | 1:1A:433:C:O2' | 2.44 | 0.43 |
| 1:1A:1652:A:OP1 | 13:1R:8:ARG:NH1 | 2.51 | 0.43 |
| 1:1A:1796:U:H2' | 1:1A:1797:C:H6 | 1.83 | 0.43 |
| 1:1A:1919:A:O2' | 32:1a:1517:G:N3 | 2.40 | 0.43 |
| 1:1A:2206:G:OP2 | 1:1A:2206:G:H4' | 2.17 | 0.43 |
| 1:1A:2691:C:O3' | 1:1A:2871:C:H4' | 2.18 | 0.43 |
| 1:1A:2820:A:OP2 | 13:1R:2:ARG:NH2 | 2.51 | 0.43 |
| 3:1D:218:ARG:HB3 | 3:1D:219:PRO:HD2 | 1.99 | 0.43 |
| 5:1F:129:PHE:HB3 | 5:1F:132:VAL:HG13 | 2.00 | 0.43 |
| 6:1G:41:GLN:HG2 | 6:1G:154:GLY:O | 2.18 | 0.43 |
| 24:12:1:MET:N | 24:12:52:ASP:OD2 | 2.40 | 0.43 |
| 30:18:63:PRO:HG2 | 30:18:64:TYR:CE2 | 2.53 | 0.43 |
| 32:1a:922:G:H4' | 36:1e:20:GLN:HA | 1.99 | 0.43 |
| 32:1a:1172:C:H2' | 32:1a:1173:G:H8 | 1.83 | 0.43 |
| 39:1h:101:PRO:HG3 | 39:1h:133:LEU:HD11 | 2.01 | 0.43 |
| 41:1j:57:LYS:HE2 | 41:1j:60:ARG:NH2 | 2.34 | 0.43 |
| 54:1y:5:G:H1' | 54:1y:69:G:N2 | 2.33 | 0.43 |
| 1:2A:284:U:H2' | 1:2A:285:C:C6 | 2.54 | 0.43 |
| 1:2A:822:U:OP2 | 61:2A:5949:HOH:O | 2.21 | 0.43 |
| 1:2A:1660:C:H2' | 1:2A:1661:G:H8 | 1.83 | 0.43 |
| 1:2A:1794:U:H2' | 1:2A:1795:C:H6 | 1.83 | 0.43 |
| 1:2A:2287:A:H2 | 1:2A:2346:A:H62 | 1.64 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 61:2A:4490:HOH:O | 3:2D:237:GLU:OE2 | 2.20 | 0.43 |
| 6:2G:36:LYS:HD3 | 6:2G:95:ARG:NH1 | 2.33 | 0.43 |
| 8:2I:62:LYS:O | 8:2I:66:GLU:HG2 | 2.18 | 0.43 |
| 19:2X:57:LEU:HD11 | 19:2X:78:LYS:HE2 | 1.99 | 0.43 |
| 20:2Y:13:VAL:HG12 | 20:2Y:74:PRO:HA | 2.00 | 0.43 |
| 24:22:10:LEU:HD21 | 24:22:59:ARG:HG2 | 1.98 | 0.43 |
| 30:28:23:VAL:HG11 | 30:28:47:LYS:HD3 | 2.00 | 0.43 |
| 32:2a:41:G:H2' | 32:2a:42:G:C8 | 2.53 | 0.43 |
| 32:2a:1004:A:N1 | 32:2a:1037:C:C2 | 2.86 | 0.43 |
| 32:2a:1004:A:C6 | 32:2a:1037:C:H1' | 2.53 | 0.43 |
| 32:2a:1096:C:O2 | 32:2a:1170:A:O2' | 2.33 | 0.43 |
| 32:2a:1251:A:H5" | 40:2i:12:GLU:OE1 | 2.19 | 0.43 |
| 32:2a:1492:A:H2' | 32:2a:1493:A:C8 | 2.53 | 0.43 |
| 32:2a:1517:G:H2' | 32:2a:1518:MA6:H8 | 1.99 | 0.43 |
| 35:2d:187:ARG:NH2 | 35:2d:193:ASP:OD2 | 2.51 | 0.43 |
| 38:2g:77:SER:HA | 38:2g:85:TYR:O | 2.19 | 0.43 |
| 39:2h:39:LEU:HB3 | 39:2h:45:ILE:HG12 | 1.99 | 0.43 |
| 1:1A:26:G:H1' | 1:1A:515:A:H61 | 1.84 | 0.43 |
| 1:1A:125:G:H1' | 29:17:48:LYS:HD3 | 2.01 | 0.43 |
| 1:1A:747:U:H1' | 18:1W:92:ARG:NH1 | 2.32 | 0.43 |
| 1:1A:1266:G:O5' | 18:1W:15:ARG:NH2 | 2.51 | 0.43 |
| 7:1H:90:LYS:HD2 | 7:1H:159:GLU:HG2 | 1.99 | 0.43 |
| 15:1T:24:PRO:HA | 15:1T:49:VAL:HG23 | 2.00 | 0.43 |
| 32:1a:826:C:H2' | 32:1a:827:U:C6 | 2.54 | 0.43 |
| 32:1a:1206:G:O4' | 34:1c:194:GLY:HA2 | 2.19 | 0.43 |
| 32:1a:1219:U:OP1 | 45:1n:19:ARG:NH1 | 2.40 | 0.43 |
| 38:1g:26:PHE:CE2 | 38:1g:30:ILE:HD11 | 2.53 | 0.43 |
| 46:1o:74:ASP:HB3 | 46:1o:77:ARG:HB2 | 2.00 | 0.43 |
| 52:1u:6:ARG:O | 52:1u:12:LYS:HE3 | 2.18 | 0.43 |
| 1:2A:210:C:H2' | 1:2A:211:A:C8 | 2.53 | 0.43 |
| 1:2A:565:C:H2' | 1:2A:566:U:O4' | 2.19 | 0.43 |
| 1:2A:589:C:H2' | 1:2A:590:A:C8 | 2.53 | 0.43 |
| 1:2A:1537:G:H2' | 1:2A:1538:G:C8 | 2.49 | 0.43 |
| 1:2A:1814:G:H2' | 1:2A:1815:A:C8 | 2.54 | 0.43 |
| 1:2A:2322:A:H2' | 1:2A:2323:G:O4' | 2.18 | 0.43 |
| 2:2B:31:C:H4' | 6:2G:29:TRP:CZ2 | 2.54 | 0.43 |
| 4:2E:59:VAL:HG21 | 4:2E:74:PRO:HB3 | 2.00 | 0.43 |
| 6:2G:135:LEU:O | 6:2G:155:MET:N | 2.40 | 0.43 |
| 13:2R:66:VAL:HG12 | 13:2R:70:LEU:HD12 | 1.99 | 0.43 |
| 15:2T:33:LYS:HB3 | 15:2T:82:LEU:HD22 | 2.00 | 0.43 |
| 15:2T:88:ILE:HG21 | 15:2T:91:ARG:NE | 2.32 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 28:26:13:CYS:SG | 28:26:47:THR:HG21 | 2.58 | 0.43 |
| 32:2a:65:U:H1' | 32:2a:66:G:OP2 | 2.18 | 0.43 |
| 32:2a:309:G:O2' | 32:2a:607:A:N1 | 2.49 | 0.43 |
| 41:2j:63:PHE:HE2 | 45:2n:45:ARG:HA | 1.83 | 0.43 |
| 44:2m:16:ASP:O | 44:2m:20:THR:HG23 | 2.18 | 0.43 |
| 44:2m:23:TYR:CZ | 44:2m:71:ARG:HG3 | 2.54 | 0.43 |
| 1:1A:53:A:H2' | 1:1A:54:G:O4' | 2.19 | 0.43 |
| 1:1A:388:G:O2' | 1:1A:389:G:N7 | 2.47 | 0.43 |
| 1:1A:1111:A:H4' | 1:1A:1112:G:OP1 | 2.19 | 0.43 |
| 1:1A:1441:G:O6 | 61:1A:6075:HOH:O | 2.21 | 0.43 |
| 1:1A:2049:G:N7 | 61:1A:6385:HOH:O | 2.37 | 0.43 |
| 1:1A:2359:C:H2' | 1:1A:2360:A:O4' | 2.19 | 0.43 |
| 1:1A:2639:A:O2' | 9:1N:97:ARG:NH2 | 2.52 | 0.43 |
| 32:1a:110:C:H2' | 32:1a:111:G:O4' | 2.18 | 0.43 |
| 32:1a:600:C:H2' | 32:1a:601:C:C6 | 2.54 | 0.43 |
| 37:1f:69:GLU:H | 37:1f:69:GLU:CD | 2.26 | 0.43 |
| 47:1p:19:ILE:N | 47:1p:37:GLY:O | 2.51 | 0.43 |
| 1:2A:752:A:H4' | 1:2A:753:C:H5' | 1.99 | 0.43 |
| 1:2A:884:C:H3' | 1:2A:885:C:H6 | 1.84 | 0.43 |
| 1:2A:1630:G:H2' | 1:2A:1631:C:C6 | 2.53 | 0.43 |
| 1:2A:2563:U:H4' | 10:2O:28:SER:HA | 2.00 | 0.43 |
| 10:2O:29:ASN:N | 10:2O:29:ASN:OD1 | 2.51 | 0.43 |
| 10:2O:49:ARG:NH1 | 32:2a:1422:G:O3' | 2.51 | 0.43 |
| 13:2R:72:ASP:HB3 | 13:2R:75:LEU:HB3 | 2.00 | 0.43 |
| 16:2U:6:THR:HG21 | 16:2U:10:ARG:HH21 | 1.84 | 0.43 |
| 32:2a:4:U:O2 | 39:2h:105:ARG:NH2 | 2.51 | 0.43 |
| 32:2a:273:A:N7 | 61:2a:3622:HOH:O | 2.37 | 0.43 |
| 32:2a:1401:G:OP1 | 53:2v:18:G:O2' | 2.33 | 0.43 |
| 33:2b:97:TRP:CH2 | 33:2b:173:ALA:HA | 2.53 | 0.43 |
| 38:2g:69:VAL:HG11 | 38:2g:134:ALA:HB1 | 2.01 | 0.43 |
| 40:2i:21:PRO:HA | 40:2i:59:PHE:HA | 2.00 | 0.43 |
| 47:2p:19:ILE:N | 47:2p:37:GLY:O | 2.51 | 0.43 |
| 1:1A:185:U:H2' | 1:1A:186:G:C8 | 2.54 | 0.43 |
| 1:1A:1470:G:N2 | 1:1A:1520:G:OP2 | 2.34 | 0.43 |
| 1:1A:1952:A:C6 | 1:1A:1953:A:N1 | 2.86 | 0.43 |
| 1:1A:2168:G:C6 | 1:1A:2171:A:C8 | 3.07 | 0.43 |
| 1:1A:2188:C:H2' | 1:1A:2189:U:O4' | 2.18 | 0.43 |
| 1:1A:2718:G:O2' | 1:1A:2847:U:OP1 | 2.32 | 0.43 |
| 4:1E:28:ALA:HB3 | 4:1E:93:VAL:HG12 | 2.01 | 0.43 |
| 7:1H:97:ARG:NE | 7:1H:104:GLU:OE1 | 2.51 | 0.43 |
| 28:16:12:GLU:HA | 28:16:19:ARG:HA | 2.01 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 32:1a:19:C:H4' | 32:1a:864:A:O4' | 2.18 | 0.43 |
| 32:1a:21:G:H2' | 32:1a:22:G:C8 | 2.54 | 0.43 |
| 32:1a:44:G:O6 | 61:1a:2377:HOH:O | 2.21 | 0.43 |
| 32:1a:269:C:H2' | 32:1a:270:A:C8 | 2.54 | 0.43 |
| 32:1a:277:C:H5" | 48:1q:68:ARG:NH2 | 2.33 | 0.43 |
| 32:1a:567:G:O6 | 43:1l:5:PRO:HD3 | 2.18 | 0.43 |
| 32:1a:743:U:H2' | 32:1a:744:C:C6 | 2.54 | 0.43 |
| 32:1a:877:C:OP1 | 39:1h:88:LYS:NZ | 2.35 | 0.43 |
| 32:1a:881:G:H2' | 32:1a:882:C:O4' | 2.19 | 0.43 |
| 32:1a:1006:C:N4 | 32:1a:1023:G:H1 | 2.11 | 0.43 |
| 32:1a:1009:G:O6 | 32:1a:1020:U:C2 | 2.72 | 0.43 |
| 32:1a:1244:C:H2' | 32:1a:1245:A:C8 | 2.53 | 0.43 |
| 32:1a:1367:C:H5' | 41:1j:60:ARG:NH1 | 2.33 | 0.43 |
| 35:1d:155:LEU:HD23 | 35:1d:155:LEU:HA | 1.82 | 0.43 |
| 44:1m:123:ALA:HB2 | 54:1w:39:PSU:H1' | 1.99 | 0.43 |
| 54:1y:15:G:H22 | 54:1y:48:C:N4 | 2.15 | 0.43 |
| 1:2A:469:G:N7 | 29:27:37:LYS:NZ | 2.63 | 0.43 |
| 1:2A:684:G:N7 | 61:2A:3918:HOH:O | 2.37 | 0.43 |
| 1:2A:855:G:H2' | 1:2A:856:C:C6 | 2.53 | 0.43 |
| 1:2A:863:A:H2' | 1:2A:864:G:C8 | 2.54 | 0.43 |
| 1:2A:1022:G:N2 | 1:2A:1023:U:O4 | 2.45 | 0.43 |
| 1:2A:1147:C:H2' | 1:2A:1148:A:H8 | 1.84 | 0.43 |
| 1:2A:1423:G:H2' | 1:2A:1424:G:H8 | 1.83 | 0.43 |
| 1:2A:2180:U:H2' | 1:2A:2181:G:O4' | 2.19 | 0.43 |
| 1:2A:2846:G:H2' | 1:2A:2847:U:O4' | 2.18 | 0.43 |
| 32:2a:160:A:H1' | 32:2a:344:A:N7 | 2.33 | 0.43 |
| 32:2a:1081:G:H5' | 36:2e:18:ARG:HB3 | 2.00 | 0.43 |
| 32:2a:1210:C:H3' | 32:2a:1211:U:H5" | 2.00 | 0.43 |
| 40:2i:77:ILE:O | 40:2i:81:ILE:HG22 | 2.19 | 0.43 |
| 42:2k:15:ALA:HA | 42:2k:76:GLY:O | 2.19 | 0.43 |
| 46:2o:82:ILE:HB | 46:2o:87:ILE:HB | 2.00 | 0.43 |
| 49:2r:36:ASN:O | 49:2r:40:LEU:HG | 2.19 | 0.43 |
| 54:2w:68:C:H2' | 54:2w:69:G:C8 | 2.54 | 0.43 |
| 1:1A:35:G:H2' | 1:1A:36:G:O4' | 2.19 | 0.43 |
| 1:1A:1638:C:H5" | 1:1A:2710:C:O2' | 2.18 | 0.43 |
| 9:1N:4:TYR:CE2 | 16:1U:100:VAL:HG11 | 2.53 | 0.43 |
| 21:1Z:136:PHE:O | 21:1Z:137:ILE:HG13 | 2.18 | 0.43 |
| 32:1a:953:G:H2' | 32:1a:954:G:O4' | 2.18 | 0.43 |
| 32:1a:1118:C:H2' | 32:1a:1119:C:H6 | 1.84 | 0.43 |
| 32:1a:1345:U:H4' | 32:1a:1346:A:H5' | 2.00 | 0.43 |
| 32:1a:1464:G:H2' | 32:1a:1465:C:C6 | 2.54 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 33:1b:27:LYS:HB2 | 33:1b:194:PRO:HD2 | 2.00 | 0.43 |
| 44:1m:108:ARG:HD3 | 44:1m:108:ARG:HA | 1.78 | 0.43 |
| 1:2A:458:G:C8 | 29:27:37:LYS:HG2 | 2.54 | 0.43 |
| 1:2A:848:G:O6 | 1:2A:928:G:H2' | 2.18 | 0.43 |
| 1:2A:1131:G:O6 | 1:2A:2040:C:H1' | 2.18 | 0.43 |
| 1:2A:1913:A:H4' | 1:2A:1914:C:O5' | 2.18 | 0.43 |
| 1:2A:2841:C:H2' | 1:2A:2842:G:C8 | 2.53 | 0.43 |
| 2:2B:68:C:H2' | 2:2B:69:G:H8 | 1.82 | 0.43 |
| 18:2W:46:PHE:O | 18:2W:50:VAL:HG23 | 2.19 | 0.43 |
| 19:2X:12:VAL:HG22 | 19:2X:29:TRP:CE2 | 2.53 | 0.43 |
| 23:21:89:GLU:O | 23:21:93:GLU:HG2 | 2.18 | 0.43 |
| 32:2a:229:U:O2' | 47:2p:23:ASP:OD2 | 2.33 | 0.43 |
| 32:2a:338:A:H2 | 32:2a:351:G:H22 | 1.66 | 0.43 |
| 32:2a:741:G:H2' | 32:2a:742:G:O4' | 2.18 | 0.43 |
| 38:2g:80:VAL:HB | 38:2g:85:TYR:HE2 | 1.84 | 0.43 |
| 44:2m:123:ALA:HB2 | 54:2w:39:PSU:H1' | 2.01 | 0.43 |
| 48:2q:53:LEU:HB3 | 48:2q:82:MET:SD | 2.58 | 0.43 |
| 1:1A:493:G:HO2' | 18:1W:8:ARG:H | 1.67 | 0.43 |
| 1:1A:1059:G:H2' | 1:1A:1060:U:C5 | 2.54 | 0.43 |
| 1:1A:1783:A:C5' | 1:1A:2608:G:H4' | 2.49 | 0.43 |
| 1:1A:2001:A:H2' | 1:1A:2002:G:C8 | 2.54 | 0.43 |
| 1:1A:2011:U:OP1 | 18:1W:42:ARG:NH1 | 2.51 | 0.43 |
| 1:1A:2135:A:H2 | 1:1A:2136:C:C2 | 2.37 | 0.43 |
| 1:1A:2156:G:H2' | 1:1A:2157:G:C2 | 2.54 | 0.43 |
| 1:1A:2327:A:H2' | 1:1A:2328:A:C8 | 2.54 | 0.43 |
| 2:1B:92:C:H5" | 21:1Z:79:ARG:NH1 | 2.33 | 0.43 |
| 5:1F:53:THR:HG22 | 5:1F:55:GLY:H | 1.83 | 0.43 |
| 11:1P:59:LEU:HD21 | 30:18:10:ALA:HA | 2.01 | 0.43 |
| 32:1a:408:A:H2' | 32:1a:409:G:O4' | 2.18 | 0.43 |
| 32:1a:815:A:N7 | 32:1a:1509:C:O2' | 2.50 | 0.43 |
| 32:1a:1025:U:O2 | 32:1a:1036:G:O6 | 2.37 | 0.43 |
| 32:1a:1144:G:H21 | 32:1a:1146:A:H62 | 1.67 | 0.43 |
| 44:1m:82:MET:O | 44:1m:93:ARG:NH2 | 2.51 | 0.43 |
| 1:2A:729:G:C8 | 3:2D:208:LYS:HD2 | 2.54 | 0.43 |
| 1:2A:744:G:H2' | 1:2A:745:G:O4' | 2.18 | 0.43 |
| 1:2A:1504:C:H2' | 1:2A:1505:C:H6 | 1.83 | 0.43 |
| 1:2A:1686:C:H2' | 1:2A:1687:G:O4' | 2.19 | 0.43 |
| 1:2A:2156:G:H2' | 1:2A:2157:G:C2 | 2.54 | 0.43 |
| 1:2A:2394:C:N3 | 54:2y:76:A:O2' | 2.41 | 0.43 |
| 1:2A:2840:C:H2' | 1:2A:2841:C:C6 | 2.54 | 0.43 |
| 2:2B:11:C:H3' | 2:2B:12:C:C6 | 2.53 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:2B:66:A:H61 | 2:2B:108:U:H2' | 1.84 | 0.43 |
| 6:2G:3:LEU:HD12 | 6:2G:8:LYS:NZ | 2.34 | 0.43 |
| 17:2V:98:GLU:OE2 | 17:2V:100:ARG:NH1 | 2.52 | 0.43 |
| 21:2Z:50:GLN:OE1 | 21:2Z:50:GLN:N | 2.51 | 0.43 |
| 32:2a:45:U:OP1 | 32:2a:307:C:O2' | 2.36 | 0.43 |
| 32:2a:757:U:H2' | 32:2a:758:G:O4' | 2.18 | 0.43 |
| 32:2a:781:A:N6 | 61:2a:3307:HOH:O | 2.45 | 0.43 |
| 32:2a:1032:G:H2' | 32:2a:1033:G:C8 | 2.54 | 0.43 |
| 32:2a:1100:C:H2' | 32:2a:1102:A:O5' | 2.19 | 0.43 |
| 32:2a:1318:A:H4' | 50:2s:10:PHE:CD2 | 2.53 | 0.43 |
| 32:2a:1380:U:C4 | 38:2g:3:ARG:HG2 | 2.54 | 0.43 |
| 36:2e:6:PHE:HB3 | 36:2e:34:VAL:HG22 | 2.00 | 0.43 |
| 36:2e:110:LEU:HB3 | 36:2e:115:VAL:HB | 2.01 | 0.43 |
| 46:2o:82:ILE:HD12 | 46:2o:88:ARG:HB2 | 2.00 | 0.43 |
| 1:1A:234:C:H2' | 1:1A:235:U:C6 | 2.54 | 0.43 |
| 1:1A:1010:A:N3 | 1:1A:1153:C:H1' | 2.33 | 0.43 |
| 1:1A:1054:A:N6 | 1:1A:1105:U:N3 | 2.49 | 0.43 |
| 1:1A:1058:G:N1 | 1:1A:1080:C:N4 | 2.34 | 0.43 |
| 1:1A:1409:C:H2' | 1:1A:1410:G:C8 | 2.54 | 0.43 |
| 1:1A:1418:G:O5' | 1:1A:1418:G:H8 | 2.02 | 0.43 |
| 1:1A:1665:A:H2' | 1:1A:1666:G:O4' | 2.19 | 0.43 |
| 20:1Y:15:VAL:HG21 | 20:1Y:42:VAL:HG11 | 2.00 | 0.43 |
| 32:1a:171:A:H2' | 32:1a:172:A:C8 | 2.54 | 0.43 |
| 32:1a:172:A:N6 | 32:1a:174:C:O2 | 2.52 | 0.43 |
| 32:1a:250:A:H4' | 32:1a:251:G:O5' | 2.18 | 0.43 |
| 32:1a:374:A:C6 | 32:1a:375:U:C4 | 3.07 | 0.43 |
| 32:1a:1229:A:O2' | 55:1x:30:G:OP1 | 2.36 | 0.43 |
| 32:1a:1328:C:H2' | 32:1a:1329:A:O4' | 2.18 | 0.43 |
| 34:1c:6:HIS:CD2 | 34:1c:8:ILE:H | 2.27 | 0.43 |
| 36:1e:69:VAL:O | 36:1e:71:LEU:HD22 | 2.19 | 0.43 |
| 47:1p:58:TYR:O | 47:1p:62:VAL:HG23 | 2.18 | 0.43 |
| 54:1w:37:MIA:H162 | 54:1w:37:MIA:H121 | 1.70 | 0.43 |
| 54:1w:63:G:H2' | 54:1w:64:A:C8 | 2.54 | 0.43 |
| 1:2A:898:C:H2' | 1:2A:899:A:H5' | 2.01 | 0.43 |
| 1:2A:1568:G:H5" | 3:2D:61:LEU:HD13 | 2.00 | 0.43 |
| 1:2A:2474:C:H5" | 1:2A:2475:C:OP2 | 2.19 | 0.43 |
| 1:2A:2689:U:H4' | 1:2A:2690:C:O5' | 2.19 | 0.43 |
| 7:2H:122:THR:O | 7:2H:134:SER:OG | 2.33 | 0.43 |
| 10:2O:64:ARG:HG2 | 10:2O:83:ALA:HB3 | 2.01 | 0.43 |
| 32:2a:46:G:H2' | 32:2a:366:C:C5 | 2.54 | 0.43 |
| 32:2a:892:A:O2' | 32:2a:1415:G:H4' | 2.19 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 32:2a:922:G:N3 | 32:2a:1398:A:H2 | 2.17 | 0.43 |
| 32:2a:989:C:H2' | 32:2a:990:C:C6 | 2.54 | 0.43 |
| 32:2a:1097:C:H1' | 32:2a:1170:A:H1' | 2.01 | 0.43 |
| 32:2a:1320:C:H2' | 32:2a:1321:C:O4' | 2.19 | 0.43 |
| 33:2b:16:HIS:CD2 | 33:2b:18:GLY:H | 2.37 | 0.43 |
| 36:2e:33:VAL:HA | 36:2e:42:GLY:O | 2.19 | 0.43 |
| 39:2h:12:ARG:HD3 | 39:2h:26:VAL:HG12 | 2.00 | 0.43 |
| 40:2i:24:GLY:HA2 | 40:2i:59:PHE:O | 2.19 | 0.43 |
| 45:2n:29:ARG:HD3 | 45:2n:40:CYS:SG | 2.58 | 0.43 |
| 1:1A:143:G:H4' | 19:1X:35:THR:HG21 | 2.00 | 0.42 |
| 1:1A:957:A:H4' | 12:1Q:74:TYR:OH | 2.19 | 0.42 |
| 1:1A:1430:C:H2' | 1:1A:1431:U:C6 | 2.53 | 0.42 |
| 1:1A:2611:U:H5' | 1:1A:2611:U:H6 | 1.84 | 0.42 |
| 1:1A:2801(A):A:H5" | 1:1A:2802:G:C8 | 2.54 | 0.42 |
| 30:18:62:LEU:HB3 | 30:18:65:GLU:HG2 | 2.01 | 0.42 |
| 32:1a:562:C:H1' | 43:1l:15:ARG:HB3 | 2.01 | 0.42 |
| 32:1a:1288:A:N3 | 32:1a:1352:C:O2' | 2.48 | 0.42 |
| 32:1a:1347:G:N2 | 32:1a:1373:G:H2' | 2.34 | 0.42 |
| 1:2A:139:G:H2' | 1:2A:140:G:N7 | 2.34 | 0.42 |
| 1:2A:877:U:O2' | 1:2A:900:A:N6 | 2.52 | 0.42 |
| 1:2A:923:C:H2' | 1:2A:924:C:H6 | 1.84 | 0.42 |
| 1:2A:1263:U:C4 | 1:2A:1264:G:C6 | 3.06 | 0.42 |
| 1:2A:1354:A:O3' | 3:2D:38:LYS:HE3 | 2.19 | 0.42 |
| 1:2A:1518:U:H2' | 1:2A:1519:G:O4' | 2.18 | 0.42 |
| 2:2B:19:G:H2' | 2:2B:20:C:O4' | 2.19 | 0.42 |
| 2:2B:42:C:O2' | 6:2G:66:GLN:HG2 | 2.19 | 0.42 |
| 3:2D:70:TRP:CE2 | 3:2D:150:LYS:HG3 | 2.54 | 0.42 |
| 7:2H:3:ARG:NH1 | 7:2H:5:GLY:H | 2.17 | 0.42 |
| 7:2H:43:VAL:HG13 | 7:2H:52:VAL:HG22 | 2.00 | 0.42 |
| 19:2X:5:TYR:CZ | 24:22:30:ARG:HB2 | 2.53 | 0.42 |
| 32:2a:932:C:H4' | 38:2g:4:ARG:CZ | 2.49 | 0.42 |
| 32:2a:1352:C:H2' | 32:2a:1353:G:C8 | 2.54 | 0.42 |
| 33:2b:31:TYR:CE2 | 33:2b:200:ILE:HG21 | 2.53 | 0.42 |
| 34:2c:123:GLN:HA | 34:2c:126:ARG:HD2 | 2.01 | 0.42 |
| 35:2d:112:VAL:HG22 | 35:2d:116:GLN:OE1 | 2.19 | 0.42 |
| 36:2e:8:GLU:HG2 | 36:2e:34:VAL:HG23 | 2.01 | 0.42 |
| 42:2k:109:VAL:CG2 | 49:2r:84:LYS:HB3 | 2.49 | 0.42 |
| 51:2t:13:LEU:O | 51:2t:17:ARG:HG3 | 2.19 | 0.42 |
| 1:1A:570:G:H2' | 1:1A:2030:A:C5 | 2.54 | 0.42 |
| 1:1A:751:A:H5' | 18:1W:90:ARG:HA | 2.01 | 0.42 |
| 1:1A:2314:C:H2' | 1:1A:2315:G:C8 | 2.54 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1A:2478:A:O2' | 1:1A:2536:G:N2 | 2.52 | 0.42 |
| 1:1A:2484:G:H1' | 12:1Q:124:LYS:HD2 | 2.00 | 0.42 |
| 13:1R:72:ASP:HB3 | 13:1R:75:LEU:HB3 | 2.01 | 0.42 |
| 14:1S:34:HIS:HD1 | 14:1S:53:SER:HG | 1.64 | 0.42 |
| 28:16:11:LEU:HD23 | 28:16:11:LEU:HA | 1.91 | 0.42 |
| 32:1a:62:U:OP1 | 32:1a:385:C:O2' | 2.31 | 0.42 |
| 32:1a:1111:A:N1 | 34:1c:177:THR:OG1 | 2.38 | 0.42 |
| 32:1a:1244:C:OP1 | 52:1u:9:ARG:HB2 | 2.19 | 0.42 |
| 37:1f:76:ALA:O | 37:1f:80:ARG:HG3 | 2.19 | 0.42 |
| 38:1g:78:ARG:HD2 | 38:1g:156:TRP:CE3 | 2.53 | 0.42 |
| 42:1k:48:ILE:O | 42:1k:50:TYR:N | 2.48 | 0.42 |
| 44:1m:96:LEU:C | 44:1m:110:ARG:HG2 | 2.44 | 0.42 |
| 1:2A:588:U:H2' | 1:2A:589:C:C6 | 2.54 | 0.42 |
| 1:2A:2389:G:H5" | 1:2A:2390:U:O4' | 2.19 | 0.42 |
| 2:2B:55:U:O3' | 6:2G:27:ASN:ND2 | 2.51 | 0.42 |
| 5:2F:32:LEU:HD13 | 5:2F:112:MET:HE1 | 2.00 | 0.42 |
| 10:2O:101:PRO:HD3 | 15:2T:68:TYR:HB2 | 2.00 | 0.42 |
| 12:2Q:20:ALA:HB2 | 21:2Z:79:ARG:HG2 | 2.00 | 0.42 |
| 12:2Q:57:HIS:NE2 | 12:2Q:116:GLU:HB3 | 2.34 | 0.42 |
| 21:2Z:30:ASN:HA | 21:2Z:89:PHE:HE1 | 1.83 | 0.42 |
| 26:24:64:GLY:C | 26:24:66:SER:N | 2.77 | 0.42 |
| 33:2b:112:VAL:HG12 | 33:2b:149:LEU:HD22 | 2.02 | 0.42 |
| 1:1A:2224:G:H4' | 1:1A:2226:C:C2 | 2.55 | 0.42 |
| 1:1A:2232:U:P | 23:11:40:ARG:HH12 | 2.43 | 0.42 |
| 7:1H:56:SER:OG | 7:1H:57:ASP:N | 2.52 | 0.42 |
| 13:1R:67:LEU:HD13 | 13:1R:76:VAL:HG21 | 2.00 | 0.42 |
| 15:1T:94:ALA:HB1 | 15:1T:99:LEU:HD21 | 2.00 | 0.42 |
| 16:1U:27:LEU:HB3 | 16:1U:31:SER:HB3 | 1.99 | 0.42 |
| 24:12:53:LEU:HD23 | 24:12:53:LEU:HA | 1.81 | 0.42 |
| 32:1a:97:G:H2' | 32:1a:98:G:O4' | 2.19 | 0.42 |
| 32:1a:472:A:H2' | 32:1a:473:G:O4' | 2.19 | 0.42 |
| 32:1a:812:C:N3 | 61:1a:2048:HOH:O | 2.37 | 0.42 |
| 32:1a:1006:C:OP2 | 32:1a:1037:C:O2' | 2.38 | 0.42 |
| 32:1a:1037:C:H2' | 32:1a:1038:C:H6 | 1.83 | 0.42 |
| 32:1a:1530:G:H4' | 32:1a:1530:G:OP1 | 2.20 | 0.42 |
| 34:1c:130:VAL:HG21 | 34:1c:157:ILE:HG23 | 2.00 | 0.42 |
| 40:1i:3:GLN:HE21 | 40:1i:20:ARG:HE | 1.66 | 0.42 |
| 42:1k:34:ASP:OD1 | 42:1k:38:ASN:N | 2.52 | 0.42 |
| 1:2A:598:G:H2' | 1:2A:599:G:O4' | 2.19 | 0.42 |
| 1:2A:996:A:H4' | 16:2U:91:ASP:OD2 | 2.19 | 0.42 |
| 1:2A:1364:G:C8 | 23:21:3:LYS:HD2 | 2.54 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:2A:1580:A:H3' | 1:2A:1581:G:C8 | 2.51 | 0.42 |
| 3:2D:69:ARG:HH11 | 3:2D:105:ILE:HG21 | 1.85 | 0.42 |
| 3:2D:242:ARG:HD2 | 3:2D:246:PRO:HG3 | 2.00 | 0.42 |
| 5:2F:184:TYR:CZ | 5:2F:188:ARG:HD2 | 2.54 | 0.42 |
| 17:2V:85:LYS:HB2 | 17:2V:85:LYS:HE3 | 1.70 | 0.42 |
| 21:2Z:126:VAL:CG1 | 21:2Z:161:VAL:HG23 | 2.49 | 0.42 |
| 24:22:49:LYS:HE2 | 24:22:49:LYS:HB3 | 1.75 | 0.42 |
| 32:2a:397:A:H3' | 32:2a:397:A:N3 | 2.34 | 0.42 |
| 32:2a:779:C:H2' | 32:2a:780:A:O4' | 2.18 | 0.42 |
| 32:2a:1321:C:H4' | 44:2m:87:TYR:CE2 | 2.53 | 0.42 |
| 34:2c:180:ALA:HB1 | 34:2c:203:PHE:CE1 | 2.54 | 0.42 |
| 37:2f:3:ARG:HB3 | 37:2f:93:SER:HB2 | 2.01 | 0.42 |
| 40:2i:28:VAL:HG22 | 40:2i:63:ILE:HB | 2.00 | 0.42 |
| 47:2p:51:VAL:HG12 | 47:2p:53:VAL:N | 2.32 | 0.42 |
| 48:2q:82:MET:O | 48:2q:86:GLU:HG2 | 2.19 | 0.42 |
| 50:2s:50:ALA:HA | 50:2s:58:VAL:O | 2.19 | 0.42 |
| 1:1A:478:A:N1 | 1:1A:500:G:H4' | 2.33 | 0.42 |
| 1:1A:1178:C:O5' | 1:1A:1178:C:H6 | 2.01 | 0.42 |
| 1:1A:1431:U:H2' | 1:1A:1432:C:C6 | 2.55 | 0.42 |
| 1:1A:1769:G:O2' | 1:1A:1958:C:OP1 | 2.28 | 0.42 |
| 1:1A:1798:U:H5' | 3:1D:259:THR:CG2 | 2.47 | 0.42 |
| 9:1N:96:GLU:CD | 9:1N:96:GLU:H | 2.27 | 0.42 |
| 13:1R:98:LEU:HB2 | 13:1R:113:LEU:HD11 | 2.02 | 0.42 |
| 14:1S:10:ARG:HG3 | 14:1S:13:ARG:NH2 | 2.33 | 0.42 |
| 20:1Y:6:HIS:HE1 | 20:1Y:72:VAL:O | 2.03 | 0.42 |
| 23:11:64:ALA:HA | 23:11:67:ILE:HG13 | 2.00 | 0.42 |
| 32:1a:60:A:N1 | 32:1a:107:G:O2' | 2.48 | 0.42 |
| 32:1a:92:C:H2' | 32:1a:93:G:C8 | 2.54 | 0.42 |
| 32:1a:438:G:H4' | 35:1d:123:HIS:CE1 | 2.54 | 0.42 |
| 32:1a:613:C:H2' | 32:1a:614:A:C8 | 2.55 | 0.42 |
| 32:1a:841:U:OP2 | 32:1a:841:U:H6 | 2.01 | 0.42 |
| 43:1l:7:ILE:O | 43:1l:11:VAL:HG23 | 2.18 | 0.42 |
| 46:1o:39:LEU:HD22 | 46:1o:56:LEU:HB2 | 2.00 | 0.42 |
| 1:2A:648:G:H2' | 1:2A:649:G:C8 | 2.54 | 0.42 |
| 1:2A:807:U:O2' | 1:2A:2060:A:N1 | 2.50 | 0.42 |
| 1:2A:2586:C:OP2 | 1:2A:2608:G:N1 | 2.42 | 0.42 |
| 1:2A:2792:G:H2' | 1:2A:2792:G:N3 | 2.35 | 0.42 |
| 4:2E:11:MET:HG2 | 4:2E:24:THR:HB | 2.00 | 0.42 |
| 10:2O:1:MET:HG3 | 10:2O:67:LYS:HG2 | 2.00 | 0.42 |
| 10:2O:64:ARG:HB2 | 10:2O:79:PHE:CD2 | 2.54 | 0.42 |
| 11:2P:101:VAL:HA | 11:2P:106:LEU:O | 2.19 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:2R:26:LYS:HE2 | 13:2R:70:LEU:O | 2.19 | 0.42 |
| 21:2Z:54:HIS:HB3 | 21:2Z:101:PRO:HD3 | 2.02 | 0.42 |
| 26:24:34:GLU:HA | 44:2m:57:ARG:NH1 | 2.34 | 0.42 |
| 27:25:16:ARG:NH1 | 27:25:17:ASP:OD1 | 2.52 | 0.42 |
| 32:2a:1359:C:O2' | 32:2a:1361:G:N7 | 2.52 | 0.42 |
| 34:2c:9:GLY:HA3 | 45:2n:49:HIS:HA | 2.01 | 0.42 |
| 35:2d:200:GLU:O | 35:2d:204:ILE:HG12 | 2.19 | 0.42 |
| 46:2o:15:PHE:CE1 | 46:2o:84:LYS:HE3 | 2.54 | 0.42 |
| 54:2y:37:MIA:H2' | 54:2y:38:A:O4' | 2.20 | 0.42 |
| 1:1A:27:G:C2 | 1:1A:512:G:N3 | 2.87 | 0.42 |
| 1:1A:1027:A:C2 | 1:1A:2488:A:H5' | 2.54 | 0.42 |
| 1:1A:1055:G:N2 | 1:1A:1104:C:N3 | 2.58 | 0.42 |
| 1:1A:2378:A:H2' | 14:1S:21:THR:HG21 | 2.02 | 0.42 |
| 1:1A:2869:G:H2' | 1:1A:2870:C:O4' | 2.19 | 0.42 |
| 2:1B:42:C:O2' | 6:1G:66:GLN:HG2 | 2.19 | 0.42 |
| 3:1D:208:LYS:HG3 | 3:1D:210:GLY:H | 1.84 | 0.42 |
| 4:1E:9:VAL:HB | 15:1T:3:ARG:HG2 | 2.02 | 0.42 |
| 10:1O:1:MET:HE2 | 10:1O:1:MET:HB3 | 1.81 | 0.42 |
| 15:1T:95:ARG:HB2 | 15:1T:96:ARG:HH12 | 1.84 | 0.42 |
| 17:1V:40:LEU:HB2 | 17:1V:46:VAL:HG22 | 2.01 | 0.42 |
| 26:14:55:ARG:H | 26:14:56:VAL:HA | 1.85 | 0.42 |
| 32:1a:253:U:H2' | 32:1a:254:G:H8 | 1.85 | 0.42 |
| 32:1a:774:G:H2' | 32:1a:775:G:O4' | 2.19 | 0.42 |
| 32:1a:1028:C:N4 | 32:1a:1033:G:H1 | 2.15 | 0.42 |
| 32:1a:1053:G:O2' | 61:1a:2107:HOH:O | 2.22 | 0.42 |
| 32:1a:1488:G:H2' | 32:1a:1489:G:C8 | 2.54 | 0.42 |
| 34:1c:122:GLU:O | 34:1c:126:ARG:NH1 | 2.47 | 0.42 |
| 1:2A:250:G:C6 | 1:2A:251:A:C6 | 3.08 | 0.42 |
| 1:2A:320:A:H4' | 1:2A:322:A:N7 | 2.34 | 0.42 |
| 1:2A:459:U:OP2 | 29:27:39:ARG:NH1 | 2.52 | 0.42 |
| 1:2A:729:G:C6 | 3:2D:208:LYS:HB2 | 2.54 | 0.42 |
| 1:2A:784:A:N6 | 3:2D:229:VAL:HG11 | 2.34 | 0.42 |
| 1:2A:1847:A:H3' | 1:2A:1848:A:H5' | 2.01 | 0.42 |
| 1:2A:2377:A:H2' | 1:2A:2378:A:C8 | 2.54 | 0.42 |
| 1:2A:2494:G:OP1 | 22:20:3:HIS:N | 2.43 | 0.42 |
| 1:2A:2612:C:OP2 | 27:25:2:ALA:N | 2.52 | 0.42 |
| 1:2A:2748:A:H2 | 7:2H:63:SER:HB3 | 1.84 | 0.42 |
| 5:2F:32:LEU:O | 5:2F:36:VAL:HG23 | 2.19 | 0.42 |
| 8:2I:26:ALA:O | 8:2I:31:LEU:HB2 | 2.20 | 0.42 |
| 11:2P:83:VAL:HG22 | 11:2P:112:LEU:HD11 | 2.01 | 0.42 |
| 14:2S:62:LYS:O | 14:2S:66:ALA:N | 2.51 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 25:23:6:VAL:HG13 | 25:23:54:VAL:HG11 | 2.01 | 0.42 |
| 32:2a:476:G:H2' | 32:2a:477:A:H8 | 1.85 | 0.42 |
| 32:2a:979:C:H41 | 32:2a:1360:A:N6 | 2.17 | 0.42 |
| 32:2a:1346:A:N1 | 32:2a:1374:A:H5" | 2.34 | 0.42 |
| 32:2a:1387:G:H2' | 32:2a:1388:C:H6 | 1.83 | 0.42 |
| 40:2i:4:TYR:CE1 | 40:2i:88:TYR:HA | 2.55 | 0.42 |
| 45:2n:14:PRO:HB2 | 45:2n:19:ARG:HB2 | 2.01 | 0.42 |
| 52:2u:6:ARG:HG2 | 52:2u:15:ARG:HE | 1.84 | 0.42 |
| 1:1A:573:G:O2' | 1:1A:574:C:H3' | 2.20 | 0.42 |
| 1:1A:744:G:OP1 | 4:1E:132:HIS:ND1 | 2.50 | 0.42 |
| 1:1A:817:C:H4' | 1:1A:932:G:C5 | 2.55 | 0.42 |
| 1:1A:1057:A:N6 | 1:1A:1081:U:H3 | 2.15 | 0.42 |
| 1:1A:1187:G:H5" | 17:1V:81:TYR:CE1 | 2.54 | 0.42 |
| 1:1A:1645:G:H5" | 1:1A:1646:C:O4' | 2.20 | 0.42 |
| 1:1A:1794:U:H2' | 1:1A:1795:C:C6 | 2.55 | 0.42 |
| 1:1A:1821:A:H2' | 1:1A:1822:G:C8 | 2.55 | 0.42 |
| 6:1G:25:TYR:CZ | 6:1G:32:PRO:HD3 | 2.54 | 0.42 |
| 6:1G:49:ASP:OD1 | 6:1G:49:ASP:N | 2.53 | 0.42 |
| 6:1G:142:PRO:HB2 | 26:14:31:ILE:HG21 | 2.01 | 0.42 |
| 9:1N:66:LYS:HB3 | 9:1N:70:LYS:HB2 | 2.00 | 0.42 |
| 11:1P:62:LEU:O | 30:18:13:ARG:HD3 | 2.20 | 0.42 |
| 19:1X:28:PHE:CE1 | 19:1X:92:LEU:HD11 | 2.55 | 0.42 |
| 25:13:23:LEU:HD13 | 25:13:50:VAL:HG11 | 2.01 | 0.42 |
| 26:14:53:GLU:O | 26:14:56:VAL:HG13 | 2.19 | 0.42 |
| 32:1a:194:C:C2' | 32:1a:195:A:H5" | 2.49 | 0.42 |
| 32:1a:390:C:H2' | 32:1a:391:G:H8 | 1.83 | 0.42 |
| 32:1a:1425:U:H2' | 32:1a:1426:C:C6 | 2.55 | 0.42 |
| 33:1b:111:ARG:HA | 33:1b:111:ARG:HD3 | 1.82 | 0.42 |
| 47:1p:14:ASN:OD1 | 47:1p:42:ARG:NH2 | 2.53 | 0.42 |
| 47:1p:37:GLY:HA3 | 47:1p:50:LYS:O | 2.19 | 0.42 |
| 54:1w:24:G:C6 | 54:1w:25:C:C4 | 3.08 | 0.42 |
| 54:1w:43:C:H2' | 54:1w:44:G:C8 | 2.55 | 0.42 |
| 54:1w:70:G:C4 | 54:1w:71:G:H1' | 2.54 | 0.42 |
| 1:2A:797:C:H2' | 1:2A:798:G:O4' | 2.20 | 0.42 |
| 1:2A:1027:A:C2 | 1:2A:2488:A:H5' | 2.54 | 0.42 |
| 1:2A:1262:A:H2 | 27:25:10:LYS:HD2 | 1.83 | 0.42 |
| 1:2A:1405:U:H2' | 1:2A:1406:U:C6 | 2.54 | 0.42 |
| 1:2A:1495:A:H2' | 1:2A:1496:A:C8 | 2.53 | 0.42 |
| 1:2A:1540:U:H2' | 1:2A:1541:G:O4' | 2.20 | 0.42 |
| 1:2A:2278:A:OP2 | 22:20:12:ASN:ND2 | 2.43 | 0.42 |
| 1:2A:2305:A:H5" | 6:2G:134:GLY:HA3 | 2.00 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:2A:2617:C:H2' | 1:2A:2618:G:O4' | 2.20 | 0.42 |
| 1:2A:2649:U:H2' | 1:2A:2650:U:C6 | 2.54 | 0.42 |
| 7:2H:56:SER:OG | 7:2H:57:ASP:N | 2.53 | 0.42 |
| 10:2O:2:ILE:HD12 | 10:2O:6:THR:HG21 | 2.01 | 0.42 |
| 11:2P:138:LEU:HG | 11:2P:143:GLY:HA3 | 2.00 | 0.42 |
| 13:2R:87:TYR:CD1 | 13:2R:90:ARG:HD2 | 2.55 | 0.42 |
| 20:2Y:14:LEU:HG | 20:2Y:15:VAL:N | 2.34 | 0.42 |
| 20:2Y:19:LYS:HB3 | 20:2Y:19:LYS:HE2 | 1.84 | 0.42 |
| 21:2Z:72:ARG:HD3 | 21:2Z:72:ARG:HA | 1.73 | 0.42 |
| 32:2a:1287:A:H2 | 32:2a:1353:G:H1' | 1.83 | 0.42 |
| 34:2c:22:TRP:CD2 | 34:2c:59:ARG:HD2 | 2.55 | 0.42 |
| 35:2d:180:GLY:O | 35:2d:181:MET:HG2 | 2.19 | 0.42 |
| 45:2n:6:LEU:O | 45:2n:10:ALA:N | 2.50 | 0.42 |
| 49:2r:21:LYS:O | 49:2r:25:THR:HG23 | 2.19 | 0.42 |
| 55:2x:8:4SU:O2 | 55:2x:21:A:C2 | 2.72 | 0.42 |
| 55:2x:47:U:H3' | 55:2x:48:C:C5' | 2.49 | 0.42 |
| 1:1A:762:U:OP1 | 61:1A:6670:HOH:O | 2.22 | 0.42 |
| 1:1A:1047:G:H2' | 1:1A:1110:G:H22 | 1.84 | 0.42 |
| 1:1A:1064:C:H2' | 1:1A:1065:U:H5' | 2.01 | 0.42 |
| 1:1A:1190:G:H5" | 11:1P:32:THR:O | 2.20 | 0.42 |
| 2:1B:83:G:OP1 | 25:13:19:GLN:NE2 | 2.49 | 0.42 |
| 4:1E:11:MET:HE2 | 4:1E:11:MET:HB3 | 1.90 | 0.42 |
| 19:1X:40:LYS:O | 19:1X:44:GLU:HG3 | 2.19 | 0.42 |
| 21:1Z:154:ASP:C | 21:1Z:155:LEU:HD12 | 2.44 | 0.42 |
| 25:13:39:ASP:OD1 | 25:13:44:ARG:NH1 | 2.52 | 0.42 |
| 32:1a:4:U:O4 | 39:1h:105:ARG:HG2 | 2.19 | 0.42 |
| 32:1a:234:C:H2' | 32:1a:235:C:H6 | 1.83 | 0.42 |
| 33:1b:146:GLN:O | 33:1b:150:SER:HB3 | 2.19 | 0.42 |
| 43:1l:60:LEU:HD21 | 43:1l:85:ILE:HD11 | 2.02 | 0.42 |
| 54:1y:46:7MG:O2' | 54:1y:48:C:OP2 | 2.33 | 0.42 |
| 1:2A:746:A:H2' | 1:2A:2612:C:H5" | 2.00 | 0.42 |
| 1:2A:2116:G:N2 | 1:2A:2162:G:OP1 | 2.52 | 0.42 |
| 1:2A:2398:U:H2' | 1:2A:2399:G:C8 | 2.55 | 0.42 |
| 1:2A:2512:C:H2' | 1:2A:2513:G:O4' | 2.19 | 0.42 |
| 5:2F:33:LEU:HD11 | 5:2F:112:MET:HB3 | 2.01 | 0.42 |
| 12:2Q:36:ALA:HA | 12:2Q:129:THR:HG22 | 2.02 | 0.42 |
| 15:2T:51:ARG:HG2 | 15:2T:62:THR:HB | 2.02 | 0.42 |
| 25:23:6:VAL:HG13 | 25:23:54:VAL:CG1 | 2.49 | 0.42 |
| 32:2a:93:G:C6 | 32:2a:96:U:C4 | 3.08 | 0.42 |
| 32:2a:259:G:H2' | 32:2a:260:G:O4' | 2.19 | 0.42 |
| 32:2a:620:C:H2' | 32:2a:621:A:O4' | 2.20 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 32:2a:1343:G:H1' | 40:2i:121:ARG:HH11 | 1.84 | 0.42 |
| 38:2g:97:GLN:O | 38:2g:101:LEU:HG | 2.20 | 0.42 |
| 43:2l:53:ARG:HB2 | 43:2l:93:LEU:HD11 | 2.02 | 0.42 |
| 43:2l:58:VAL:HG12 | 43:2l:60:LEU:HD12 | 2.02 | 0.42 |
| 53:2v:22:U:H2' | 53:2v:23:A:C8 | 2.54 | 0.42 |
| 54:2w:14:A:C2 | 54:2w:22:G:H1' | 2.55 | 0.42 |
| 1:1A:27:G:O2' | 1:1A:28:A:OP2 | 2.35 | 0.42 |
| 1:1A:686:G:N2 | 1:1A:788:A:H61 | 2.18 | 0.42 |
| 1:1A:1069:A:H1' | 1:1A:1096:A:H4' | 2.02 | 0.42 |
| 1:1A:1274:A:N3 | 1:1A:1297:C:H1' | 2.35 | 0.42 |
| 1:1A:1465:G:O2' | 1:1A:1545:A:N1 | 2.52 | 0.42 |
| 2:1B:28:C:H2' | 2:1B:29:A:O4' | 2.20 | 0.42 |
| 14:1S:10:ARG:HG3 | 14:1S:13:ARG:HH22 | 1.85 | 0.42 |
| 16:1U:47:TYR:HA | 16:1U:50:ARG:NH2 | 2.34 | 0.42 |
| 18:1W:65:LEU:HB2 | 18:1W:68:ARG:HD2 | 2.01 | 0.42 |
| 20:1Y:28:LYS:HD2 | 20:1Y:40:GLU:OE1 | 2.20 | 0.42 |
| 20:1Y:106:LEU:O | 20:1Y:107:ASP:HB2 | 2.19 | 0.42 |
| 32:1a:461:A:O2' | 32:1a:470:C:H5' | 2.20 | 0.42 |
| 32:1a:601:C:H2' | 32:1a:602:A:C8 | 2.53 | 0.42 |
| 32:1a:629:G:H2' | 32:1a:630:G:O4' | 2.20 | 0.42 |
| 32:1a:1064:G:H4' | 32:1a:1065:U:OP1 | 2.19 | 0.42 |
| 32:1a:1320:C:O2 | 50:1s:36:ARG:NH2 | 2.52 | 0.42 |
| 39:1h:110:ALA:HB3 | 39:1h:121:ASP:HB3 | 2.02 | 0.42 |
| 54:1y:18:G:N2 | 54:1y:57:G:C5 | 2.88 | 0.42 |
| 1:2A:297:C:H2' | 1:2A:298:G:O4' | 2.20 | 0.42 |
| 1:2A:729:G:O5' | 3:2D:208:LYS:NZ | 2.53 | 0.42 |
| 1:2A:1022:G:OP2 | 9:2N:69:GLN:NE2 | 2.46 | 0.42 |
| 1:2A:1832:C:H2' | 1:2A:1833:U:O4' | 2.20 | 0.42 |
| 1:2A:2133:G:C6 | 1:2A:2157:G:C6 | 3.08 | 0.42 |
| 1:2A:2758:A:C4 | 7:2H:67:LEU:HD21 | 2.55 | 0.42 |
| 2:2B:15:A:OP2 | 2:2B:69:G:N2 | 2.53 | 0.42 |
| 4:2E:101:ARG:CZ | 4:2E:171:GLU:HB2 | 2.50 | 0.42 |
| 4:2E:181:LEU:HA | 4:2E:181:LEU:HD12 | 1.74 | 0.42 |
| 10:2O:7:TYR:CZ | 10:2O:44:LYS:HG3 | 2.55 | 0.42 |
| 15:2T:19:LEU:HD13 | 15:2T:86:ILE:HD12 | 2.02 | 0.42 |
| 16:2U:88:ILE:HG22 | 16:2U:90:VAL:HG23 | 2.01 | 0.42 |
| 21:2Z:149:SER:HG | 21:2Z:170:THR:HG1 | 1.64 | 0.42 |
| 32:2a:156:G:H1 | 32:2a:165:C:H42 | 1.68 | 0.42 |
| 32:2a:779:C:O2' | 42:2k:120:ARG:NH1 | 2.46 | 0.42 |
| 32:2a:1324:A:O4' | 32:2a:1362:C:H4' | 2.20 | 0.42 |
| 32:2a:1502:A:C8 | 32:2a:1505:G:N2 | 2.87 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 33:2b:111:ARG:HH11 | 33:2b:111:ARG:HA | 1.84 | 0.42 |
| 36:2e:78:HIS:HB2 | 39:2h:104:ARG:HG2 | 2.02 | 0.42 |
| 38:2g:69:VAL:HA | 38:2g:138:LYS:HD3 | 2.02 | 0.42 |
| 44:2m:87:TYR:CZ | 44:2m:91:ARG:HD2 | 2.55 | 0.42 |
| 45:2n:21:TYR:OH | 45:2n:23:ARG:NH2 | 2.45 | 0.42 |
| 54:2y:69:G:H2' | 54:2y:70:G:O4' | 2.19 | 0.42 |
| 1:1A:196:A:H2' | 1:1A:196:A:N3 | 2.35 | 0.42 |
| 1:1A:271(E):U:H2' | 1:1A:271(F):C:C6 | 2.55 | 0.42 |
| 1:1A:284:U:H2' | 1:1A:285:C:C6 | 2.55 | 0.42 |
| 1:1A:1653:G:O3' | 13:1R:2:ARG:HB2 | 2.19 | 0.42 |
| 61:1A:5688:HOH:O | 11:1P:43:GLY:HA3 | 2.20 | 0.42 |
| 3:1D:147:LEU:HD13 | 3:1D:155:LEU:HD21 | 2.02 | 0.42 |
| 5:1F:125:LEU:HD21 | 5:1F:199:TRP:CD2 | 2.55 | 0.42 |
| 25:13:3:ARG:HB2 | 25:13:59:VAL:HG23 | 2.01 | 0.42 |
| 25:13:19:GLN:OE1 | 25:13:52:HIS:NE2 | 2.44 | 0.42 |
| 32:1a:134:A:H61 | 47:1p:25:ARG:HH12 | 1.67 | 0.42 |
| 32:1a:857:C:H2' | 32:1a:858:G:O4' | 2.20 | 0.42 |
| 32:1a:1004:A:C5' | 32:1a:1024:G:H1 | 2.30 | 0.42 |
| 37:1f:97:PHE:HD2 | 49:1r:31:LEU:HD11 | 1.85 | 0.42 |
| 42:1k:99:GLN:HA | 42:1k:105:VAL:HG21 | 2.02 | 0.42 |
| 44:1m:118:ALA:HB2 | 55:1x:28:C:H4' | 2.01 | 0.42 |
| 54:1y:18:G:C2 | 54:1y:58:A:C5 | 3.08 | 0.42 |
| 1:2A:631:A:H1' | 11:2P:66:GLY:HA2 | 2.02 | 0.42 |
| 1:2A:1429:G:H2' | 1:2A:1430:C:C6 | 2.54 | 0.42 |
| 1:2A:1477:A:H2' | 1:2A:1478:G:O4' | 2.20 | 0.42 |
| 1:2A:2658:C:H5' | 7:2H:160:LYS:HZ2 | 1.84 | 0.42 |
| 6:2G:27:ASN:HB3 | 6:2G:30:GLU:HB2 | 2.01 | 0.42 |
| 7:2H:152:ARG:HD3 | 7:2H:152:ARG:HA | 1.86 | 0.42 |
| 14:2S:20:ARG:HA | 14:2S:20:ARG:HD2 | 1.94 | 0.42 |
| 21:2Z:128:VAL:HG23 | 21:2Z:160:GLY:O | 2.20 | 0.42 |
| 21:2Z:158:PRO:HA | 21:2Z:159:PRO:HD3 | 1.97 | 0.42 |
| 32:2a:391:G:N7 | 61:2a:3610:HOH:O | 2.37 | 0.42 |
| 32:2a:781:A:OP1 | 32:2a:1523:G:H5' | 2.20 | 0.42 |
| 41:2j:27:ALA:HB3 | 41:2j:34:VAL:HG12 | 2.01 | 0.42 |
| 55:2x:61:C:H2' | 55:2x:62:C:H6 | 1.84 | 0.42 |
| 1:1A:106:C:HO2' | 1:1A:294:A:HO2' | 1.66 | 0.42 |
| 1:1A:129:C:H2' | 1:1A:130:C:H6 | 1.85 | 0.42 |
| 1:1A:251:A:C5 | 1:1A:252:G:H1' | 2.54 | 0.42 |
| 1:1A:479:A:N3 | 1:1A:481:G:H5" | 2.35 | 0.42 |
| 1:1A:607:U:OP1 | 5:1F:102:PRO:HA | 2.20 | 0.42 |
| 1:1A:1156:A:OP1 | 16:1U:55:ARG:NH1 | 2.45 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1A:1216:G:O6 | 61:1A:4803:HOH:O | 2.21 | 0.42 |
| 1:1A:2040:C:H2' | 1:1A:2041:U:O4' | 2.20 | 0.42 |
| 1:1A:2141:G:C6 | 1:1A:2142:C:C2 | 3.07 | 0.42 |
| 1:1A:2846:G:H2' | 1:1A:2847:U:O4' | 2.20 | 0.42 |
| 6:1G:62:LEU:HA | 26:14:27:THR:HG21 | 2.02 | 0.42 |
| 8:1I:26:ALA:O | 8:1I:31:LEU:HB2 | 2.20 | 0.42 |
| 9:1N:62:VAL:CG1 | 9:1N:66:LYS:HB2 | 2.50 | 0.42 |
| 14:1S:15:ARG:C | 14:1S:19:LYS:HZ3 | 2.27 | 0.42 |
| 18:1W:36:LEU:HD13 | 18:1W:48:ALA:HA | 2.02 | 0.42 |
| 18:1W:46:PHE:O | 18:1W:50:VAL:HG23 | 2.20 | 0.42 |
| 30:18:30:ARG:O | 61:18:207:HOH:O | 2.22 | 0.42 |
| 32:1a:524:G:H2' | 32:1a:525:C:C6 | 2.54 | 0.42 |
| 32:1a:828:A:H2' | 32:1a:829:G:O4' | 2.19 | 0.42 |
| 32:1a:1008:C:N3 | 32:1a:1021:G:C6 | 2.87 | 0.42 |
| 32:1a:1295:G:O2' | 44:1m:14:ARG:NH1 | 2.52 | 0.42 |
| 32:1a:1463:C:H2' | 32:1a:1464:G:O4' | 2.19 | 0.42 |
| 33:1b:178:ARG:NH2 | 39:1h:74:PRO:HB3 | 2.34 | 0.42 |
| 35:1d:200:GLU:O | 35:1d:204:ILE:HG12 | 2.19 | 0.42 |
| 36:1e:82:VAL:HG21 | 36:1e:138:ALA:HA | 2.02 | 0.42 |
| 53:1v:16:A:H2' | 53:1v:17:U:O4' | 2.20 | 0.42 |
| 1:2A:359:A:H2' | 1:2A:360:G:O4' | 2.20 | 0.42 |
| 1:2A:1639:U:H4' | 1:2A:2699:C:H4' | 2.02 | 0.42 |
| 1:2A:1713:U:H2' | 1:2A:1714:G:H8 | 1.84 | 0.42 |
| 1:2A:1778:U:H2' | 1:2A:1784:A:N6 | 2.35 | 0.42 |
| 1:2A:1902:C:H5' | 3:2D:246:PRO:HD3 | 2.02 | 0.42 |
| 1:2A:2313:C:H2' | 1:2A:2314:C:C6 | 2.55 | 0.42 |
| 6:2G:16:ARG:O | 6:2G:20:ILE:HG13 | 2.19 | 0.42 |
| 26:24:18:CYS:SG | 26:24:20:ASN:HB2 | 2.60 | 0.42 |
| 32:2a:72:C:H2' | 32:2a:73:G:C8 | 2.55 | 0.42 |
| 32:2a:266:G:H2' | 32:2a:266:G:N3 | 2.35 | 0.42 |
| 32:2a:986:A:O2' | 50:2s:55:LYS:HA | 2.19 | 0.42 |
| 32:2a:991:U:C4 | 32:2a:1212:U:H1' | 2.54 | 0.42 |
| 32:2a:1128:C:O2' | 32:2a:1147:C:N3 | 2.37 | 0.42 |
| 32:2a:1151:A:O2' | 32:2a:1152:A:O5' | 2.32 | 0.42 |
| 34:2c:52:LEU:HD12 | 34:2c:53:ALA:H | 1.85 | 0.42 |
| 51:2t:50:GLU:O | 51:2t:100:ILE:HD11 | 2.20 | 0.42 |
| 55:2x:37:A:H2' | 55:2x:38:A:O4' | 2.20 | 0.42 |
| 1:1A:669:G:N2 | 61:1A:4261:HOH:O | 2.44 | 0.41 |
| 1:1A:1156:A:C8 | 16:1U:51:LYS:HD2 | 2.54 | 0.41 |
| 1:1A:1588:C:H2' | 1:1A:1589:C:H6 | 1.84 | 0.41 |
| 1:1A:2032:G:OP2 | 1:1A:2454:G:O2' | 2.29 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1A:2849:U:OP2 | 15:1T:95:ARG:NH1 | 2.53 | 0.41 |
| 8:1I:50:ARG:CZ | 8:1I:50:ARG:HB3 | 2.50 | 0.41 |
| 15:1T:33:LYS:HD3 | 15:1T:82:LEU:HD22 | 2.02 | 0.41 |
| 15:1T:95:ARG:HB2 | 15:1T:96:ARG:NH1 | 2.35 | 0.41 |
| 21:1Z:44:PHE:CZ | 21:1Z:86:VAL:HG11 | 2.55 | 0.41 |
| 24:12:51:ARG:HD3 | 24:12:55:ARG:NH1 | 2.35 | 0.41 |
| 25:13:31:LEU:HD23 | 25:13:31:LEU:HA | 1.92 | 0.41 |
| 27:15:16:ARG:NH1 | 27:15:17:ASP:OD1 | 2.53 | 0.41 |
| 32:1a:454:C:H3' | 32:1a:455:C:C6 | 2.55 | 0.41 |
| 32:1a:629:G:H3' | 32:1a:630:G:H5" | 2.01 | 0.41 |
| 32:1a:688:G:H5' | 42:1k:46:GLY:C | 2.45 | 0.41 |
| 32:1a:926:G:O2' | 53:1v:13:A:N3 | 2.50 | 0.41 |
| 32:1a:1429:C:H2' | 32:1a:1430:C:C6 | 2.55 | 0.41 |
| 34:1c:131:ARG:NE | 34:1c:135:LYS:HE3 | 2.33 | 0.41 |
| 40:1i:28:VAL:HG22 | 40:1i:63:ILE:HB | 2.01 | 0.41 |
| 1:2A:784:A:OP1 | 1:2A:2588:G:H5" | 2.19 | 0.41 |
| 1:2A:948:G:H21 | 1:2A:985:C:P | 2.43 | 0.41 |
| 1:2A:2011:U:H2' | 1:2A:2012:G:O4' | 2.20 | 0.41 |
| 1:2A:2138:C:H2' | 1:2A:2139:C:O4' | 2.20 | 0.41 |
| 1:2A:2166:G:N7 | 1:2A:2168:G:N2 | 2.68 | 0.41 |
| 1:2A:2320:A:N3 | 1:2A:2320:A:H2' | 2.34 | 0.41 |
| 1:2A:2533:A:OP1 | 1:2A:2665:A:O2' | 2.37 | 0.41 |
| 2:2B:30:C:H2' | 2:2B:31:C:H5' | 2.02 | 0.41 |
| 2:2B:50:G:P | 14:2S:62:LYS:HB2 | 2.60 | 0.41 |
| 5:2F:110:LEU:HD11 | 5:2F:181:LEU:HG | 2.02 | 0.41 |
| 13:2R:29:LEU:HD12 | 13:2R:29:LEU:HA | 1.85 | 0.41 |
| 20:2Y:87:LYS:HB3 | 20:2Y:95:LYS:HD2 | 2.01 | 0.41 |
| 32:2a:24:U:H2' | 32:2a:25:C:C6 | 2.55 | 0.41 |
| 32:2a:742:G:P | 46:2o:35:ARG:HH22 | 2.42 | 0.41 |
| 32:2a:1469:G:H2' | 32:2a:1470:G:C8 | 2.55 | 0.41 |
| 33:2b:109:SER:O | 33:2b:112:VAL:HG22 | 2.19 | 0.41 |
| 1:1A:271(H):G:H4' | 23:11:81:LYS:HG2 | 2.02 | 0.41 |
| 1:1A:271(V):G:O6 | 61:1A:5975:HOH:O | 2.22 | 0.41 |
| 1:1A:596:G:H2' | 1:1A:597:U:O4' | 2.20 | 0.41 |
| 1:1A:784:A:C6 | 3:1D:229:VAL:HG11 | 2.55 | 0.41 |
| 1:1A:996:A:O3' | 16:1U:91:ASP:HB2 | 2.20 | 0.41 |
| 1:1A:2432:A:N9 | 23:11:33:LYS:HD3 | 2.35 | 0.41 |
| 6:1G:28:VAL:O | 6:1G:31:VAL:HG12 | 2.20 | 0.41 |
| 8:1I:60:GLU:HG3 | 8:1I:61:ARG:NH1 | 2.35 | 0.41 |
| 11:1P:128:HIS:NE2 | 11:1P:148:LEU:HD11 | 2.35 | 0.41 |
| 26:14:49:PHE:HD1 | 26:14:49:PHE:HA | 1.73 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 32:1a:452:A:H4' | 47:1p:72:ARG:CZ | 2.50 | 0.41 |
| 32:1a:593:G:H2' | 32:1a:594:G:O4' | 2.19 | 0.41 |
| 32:1a:1065:U:H1' | 32:1a:1066:C:OP2 | 2.20 | 0.41 |
| 32:1a:1221:G:O3' | 50:1s:77:THR:OG1 | 2.34 | 0.41 |
| 32:1a:1429:C:H2' | 32:1a:1430:C:H6 | 1.85 | 0.41 |
| 35:1d:18:LYS:CG | 60:1d:302:SF4:S1 | 3.08 | 0.41 |
| 36:1e:12:LEU:HB3 | 36:1e:31:LEU:HB2 | 2.02 | 0.41 |
| 37:1f:55:ASP:HB2 | 37:1f:86:ARG:HH12 | 1.84 | 0.41 |
| 55:1x:50:U:H3 | 55:1x:64:G:H1 | 1.66 | 0.41 |
| 54:1y:47:U:O2' | 54:1y:50:U:OP1 | 2.31 | 0.41 |
| 1:2A:56:A:H2' | 1:2A:57:C:O4' | 2.21 | 0.41 |
| 1:2A:1939:5MU:OP1 | 1:2A:2604:U:O2' | 2.36 | 0.41 |
| 1:2A:2419:U:H2' | 1:2A:2420:C:C6 | 2.56 | 0.41 |
| 1:2A:2558:C:H2' | 1:2A:2559:C:O4' | 2.20 | 0.41 |
| 1:2A:2643:G:H2' | 1:2A:2644:G:O4' | 2.19 | 0.41 |
| 1:2A:2697:G:H2' | 1:2A:2698:U:O4' | 2.21 | 0.41 |
| 2:2B:75:G:H1 | 21:2Z:73:GLN:NE2 | 2.19 | 0.41 |
| 7:2H:56:SER:HB3 | 7:2H:61:HIS:HD1 | 1.83 | 0.41 |
| 15:2T:73:GLU:OE2 | 15:2T:103:ARG:NE | 2.53 | 0.41 |
| 26:24:40:HIS:O | 26:24:44:THR:HG22 | 2.20 | 0.41 |
| 32:2a:434:U:H2' | 32:2a:435:C:H6 | 1.85 | 0.41 |
| 32:2a:1061:G:H1' | 41:2j:56:HIS:CE1 | 2.55 | 0.41 |
| 35:2d:149:ALA:HB3 | 35:2d:152:SER:HB2 | 2.01 | 0.41 |
| 44:2m:13:LYS:O | 44:2m:45:VAL:HG23 | 2.21 | 0.41 |
| 48:2q:21:VAL:HG21 | 48:2q:59:ILE:HG21 | 2.01 | 0.41 |
| 49:2r:44:LEU:HD11 | 49:2r:79:LEU:HD13 | 2.02 | 0.41 |
| 53:2v:14:A:H2' | 53:2v:14:A:N3 | 2.35 | 0.41 |
| 54:2w:31:A:H2' | 54:2w:32:PSU:O4' | 2.20 | 0.41 |
| 1:1A:1119:C:N4 | 61:1A:6713:HOH:O | 2.53 | 0.41 |
| 1:1A:1866:C:H2' | 1:1A:1876:A:O4' | 2.20 | 0.41 |
| 1:1A:2206:G:H5" | 1:1A:2207:G:N7 | 2.35 | 0.41 |
| 1:1A:2376:A:H2' | 1:1A:2377:A:O4' | 2.20 | 0.41 |
| 1:1A:2715:C:H2' | 1:1A:2716:U:C6 | 2.56 | 0.41 |
| 32:1a:270:A:H2' | 32:1a:271:C:O4' | 2.20 | 0.41 |
| 32:1a:309:G:O2' | 32:1a:607:A:N1 | 2.53 | 0.41 |
| 32:1a:375:U:OP1 | 47:1p:69:THR:HG21 | 2.19 | 0.41 |
| 32:1a:672:U:H2' | 32:1a:673:G:C8 | 2.56 | 0.41 |
| 32:1a:749:C:H2' | 32:1a:750:G:H8 | 1.85 | 0.41 |
| 32:1a:1060:C:H2' | 32:1a:1061:G:H8 | 1.86 | 0.41 |
| 32:1a:1134:G:N3 | 32:1a:1134:G:H2' | 2.35 | 0.41 |
| 32:1a:1519:MA6:H5" | 32:1a:1520:G:OP2 | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 47:1p:48:TRP:HH2 | 47:1p:76:GLN:HE22 | 1.67 | 0.41 |
| 54:1y:28:G:N2 | 54:1y:42:C:N3 | 2.53 | 0.41 |
| 1:2A:288:C:H2' | 1:2A:289:A:C8 | 2.54 | 0.41 |
| 1:2A:307:G:N2 | 1:2A:330:A:H62 | 2.16 | 0.41 |
| 1:2A:597:U:H2' | 1:2A:598:G:H8 | 1.86 | 0.41 |
| 1:2A:1235:G:C6 | 1:2A:1236:G:N1 | 2.87 | 0.41 |
| 1:2A:1364:G:N7 | 23:21:3:LYS:HD2 | 2.36 | 0.41 |
| 1:2A:1510:G:H2' | 1:2A:1511:C:O4' | 2.20 | 0.41 |
| 1:2A:1619:G:N2 | 29:27:1:MET:O | 2.47 | 0.41 |
| 1:2A:1770:G:H4' | 1:2A:1938:A:OP1 | 2.20 | 0.41 |
| 1:2A:2185:C:H2' | 1:2A:2186:G:O4' | 2.21 | 0.41 |
| 1:2A:2419:U:H2' | 1:2A:2420:C:H6 | 1.85 | 0.41 |
| 2:2B:43:C:O4' | 6:2G:66:GLN:NE2 | 2.53 | 0.41 |
| 3:2D:159:ALA:HB1 | 3:2D:198:ASN:O | 2.20 | 0.41 |
| 6:2G:5:VAL:HG22 | 6:2G:8:LYS:HE2 | 2.02 | 0.41 |
| 9:2N:99:LEU:HD23 | 9:2N:99:LEU:HA | 1.84 | 0.41 |
| 32:2a:792:A:H4' | 32:2a:793:U:H5" | 2.01 | 0.41 |
| 32:2a:1084:G:H5' | 32:2a:1102:A:OP2 | 2.21 | 0.41 |
| 32:2a:1286:A:H2 | 52:2u:18:TYR:OH | 2.02 | 0.41 |
| 32:2a:1370:G:N7 | 40:2i:109:VAL:HG11 | 2.35 | 0.41 |
| 32:2a:1411:C:H2' | 32:2a:1412:C:C6 | 2.55 | 0.41 |
| 33:2b:80:ILE:HD13 | 33:2b:211:ILE:HG22 | 2.02 | 0.41 |
| 33:2b:111:ARG:HA | 33:2b:111:ARG:HD3 | 1.80 | 0.41 |
| 34:2c:54:ARG:H | 34:2c:69:HIS:HB2 | 1.84 | 0.41 |
| 34:2c:111:LEU:HD21 | 34:2c:146:ALA:HB2 | 2.00 | 0.41 |
| 34:2c:122:GLU:O | 34:2c:126:ARG:HG3 | 2.20 | 0.41 |
| 34:2c:164:ARG:NH2 | 34:2c:166:GLU:OE1 | 2.53 | 0.41 |
| 35:2d:92:VAL:O | 35:2d:96:LEU:HD13 | 2.20 | 0.41 |
| 37:2f:91:VAL:HG11 | 49:2r:72:ARG:NH1 | 2.35 | 0.41 |
| 37:2f:100:ASN:HB2 | 49:2r:28:GLU:HA | 2.01 | 0.41 |
| 41:2j:6:ILE:HB | 41:2j:72:VAL:HG23 | 2.01 | 0.41 |
| 44:2m:85:GLY:HA2 | 44:2m:93:ARG:NH2 | 2.35 | 0.41 |
| 49:2r:22:VAL:HB | 49:2r:56:THR:HA | 2.02 | 0.41 |
| 54:2y:2:C:H2' | 54:2y:3:C:H6 | 1.86 | 0.41 |
| 1:1A:129:C:H2' | 1:1A:130:C:C6 | 2.55 | 0.41 |
| 1:1A:238:C:H2' | 1:1A:239:U:O4' | 2.21 | 0.41 |
| 1:1A:249:C:O2 | 30:18:12:LYS:NZ | 2.36 | 0.41 |
| 1:1A:1178:C:H2' | 1:1A:1179:C:C6 | 2.55 | 0.41 |
| 1:1A:1853:A:H2' | 1:1A:1854:A:C8 | 2.55 | 0.41 |
| 1:1A:1913:A:C8 | 32:1a:1494:G:H4' | 2.56 | 0.41 |
| 2:1B:1:U:HO2' | 2:1B:2:C:P | 2.42 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:1D:146:GLU:HG2 | 3:1D:152:GLY:C | 2.46 | 0.41 |
| 4:1E:52:LEU:HA | 4:1E:53:PRO:HD3 | 1.91 | 0.41 |
| 13:1R:28:LEU:HD22 | 13:1R:44:LEU:HD13 | 2.03 | 0.41 |
| 26:14:16:CYS:SG | 26:14:17:GLY:N | 2.93 | 0.41 |
| 32:1a:1104:G:O2' | 33:1b:111:ARG:NH2 | 2.53 | 0.41 |
| 32:1a:1346:A:O3' | 32:1a:1347:G:H4' | 2.20 | 0.41 |
| 33:1b:60:ASP:OD1 | 33:1b:64:ARG:NH2 | 2.53 | 0.41 |
| 34:1c:131:ARG:HH21 | 34:1c:135:LYS:HE3 | 1.85 | 0.41 |
| 38:1g:104:LEU:HD12 | 38:1g:134:ALA:HB1 | 2.01 | 0.41 |
| 47:1p:4:ILE:HG13 | 47:1p:64:ALA:HB1 | 2.02 | 0.41 |
| 54:1w:22:G:H5' | 54:1w:23:A:OP2 | 2.21 | 0.41 |
| 54:1y:20:U:O3' | 54:1y:21:A:H4' | 2.21 | 0.41 |
| 1:2A:116:C:H2' | 1:2A:117:G:O4' | 2.21 | 0.41 |
| 1:2A:579:G:H2' | 1:2A:580:C:C6 | 2.54 | 0.41 |
| 1:2A:896:A:H1' | 54:2w:56:C:H5' | 2.02 | 0.41 |
| 1:2A:1996:C:H4' | 1:2A:1997:G:OP1 | 2.19 | 0.41 |
| 1:2A:2543:G:H2' | 1:2A:2544:G:C8 | 2.56 | 0.41 |
| 1:2A:2679:A:H4' | 4:2E:165:VAL:HG11 | 2.01 | 0.41 |
| 1:2A:2712:U:O2' | 1:2A:2713:A:H5' | 2.21 | 0.41 |
| 2:2B:42:C:O2 | 6:2G:93:THR:N | 2.33 | 0.41 |
| 8:2I:93:THR:H | 8:2I:96:ASP:HB2 | 1.85 | 0.41 |
| 9:2N:67:LEU:HD12 | 9:2N:87:LEU:HD22 | 2.02 | 0.41 |
| 14:2S:53:SER:O | 14:2S:57:LYS:N | 2.47 | 0.41 |
| 32:2a:751:U:H4' | 46:2o:24:SER:HA | 2.01 | 0.41 |
| 32:2a:1010:G:H2' | 32:2a:1011:G:C8 | 2.55 | 0.41 |
| 32:2a:1375:A:O2' | 38:2g:29:LYS:NZ | 2.52 | 0.41 |
| 34:2c:135:LYS:HZ3 | 36:2e:52:PRO:HG2 | 1.86 | 0.41 |
| 40:2i:23:ASN:N | 40:2i:60:ASP:OD1 | 2.53 | 0.41 |
| 44:2m:34:LEU:HD13 | 44:2m:41:PRO:HB3 | 2.02 | 0.41 |
| 47:2p:74:LEU:HG | 47:2p:79:VAL:HG21 | 2.02 | 0.41 |
| 48:2q:12:SER:HB3 | 48:2q:20:THR:HB | 2.02 | 0.41 |
| 1:1A:83:G:N7 | 61:1A:7268:HOH:O | 2.37 | 0.41 |
| 1:1A:582:G:H2' | 1:1A:583:G:C8 | 2.55 | 0.41 |
| 1:1A:1766:U:H2' | 1:1A:1767:C:C6 | 2.55 | 0.41 |
| 1:1A:1837:C:OP1 | 32:1a:784:C:H4' | 2.21 | 0.41 |
| 1:1A:1997:G:H5" | 4:1E:117:MET:CE | 2.51 | 0.41 |
| 4:1E:116:VAL:HG13 | 4:1E:122:PHE:HB2 | 2.02 | 0.41 |
| 5:1F:24:LEU:HD23 | 5:1F:115:ALA:HA | 2.03 | 0.41 |
| 9:1N:14:VAL:HG11 | 9:1N:138:LEU:HD12 | 2.01 | 0.41 |
| 22:10:10:THR:HA | 61:10:205:HOH:O | 2.20 | 0.41 |
| 32:1a:250:A:H5' | 32:1a:252:U:O4' | 2.21 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 32:1a:404:U:H2' | 32:1a:405:U:C6 | 2.55 | 0.41 |
| 32:1a:413:G:H21 | 32:1a:428:G:H1' | 1.86 | 0.41 |
| 32:1a:445:G:H2' | 32:1a:446:G:C8 | 2.55 | 0.41 |
| 32:1a:769:G:N7 | 61:1a:2041:HOH:O | 2.36 | 0.41 |
| 32:1a:1521:G:N3 | 61:1a:2054:HOH:O | 2.37 | 0.41 |
| 33:1b:16:HIS:HB2 | 33:1b:204:ASN:CB | 2.50 | 0.41 |
| 45:1n:24:CYS:HB3 | 45:1n:29:ARG:H | 1.86 | 0.41 |
| 48:1q:64:PRO:HB3 | 48:1q:70:ARG:NH1 | 2.36 | 0.41 |
| 50:1s:80:TYR:O | 50:1s:81:ARG:HG2 | 2.21 | 0.41 |
| 1:2A:265:A:C8 | 1:2A:266:G:H1' | 2.55 | 0.41 |
| 1:2A:493:G:H2' | 1:2A:494:G:O4' | 2.21 | 0.41 |
| 1:2A:569:U:H1' | 1:2A:947:G:O4' | 2.21 | 0.41 |
| 1:2A:852:G:H2' | 1:2A:853:G:H8 | 1.84 | 0.41 |
| 1:2A:1278:A:H2' | 1:2A:1279:G:C8 | 2.56 | 0.41 |
| 1:2A:1471:A:OP2 | 1:2A:1519:G:N2 | 2.41 | 0.41 |
| 1:2A:2046:G:O5' | 27:25:19:ARG:HA | 2.19 | 0.41 |
| 1:2A:2690:C:N4 | 1:2A:2713:A:H1' | 2.35 | 0.41 |
| 6:2G:3:LEU:HD12 | 6:2G:8:LYS:HZ1 | 1.85 | 0.41 |
| 13:2R:62:ALA:O | 13:2R:66:VAL:HG23 | 2.21 | 0.41 |
| 16:2U:29:SER:OG | 16:2U:30:LYS:NZ | 2.44 | 0.41 |
| 20:2Y:20:TYR:CE2 | 20:2Y:43:ASN:HA | 2.56 | 0.41 |
| 32:2a:683:G:H2' | 32:2a:684:A:O4' | 2.20 | 0.41 |
| 32:2a:737:A:H2' | 32:2a:738:C:H6 | 1.84 | 0.41 |
| 32:2a:1023:G:H3' | 32:2a:1024:G:H8 | 1.85 | 0.41 |
| 33:2b:163:PHE:HD1 | 33:2b:185:ILE:HG13 | 1.85 | 0.41 |
| 35:2d:33:MET:HB2 | 60:2d:302:SF4:S2 | 2.60 | 0.41 |
| 43:2l:92:0TD:H4 | 43:2l:92:0TD:H8 | 1.74 | 0.41 |
| 1:1A:38:A:H2' | 1:1A:39:C:C6 | 2.55 | 0.41 |
| 1:1A:548:A:H61 | 17:1V:18:LEU:HA | 1.86 | 0.41 |
| 1:1A:1862:G:H2' | 1:1A:1863:G:C8 | 2.53 | 0.41 |
| 1:1A:2646:C:H2' | 1:1A:2647:U:O4' | 2.20 | 0.41 |
| 3:1D:80:ALA:HB3 | 3:1D:94:LEU:HD13 | 2.03 | 0.41 |
| 14:1S:43:GLU:OE2 | 22:10:49:LYS:HE3 | 2.20 | 0.41 |
| 24:12:2:LYS:O | 24:12:6:VAL:HG23 | 2.21 | 0.41 |
| 24:12:51:ARG:O | 24:12:55:ARG:HG2 | 2.20 | 0.41 |
| 32:1a:109:A:C6 | 32:1a:326:G:C6 | 3.08 | 0.41 |
| 33:1b:97:TRP:HZ2 | 33:1b:102:LEU:HD13 | 1.86 | 0.41 |
| 33:1b:114:ARG:NH1 | 33:1b:117:GLU:OE1 | 2.52 | 0.41 |
| 33:1b:158:LEU:HA | 33:1b:159:PRO:HD3 | 1.96 | 0.41 |
| 34:1c:73:PRO:O | 34:1c:77:ILE:HG12 | 2.21 | 0.41 |
| 34:1c:180:ALA:HB1 | 34:1c:203:PHE:CE1 | 2.55 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 36:1e:90:VAL:O | 36:1e:120:THR:HA | 2.19 | 0.41 |
| 54:1y:60:U:O2' | 54:1y:61:C:H5' | 2.21 | 0.41 |
| 1:2A:253:C:H2' | 1:2A:254:G:O4' | 2.21 | 0.41 |
| 1:2A:570:G:H2' | 1:2A:2030:A:C5 | 2.55 | 0.41 |
| 1:2A:940:G:N3 | 1:2A:1191:G:H4' | 2.36 | 0.41 |
| 1:2A:1368:G:OP1 | 29:27:28:ARG:NH2 | 2.53 | 0.41 |
| 1:2A:1783:A:H5' | 1:2A:2608:G:H4' | 2.03 | 0.41 |
| 1:2A:2165:G:H2' | 1:2A:2166:G:O4' | 2.20 | 0.41 |
| 1:2A:2313:C:H2' | 1:2A:2314:C:H6 | 1.85 | 0.41 |
| 1:2A:2431:U:O2' | 1:2A:2433:A:N7 | 2.46 | 0.41 |
| 1:2A:2648:C:H2' | 1:2A:2649:U:C6 | 2.55 | 0.41 |
| 1:2A:2812:G:H2' | 1:2A:2813:A:C8 | 2.55 | 0.41 |
| 3:2D:260:ARG:NH1 | 3:2D:267:SER:OG | 2.54 | 0.41 |
| 9:2N:103:VAL:O | 9:2N:107:LEU:HG | 2.20 | 0.41 |
| 10:2O:2:ILE:HB | 10:2O:33:ALA:HB3 | 2.01 | 0.41 |
| 32:2a:417:C:H2' | 32:2a:418:C:C6 | 2.55 | 0.41 |
| 32:2a:953:G:H5' | 32:2a:965:A:N6 | 2.25 | 0.41 |
| 32:2a:1347:G:H5" | 40:2i:107:ARG:HB3 | 2.02 | 0.41 |
| 35:2d:100:ARG:O | 35:2d:104:VAL:HG23 | 2.21 | 0.41 |
| 35:2d:150:GLU:OE1 | 35:2d:150:GLU:N | 2.50 | 0.41 |
| 47:2p:37:GLY:HA3 | 47:2p:50:LYS:O | 2.21 | 0.41 |
| 1:1A:620:G:N3 | 1:1A:620:G:H5' | 2.36 | 0.41 |
| 1:1A:764:A:O4' | 3:1D:213:ARG:HG3 | 2.21 | 0.41 |
| 1:1A:2695:C:H2' | 1:1A:2696:U:C6 | 2.56 | 0.41 |
| 10:1O:76:ALA:HB3 | 15:1T:75:ILE:HD12 | 2.02 | 0.41 |
| 13:1R:24:GLN:HB3 | 13:1R:44:LEU:HD11 | 2.01 | 0.41 |
| 21:1Z:54:HIS:CG | 21:1Z:101:PRO:HG3 | 2.56 | 0.41 |
| 28:16:25:LYS:HE3 | 28:16:27:LYS:HA | 2.03 | 0.41 |
| 32:1a:192:U:O3' | 51:1t:57:ARG:HD2 | 2.20 | 0.41 |
| 32:1a:510:A:H5" | 35:1d:49:ARG:HH12 | 1.86 | 0.41 |
| 32:1a:544:G:OP2 | 35:1d:66:ARG:NH2 | 2.54 | 0.41 |
| 32:1a:944:G:O6 | 32:1a:1337:G:H8 | 2.03 | 0.41 |
| 32:1a:960:U:H2' | 32:1a:1225:A:H62 | 1.86 | 0.41 |
| 32:1a:1003:G:C4 | 32:1a:1004:A:H2 | 2.38 | 0.41 |
| 32:1a:1123:A:O2' | 41:1j:37:PRO:O | 2.34 | 0.41 |
| 40:1i:18:PHE:HB2 | 40:1i:62:TYR:O | 2.20 | 0.41 |
| 48:1q:28:PRO:HA | 48:1q:35:VAL:HA | 2.02 | 0.41 |
| 1:2A:199:A:OP1 | 61:2A:5372:HOH:O | 2.22 | 0.41 |
| 1:2A:262:A:H2' | 1:2A:263:C:O4' | 2.20 | 0.41 |
| 1:2A:271(D):G:H2' | 1:2A:271(E):U:C6 | 2.55 | 0.41 |
| 1:2A:921:G:C6 | 1:2A:922:U:C4 | 3.09 | 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:2584:U:H2' | 1:2A:2585:U:H2' | 2.03 | 0.41 |
| 1:2A:2822:G:OP2 | 61:2A:6428:HOH:O | 2.21 | 0.41 |
| 1:2A:2836:U:H2' | 1:2A:2837:G:H8 | 1.82 | 0.41 |
| 2:2B:67:G:H2' | 2:2B:68:C:C6 | 2.55 | 0.41 |
| 10:2O:107:ARG:HG3 | 10:2O:112:MET:HE1 | 2.02 | 0.41 |
| 15:2T:39:ARG:HH12 | 15:2T:41:ARG:HB3 | 1.86 | 0.41 |
| 19:2X:44:GLU:O | 19:2X:48:LYS:N | 2.50 | 0.41 |
| 32:2a:1003:G:C5 | 32:2a:1004:A:C2 | 3.09 | 0.41 |
| 32:2a:1086:U:H2' | 32:2a:1087:G:H8 | 1.85 | 0.41 |
| 32:2a:1134:G:H1 | 32:2a:1140:C:H42 | 1.68 | 0.41 |
| 34:2c:120:VAL:HG13 | 34:2c:133:ALA:HB1 | 2.02 | 0.41 |
| 37:2f:50:TYR:CE2 | 49:2r:77:GLY:HA2 | 2.55 | 0.41 |
| 39:2h:17:THR:HA | 39:2h:65:TYR:HE1 | 1.85 | 0.41 |
| 50:2s:28:LYS:HB3 | 50:2s:29:ARG:CA | 2.51 | 0.41 |
| 1:1A:629:G:H1' | 1:1A:639:U:H1' | 2.03 | 0.41 |
| 1:1A:644:A:H4' | 1:1A:645:C:H5 | 1.85 | 0.41 |
| 1:1A:646:A:H2' | 1:1A:647:G:O4' | 2.20 | 0.41 |
| 1:1A:755:C:H2' | 1:1A:756:C:C6 | 2.55 | 0.41 |
| 1:1A:783:A:O2' | 1:1A:785:G:OP1 | 2.30 | 0.41 |
| 1:1A:1086:A:H3' | 1:1A:1086:A:N3 | 2.35 | 0.41 |
| 1:1A:1093:G:H3' | 1:1A:1094:U:H5" | 2.02 | 0.41 |
| 1:1A:1188:U:H4' | 17:1V:79:VAL:HG22 | 2.02 | 0.41 |
| 1:1A:1288:U:O4 | 13:1R:106:GLY:HA3 | 2.21 | 0.41 |
| 1:1A:1310:G:OP2 | 29:17:9:ARG:NH2 | 2.54 | 0.41 |
| 1:1A:1957:C:H2' | 1:1A:1958:C:C6 | 2.56 | 0.41 |
| 1:1A:2379:G:O2' | 14:1S:17:ARG:NH2 | 2.54 | 0.41 |
| 61:1A:6401:HOH:O | 25:13:13:ILE:O | 2.22 | 0.41 |
| 61:1A:4469:HOH:O | 55:1x:76:A:H1' | 2.21 | 0.41 |
| 4:1E:37:ARG:HD2 | 4:1E:42:ASP:CG | 2.45 | 0.41 |
| 15:1T:26:ASP:O | 15:1T:49:VAL:HG22 | 2.21 | 0.41 |
| 15:1T:27:THR:HB | 15:1T:90:GLN:HB3 | 2.03 | 0.41 |
| 26:14:64:GLY:C | 26:14:66:SER:N | 2.75 | 0.41 |
| 30:18:23:VAL:HG13 | 30:18:47:LYS:HB3 | 2.02 | 0.41 |
| 32:1a:78:G:C6 | 32:1a:91:C:C4 | 3.08 | 0.41 |
| 32:1a:156:G:H2' | 32:1a:157:G:C8 | 2.56 | 0.41 |
| 32:1a:221:C:H2' | 32:1a:222:U:H6 | 1.85 | 0.41 |
| 32:1a:1316:G:N1 | 32:1a:1319:A:OP2 | 2.53 | 0.41 |
| 33:1b:115:LEU:HD21 | 33:1b:153:ARG:NH1 | 2.36 | 0.41 |
| 33:1b:204:ASN:OD1 | 33:1b:206:ASP:N | 2.44 | 0.41 |
| 36:1e:102:ALA:HB1 | 36:1e:106:PRO:HB2 | 2.03 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 38:1g:27:ILE:HA | 38:1g:30:ILE:HD12 | 2.02 | 0.41 |
| 42:1k:98:LEU:O | 42:1k:101:SER:OG | 2.25 | 0.41 |
| 55:1x:23:C:H2' | 55:1x:24:U:C6 | 2.56 | 0.41 |
| 1:2A:26:G:C6 | 1:2A:27:G:N1 | 2.89 | 0.41 |
| 1:2A:747:U:O2' | 18:2W:92:ARG:NH2 | 2.44 | 0.41 |
| 1:2A:984:A:H5" | 1:2A:985:C:H5 | 1.86 | 0.41 |
| 1:2A:1031:G:H21 | 31:29:36:GLN:HE22 | 1.67 | 0.41 |
| 1:2A:1856:G:H1 | 1:2A:1886:C:H42 | 1.68 | 0.41 |
| 1:2A:1999:C:H5" | 1:2A:2723:C:O2' | 2.21 | 0.41 |
| 1:2A:2135:A:H5' | 1:2A:2159:G:H1' | 2.03 | 0.41 |
| 1:2A:2334:G:O6 | 22:20:74:ARG:NH1 | 2.46 | 0.41 |
| 1:2A:2745:C:C4 | 1:2A:2746:U:C4 | 3.09 | 0.41 |
| 61:2A:6160:HOH:O | 19:2X:57:LEU:HA | 2.20 | 0.41 |
| 4:2E:170:LEU:HB3 | 4:2E:184:VAL:CG2 | 2.51 | 0.41 |
| 6:2G:63:ILE:HD13 | 6:2G:141:PHE:CD2 | 2.55 | 0.41 |
| 6:2G:100:TRP:O | 6:2G:104:GLU:HB2 | 2.20 | 0.41 |
| 23:21:64:ALA:HA | 23:21:67:ILE:HG13 | 2.03 | 0.41 |
| 30:28:63:PRO:HG2 | 30:28:64:TYR:CE2 | 2.56 | 0.41 |
| 32:2a:63:C:H42 | 32:2a:104:G:H1 | 1.67 | 0.41 |
| 32:2a:473:G:H2' | 32:2a:474:G:H8 | 1.86 | 0.41 |
| 32:2a:921:U:O2 | 36:2e:19:MET:HB2 | 2.20 | 0.41 |
| 33:2b:51:LEU:O | 33:2b:55:PHE:HB2 | 2.20 | 0.41 |
| 34:2c:131:ARG:HH11 | 34:2c:166:GLU:HG3 | 1.85 | 0.41 |
| 35:2d:77:ASN:HD22 | 35:2d:77:ASN:HA | 1.62 | 0.41 |
| 35:2d:156:GLU:HG3 | 35:2d:159:ARG:NH2 | 2.36 | 0.41 |
| 39:2h:20:TYR:CZ | 39:2h:75:ARG:HB3 | 2.56 | 0.41 |
| 39:2h:119:LEU:HB3 | 39:2h:123:GLU:HB2 | 2.01 | 0.41 |
| 44:2m:82:MET:HG2 | 44:2m:89:GLY:O | 2.21 | 0.41 |
| 1:1A:536:A:H2' | 1:1A:537:C:C6 | 2.56 | 0.41 |
| 1:1A:589:C:H2' | 1:1A:590:A:C8 | 2.56 | 0.41 |
| 1:1A:662:G:H5' | 11:1P:14:LYS:O | 2.21 | 0.41 |
| 1:1A:735:A:N7 | 1:1A:761:A:H2 | 2.19 | 0.41 |
| 1:1A:996:A:H4' | 16:1U:91:ASP:OD2 | 2.21 | 0.41 |
| 1:1A:1183:G:O2' | 25:13:29:ARG:NH1 | 2.54 | 0.41 |
| 1:1A:1239:G:H2' | 1:1A:1240:U:O4' | 2.21 | 0.41 |
| 1:1A:1889:A:H2' | 1:1A:1890:A:C8 | 2.56 | 0.41 |
| 1:1A:1932:A:H2' | 1:1A:1933:G:O4' | 2.21 | 0.41 |
| 1:1A:2105:C:H2' | 1:1A:2106:G:H8 | 1.83 | 0.41 |
| 1:1A:2140:C:H2' | 1:1A:2141:G:C8 | 2.55 | 0.41 |
| 1:1A:2233:U:H2' | 1:1A:2234:G:C8 | 2.56 | 0.41 |
| 1:1A:2352:A:N6 | 1:1A:2365:G:O2' | 2.53 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1A:2732:G:OP1 | 4:1E:203:LYS:NZ | 2.48 | 0.41 |
| 61:1A:5688:HOH:O | 11:1P:42:SER:O | 2.21 | 0.41 |
| 11:1P:135:LEU:HD23 | 11:1P:135:LEU:HA | 1.85 | 0.41 |
| 13:1R:2:ARG:HG2 | 13:1R:5:LYS:HB2 | 2.03 | 0.41 |
| 16:1U:8:VAL:HG23 | 16:1U:11:ARG:HH21 | 1.86 | 0.41 |
| 21:1Z:92:SER:O | 21:1Z:130:PRO:HG2 | 2.20 | 0.41 |
| 30:18:26:LYS:HB2 | 30:18:44:LYS:O | 2.21 | 0.41 |
| 32:1a:152:A:N6 | 32:1a:170:U:C2 | 2.88 | 0.41 |
| 32:1a:376:G:OP2 | 47:1p:67:THR:HG21 | 2.21 | 0.41 |
| 32:1a:413:G:O6 | 35:1d:35:ARG:HD3 | 2.21 | 0.41 |
| 32:1a:652:U:O4 | 32:1a:752:G:O2' | 2.34 | 0.41 |
| 32:1a:739:C:O2' | 46:1o:42:HIS:ND1 | 2.53 | 0.41 |
| 32:1a:888:G:H8 | 32:1a:888:G:O5' | 2.04 | 0.41 |
| 32:1a:921:U:H2' | 32:1a:922:G:O4' | 2.21 | 0.41 |
| 32:1a:947:G:C6 | 32:1a:948:C:C4 | 3.09 | 0.41 |
| 32:1a:1026:G:C8 | 32:1a:1027:C:O2 | 2.73 | 0.41 |
| 32:1a:1201:A:H1' | 32:1a:1202:G:OP2 | 2.21 | 0.41 |
| 32:1a:1350:A:O2' | 38:1g:33:ASP:OD1 | 2.28 | 0.41 |
| 32:1a:1381:U:H1' | 38:1g:79:ARG:HG2 | 2.02 | 0.41 |
| 32:1a:1510:U:H1' | 32:1a:1526:G:N2 | 2.36 | 0.41 |
| 33:1b:128:GLU:HG3 | 33:1b:135:GLN:HE22 | 1.86 | 0.41 |
| 36:1e:59:GLY:O | 36:1e:63:ARG:HG3 | 2.20 | 0.41 |
| 38:1g:18:TYR:CE1 | 38:1g:59:LEU:HB2 | 2.56 | 0.41 |
| 41:1j:13:HIS:O | 41:1j:17:ASP:N | 2.38 | 0.41 |
| 42:1k:86:GLY:O | 42:1k:91:ARG:HD3 | 2.21 | 0.41 |
| 43:1l:54:LYS:HG2 | 43:1l:75:HIS:HD2 | 1.85 | 0.41 |
| 1:2A:355:G:H2' | 1:2A:356:G:O4' | 2.21 | 0.41 |
| 1:2A:656:G:H2' | 1:2A:657:U:O4' | 2.20 | 0.41 |
| 1:2A:723:G:H2' | 1:2A:724:U:O4' | 2.21 | 0.41 |
| 1:2A:1031:G:N2 | 31:29:36:GLN:HE22 | 2.18 | 0.41 |
| 1:2A:1599:C:H2' | 1:2A:1600:C:C6 | 2.56 | 0.41 |
| 1:2A:2218:U:H1' | 23:21:52:ARG:HH12 | 1.86 | 0.41 |
| 1:2A:2295:C:H41 | 14:2S:13:ARG:NH1 | 2.18 | 0.41 |
| 1:2A:2300:G:C6 | 1:2A:2301:C:C4 | 3.09 | 0.41 |
| 1:2A:2579:C:OP1 | 61:2A:3903:HOH:O | 2.22 | 0.41 |
| 1:2A:2784:C:H2' | 1:2A:2785:C:C6 | 2.55 | 0.41 |
| 2:2B:59:A:H2' | 2:2B:60:C:O4' | 2.21 | 0.41 |
| 3:2D:211:ARG:HG3 | 3:2D:214:TRP:CE3 | 2.55 | 0.41 |
| 4:2E:12:THR:HG21 | 15:2T:11:GLU:HG2 | 2.03 | 0.41 |
| 6:2G:51:ARG:HD3 | 6:2G:52:ILE:H | 1.85 | 0.41 |
| 10:2O:70:LYS:HB3 | 10:2O:70:LYS:HE2 | 1.92 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 15:2T:102:ILE:HB | 15:2T:110:ILE:HG12 | 2.03 | 0.41 |
| 17:2V:3:ALA:HB3 | 17:2V:14:VAL:HG23 | 2.03 | 0.41 |
| 17:2V:62:LEU:HD23 | 17:2V:93:GLU:HG2 | 2.03 | 0.41 |
| 23:21:83:GLU:OE1 | 23:21:83:GLU:N | 2.54 | 0.41 |
| 24:22:1:MET:N | 24:22:52:ASP:OD1 | 2.51 | 0.41 |
| 28:26:8:LYS:HG2 | 30:28:34:TRP:CD1 | 2.56 | 0.41 |
| 32:2a:14:U:H5" | 61:2a:3452:HOH:O | 2.19 | 0.41 |
| 32:2a:147:G:H1 | 32:2a:175:C:H42 | 1.69 | 0.41 |
| 32:2a:509:A:H2' | 32:2a:510:A:C8 | 2.56 | 0.41 |
| 32:2a:577:G:C8 | 32:2a:816:A:C6 | 3.08 | 0.41 |
| 32:2a:612:C:N4 | 61:2a:3560:HOH:O | 2.53 | 0.41 |
| 32:2a:664:G:N2 | 32:2a:741:G:H1 | 2.09 | 0.41 |
| 32:2a:714:G:H2' | 32:2a:715:A:C8 | 2.56 | 0.41 |
| 32:2a:1094:G:O2' | 32:2a:1108:G:N2 | 2.47 | 0.41 |
| 32:2a:1161:C:H2' | 32:2a:1162:C:C6 | 2.56 | 0.41 |
| 32:2a:1251:A:H2' | 32:2a:1252:A:C8 | 2.56 | 0.41 |
| 32:2a:1502:A:H5' | 32:2a:1504:G:N7 | 2.36 | 0.41 |
| 33:2b:97:TRP:HZ2 | 33:2b:102:LEU:HD13 | 1.86 | 0.41 |
| 33:2b:168:THR:OG1 | 33:2b:191:ASP:O | 2.34 | 0.41 |
| 35:2d:38:TYR:CE1 | 35:2d:45:GLN:HG3 | 2.56 | 0.41 |
| 37:2f:11:ASN:HB3 | 37:2f:14:LEU:HG | 2.02 | 0.41 |
| 37:2f:97:PHE:CE1 | 49:2r:61:LYS:HE2 | 2.56 | 0.41 |
| 44:2m:91:ARG:HG2 | 44:2m:96:LEU:HB2 | 2.03 | 0.41 |
| 54:2w:10:G:N2 | 54:2w:11:C:C2 | 2.89 | 0.41 |
| 54:2w:56:C:H2' | 54:2w:57:G:O4' | 2.20 | 0.41 |
| 1:1A:969:U:H2' | 1:1A:970:C:C6 | 2.56 | 0.41 |
| 1:1A:1063:G:C5 | 1:1A:1064:C:N4 | 2.89 | 0.41 |
| 1:1A:1286:A:C6 | 1:1A:1329:U:C2 | 3.09 | 0.41 |
| 1:1A:2364:C:OP1 | 22:10:55:ARG:NH1 | 2.54 | 0.41 |
| 1:1A:2448:A:OP1 | 61:1A:6393:HOH:O | 2.22 | 0.41 |
| 61:1A:4208:HOH:O | 22:10:41:ARG:HA | 2.21 | 0.41 |
| 3:1D:168:ARG:HA | 3:1D:173:VAL:HA | 2.03 | 0.41 |
| 5:1F:150:GLY:HA2 | 5:1F:172:TRP:CD2 | 2.55 | 0.41 |
| 11:1P:88:LEU:HD11 | 11:1P:114:ILE:HD12 | 2.03 | 0.41 |
| 12:1Q:38:GLU:HG3 | 12:1Q:127:ILE:HB | 2.02 | 0.41 |
| 14:1S:87:PHE:CZ | 14:1S:102:ALA:HB2 | 2.55 | 0.41 |
| 32:1a:130:A:O2' | 32:1a:131:C:O5' | 2.33 | 0.41 |
| 32:1a:156:G:H2' | 32:1a:157:G:H8 | 1.86 | 0.41 |
| 32:1a:840:C:H4' | 32:1a:841:U:OP1 | 2.20 | 0.41 |
| 32:1a:1039:C:H2' | 32:1a:1040:U:C6 | 2.56 | 0.41 |
| 32:1a:1151:A:O2' | 32:1a:1152:A:H8 | 2.03 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 32:1a:1183:A:O2' | 32:1a:1184:G:OP1 | 2.37 | 0.41 |
| 35:1d:11:LEU:HG | 35:1d:66:ARG:HD3 | 2.03 | 0.41 |
| 43:1l:53:ARG:HB2 | 43:1l:93:LEU:HD11 | 2.02 | 0.41 |
| 44:1m:65:LYS:HB2 | 44:1m:65:LYS:HE3 | 1.91 | 0.41 |
| 48:1q:50:LYS:HE3 | 48:1q:51:TYR:CE2 | 2.56 | 0.41 |
| 50:1s:80:TYR:C | 50:1s:82:GLY:H | 2.29 | 0.41 |
| 54:1w:9:A:C6 | 54:1w:45:U:C4 | 3.09 | 0.41 |
| 54:1w:50:U:O4 | 54:1w:64:A:N1 | 2.54 | 0.41 |
| 55:1x:25:C:H2' | 55:1x:26:G:O4' | 2.20 | 0.41 |
| 55:1x:66:C:H2' | 55:1x:67:C:O4' | 2.20 | 0.41 |
| 1:2A:380:U:H2' | 1:2A:381:G:C8 | 2.55 | 0.41 |
| 1:2A:2356:C:H2' | 1:2A:2357:U:O4' | 2.21 | 0.41 |
| 1:2A:2400:G:H2' | 1:2A:2401:U:H6 | 1.86 | 0.41 |
| 4:2E:12:THR:HG22 | 4:2E:13:ARG:H | 1.86 | 0.41 |
| 6:2G:41:GLN:HG2 | 6:2G:154:GLY:O | 2.21 | 0.41 |
| 32:2a:528:C:H41 | 43:2l:49:ASN:ND2 | 2.20 | 0.41 |
| 32:2a:540:G:H2' | 32:2a:541:G:O4' | 2.21 | 0.41 |
| 32:2a:577:G:H2' | 32:2a:578:C:H6 | 1.86 | 0.41 |
| 32:2a:826:C:H2' | 32:2a:827:U:C6 | 2.55 | 0.41 |
| 32:2a:1030(A):G:C2 | 32:2a:1030(C):G:H5" | 2.55 | 0.41 |
| 32:2a:1353:G:H2' | 32:2a:1354:C:H6 | 1.86 | 0.41 |
| 33:2b:167:PRO:HD3 | 33:2b:187:LEU:O | 2.20 | 0.41 |
| 35:2d:61:LYS:HD2 | 35:2d:207:TYR:OH | 2.21 | 0.41 |
| 35:2d:110:PHE:N | 35:2d:110:PHE:CD1 | 2.89 | 0.41 |
| 39:2h:26:VAL:O | 39:2h:59:LEU:N | 2.51 | 0.41 |
| 44:2m:25:ILE:HG13 | 44:2m:66:LEU:HD22 | 2.02 | 0.41 |
| 50:2s:20:LEU:HA | 50:2s:20:LEU:HD23 | 1.86 | 0.41 |
| 54:2y:72:C:H2' | 54:2y:73:A:O4' | 2.21 | 0.41 |
| 1:1A:228:A:H3' | 1:1A:229:A:C5' | 2.49 | 0.40 |
| 1:1A:942:G:OP2 | 11:1P:39:LYS:HE2 | 2.21 | 0.40 |
| 1:1A:1336:A:H2' | 1:1A:1337:G:C8 | 2.56 | 0.40 |
| 1:1A:1655:A:H3' | 1:1A:1656:C:C6 | 2.56 | 0.40 |
| 1:1A:1789:A:H5" | 3:1D:220:HIS:O | 2.21 | 0.40 |
| 1:1A:1920:4OC:H6 | 1:1A:1920:4OC:O5' | 2.21 | 0.40 |
| 1:1A:2408:U:H2' | 1:1A:2409:G:C8 | 2.56 | 0.40 |
| 4:1E:9:VAL:HG13 | 4:1E:25:VAL:O | 2.21 | 0.40 |
| 7:1H:3:ARG:NH2 | 7:1H:65:HIS:HB3 | 2.37 | 0.40 |
| 9:1N:108:PRO:O | 9:1N:113:GLY:HA3 | 2.21 | 0.40 |
| 10:1O:86:ILE:HG22 | 10:1O:94:ARG:HD3 | 2.03 | 0.40 |
| 14:1S:5:THR:OG1 | 14:1S:8:GLU:HG2 | 2.21 | 0.40 |
| 18:1W:18:ARG:HG2 | 18:1W:76:VAL:HB | 2.02 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 32:1a:359:U:H2' | 32:1a:360:A:C8 | 2.56 | 0.40 |
| 32:1a:993:G:H2' | 32:1a:995:C:H41 | 1.86 | 0.40 |
| 32:1a:999:C:H42 | 32:1a:1042:G:H1 | 1.68 | 0.40 |
| 32:1a:1312:G:N7 | 50:1s:2:PRO:HD2 | 2.35 | 0.40 |
| 32:1a:1379:G:OP1 | 38:1g:6:ARG:NH1 | 2.55 | 0.40 |
| 32:1a:1509:C:H2' | 32:1a:1510:U:O4' | 2.21 | 0.40 |
| 40:1i:100:GLY:O | 40:1i:103:THR:HG22 | 2.21 | 0.40 |
| 43:1l:113:ARG:HD2 | 43:1l:113:ARG:HA | 1.93 | 0.40 |
| 54:1y:4:C:H2' | 54:1y:5:G:O4' | 2.21 | 0.40 |
| 1:2A:136:G:H2' | 1:2A:137:C:C6 | 2.56 | 0.40 |
| 1:2A:271(Z):C:OP2 | 61:2A:6005:HOH:O | 2.22 | 0.40 |
| 1:2A:1252:G:N2 | 16:2U:37:GLU:OE2 | 2.48 | 0.40 |
| 1:2A:1266:G:O2' | 1:2A:2012:G:O6 | 2.19 | 0.40 |
| 1:2A:2053:G:OP2 | 61:2A:4832:HOH:O | 2.22 | 0.40 |
| 12:2Q:2:LEU:HD12 | 12:2Q:69:PHE:CE1 | 2.57 | 0.40 |
| 12:2Q:34:LEU:HB2 | 12:2Q:118:LEU:HD22 | 2.03 | 0.40 |
| 15:2T:64:ARG:HB2 | 15:2T:73:GLU:HG2 | 2.02 | 0.40 |
| 15:2T:118:ARG:HB3 | 32:2a:1442(A):G:C5 | 2.57 | 0.40 |
| 32:2a:580:U:H5" | 46:2o:58:MET:HG2 | 2.03 | 0.40 |
| 32:2a:1060:C:H2' | 32:2a:1061:G:H8 | 1.87 | 0.40 |
| 32:2a:1068:G:H8 | 32:2a:1068:G:OP2 | 2.03 | 0.40 |
| 32:2a:1219:U:OP1 | 45:2n:19:ARG:NH1 | 2.30 | 0.40 |
| 33:2b:28:PHE:CD1 | 33:2b:194:PRO:HG3 | 2.55 | 0.40 |
| 34:2c:151:VAL:HG22 | 34:2c:200:ALA:HA | 2.03 | 0.40 |
| 35:2d:4:TYR:O | 35:2d:5:ILE:HG22 | 2.21 | 0.40 |
| 35:2d:61:LYS:HE3 | 35:2d:61:LYS:HB3 | 1.95 | 0.40 |
| 36:2e:78:HIS:HE1 | 36:2e:143:ARG:N | 2.19 | 0.40 |
| 43:2l:10:LEU:HB3 | 48:2q:32:TYR:CE2 | 2.56 | 0.40 |
| 1:1A:30:G:H2' | 1:1A:31:C:C6 | 2.56 | 0.40 |
| 1:1A:330:A:N7 | 1:1A:1210:A:O2' | 2.35 | 0.40 |
| 1:1A:857:C:N4 | 1:1A:858:U:O4 | 2.55 | 0.40 |
| 1:1A:1106:G:H2' | 1:1A:1107:G:O4' | 2.21 | 0.40 |
| 1:1A:1156:A:OP2 | 61:1A:6455:HOH:O | 2.21 | 0.40 |
| 1:1A:1570:A:H2' | 1:1A:1571:A:C8 | 2.56 | 0.40 |
| 1:1A:1862:G:C2 | 1:1A:1881:C:C2 | 3.09 | 0.40 |
| 1:1A:2142:C:H2' | 1:1A:2143:C:C6 | 2.56 | 0.40 |
| 1:1A:2280:G:O2' | 1:1A:2388:A:N1 | 2.45 | 0.40 |
| 1:1A:2443:C:OP1 | 5:1F:68:LYS:HD3 | 2.21 | 0.40 |
| 5:1F:135:LYS:HE3 | 5:1F:135:LYS:HB3 | 1.90 | 0.40 |
| 7:1H:127:GLU:CD | 7:1H:130:ARG:HE | 2.29 | 0.40 |
| 9:1N:61:ARG:HD3 | 9:1N:61:ARG:HA | 1.87 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 20:1Y:19:LYS:HE2 | 20:1Y:19:LYS:HB3 | 1.78 | 0.40 |
| 32:1a:16:A:N1 | 32:1a:919:A:H2 | 2.19 | 0.40 |
| 32:1a:626:U:C2 | 32:1a:627:G:C8 | 3.10 | 0.40 |
| 32:1a:1139:G:H4' | 32:1a:1140:C:H5' | 2.03 | 0.40 |
| 32:1a:1241:G:H2' | 32:1a:1242:C:C6 | 2.57 | 0.40 |
| 33:1b:9:GLU:HA | 33:1b:48:MET:SD | 2.61 | 0.40 |
| 34:1c:148:GLY:HA3 | 34:1c:172:ARG:O | 2.22 | 0.40 |
| 55:1x:32:5MC:HM52 | 55:1x:33:U:O4 | 2.21 | 0.40 |
| 1:2A:271:A:N6 | 1:2A:271(X):G:H1' | 2.37 | 0.40 |
| 1:2A:643:A:N1 | 1:2A:2369:A:O2' | 2.50 | 0.40 |
| 1:2A:1353:A:H2' | 1:2A:1354:A:C8 | 2.56 | 0.40 |
| 1:2A:1448:G:H2' | 1:2A:1449:A:C8 | 2.57 | 0.40 |
| 1:2A:2119:A:H2 | 1:2A:2171:A:H5' | 1.86 | 0.40 |
| 1:2A:2758:A:C2 | 1:2A:2759:G:H1' | 2.56 | 0.40 |
| 5:2F:140:LEU:HD11 | 5:2F:170:LEU:HD11 | 2.03 | 0.40 |
| 9:2N:104:LYS:HA | 9:2N:107:LEU:HD12 | 2.02 | 0.40 |
| 10:2O:4:PRO:HD3 | 10:2O:24:VAL:HG23 | 2.02 | 0.40 |
| 22:20:11:ARG:O | 22:20:14:ARG:NH2 | 2.54 | 0.40 |
| 24:22:51:ARG:O | 24:22:55:ARG:HG2 | 2.21 | 0.40 |
| 24:22:64:LEU:HD11 | 24:22:68:ARG:NH2 | 2.35 | 0.40 |
| 25:23:11:SER:HA | 25:23:31:LEU:HD21 | 2.02 | 0.40 |
| 32:2a:113:G:O2' | 32:2a:354:G:H5' | 2.22 | 0.40 |
| 32:2a:860:A:H2' | 32:2a:861:G:O4' | 2.21 | 0.40 |
| 32:2a:1015:A:H1' | 32:2a:1219:U:H5' | 2.03 | 0.40 |
| 32:2a:1298:C:C5 | 38:2g:114:ARG:HD3 | 2.57 | 0.40 |
| 32:2a:1410:G:H2' | 32:2a:1411:C:C6 | 2.56 | 0.40 |
| 34:2c:164:ARG:HG2 | 34:2c:165:THR:H | 1.86 | 0.40 |
| 37:2f:37:VAL:HA | 37:2f:65:VAL:HG12 | 2.04 | 0.40 |
| 41:2j:57:LYS:HE2 | 41:2j:60:ARG:NH2 | 2.35 | 0.40 |
| 46:2o:39:LEU:HD12 | 46:2o:59:MET:HE3 | 2.03 | 0.40 |
| 50:2s:27:GLU:OE1 | 50:2s:27:GLU:N | 2.52 | 0.40 |
| 1:1A:580:C:H2' | 1:1A:581:C:C6 | 2.56 | 0.40 |
| 1:1A:695:G:OP1 | 1:1A:1380:G:O2' | 2.35 | 0.40 |
| 1:1A:781:A:OP1 | 3:1D:218:ARG:NH2 | 2.55 | 0.40 |
| 1:1A:858:U:O2 | 1:1A:2268:A:H2' | 2.21 | 0.40 |
| 1:1A:1038:C:H42 | 1:1A:1117:G:H1 | 1.67 | 0.40 |
| 1:1A:1608:A:H1' | 1:1A:1610:A:OP2 | 2.22 | 0.40 |
| 5:1F:197:ASP:O | 5:1F:201:VAL:HG13 | 2.21 | 0.40 |
| 15:1T:127:ALA:C | 15:1T:129:ARG:N | 2.77 | 0.40 |
| 32:1a:34:C:H2' | 32:1a:35:G:H8 | 1.87 | 0.40 |
| 32:1a:376:G:O3' | 47:1p:5:ARG:NH1 | 2.43 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 32:1a:803:G:OP1 | 61:1a:2104:HOH:O | 2.21 | 0.40 |
| 32:1a:1376:U:H2' | 32:1a:1377:A:H8 | 1.86 | 0.40 |
| 43:1l:54:LYS:N | 43:1l:54:LYS:HD2 | 2.36 | 0.40 |
| 1:2A:109:G:H2' | 1:2A:110:G:O4' | 2.22 | 0.40 |
| 1:2A:297:C:OP1 | 20:2Y:87:LYS:HG3 | 2.20 | 0.40 |
| 1:2A:527:C:H4' | 1:2A:528:A:O5' | 2.21 | 0.40 |
| 1:2A:847:U:H5' | 1:2A:848:G:OP2 | 2.21 | 0.40 |
| 1:2A:857:C:H4' | 22:20:23:VAL:HG21 | 2.03 | 0.40 |
| 1:2A:902:C:H2' | 1:2A:903:C:H6 | 1.86 | 0.40 |
| 1:2A:1027:A:N6 | 1:2A:1126:A:C4 | 2.90 | 0.40 |
| 1:2A:1147:C:H2' | 1:2A:1148:A:C8 | 2.56 | 0.40 |
| 1:2A:1270:C:H5" | 1:2A:1271:G:O5' | 2.22 | 0.40 |
| 1:2A:1614:A:H8 | 1:2A:1614:A:P | 2.44 | 0.40 |
| 1:2A:2324:C:H2' | 1:2A:2385:C:H5 | 1.87 | 0.40 |
| 1:2A:2652:C:H42 | 1:2A:2668:G:H1 | 1.69 | 0.40 |
| 7:2H:25:LYS:HE2 | 7:2H:27:LYS:NZ | 2.36 | 0.40 |
| 7:2H:143:GLN:NE2 | 7:2H:147:ASN:OD1 | 2.54 | 0.40 |
| 16:2U:65:ILE:HD13 | 16:2U:95:LEU:HD23 | 2.04 | 0.40 |
| 19:2X:84:ALA:HB3 | 19:2X:87:GLN:CD | 2.46 | 0.40 |
| 21:2Z:80:ARG:HB3 | 21:2Z:82:ARG:HD3 | 2.04 | 0.40 |
| 32:2a:575:G:O4' | 32:2a:881:G:N2 | 2.54 | 0.40 |
| 32:2a:701:C:OP1 | 32:2a:702:A:O2' | 2.19 | 0.40 |
| 32:2a:783:C:H2' | 32:2a:784:C:C6 | 2.55 | 0.40 |
| 32:2a:918:A:H2' | 32:2a:919:A:O4' | 2.22 | 0.40 |
| 32:2a:990:C:H2' | 32:2a:991:U:C6 | 2.57 | 0.40 |
| 32:2a:1085:U:H3' | 32:2a:1086:U:C5 | 2.57 | 0.40 |
| 32:2a:1177:G:H2' | 32:2a:1178:G:O4' | 2.21 | 0.40 |
| 32:2a:1359:C:OP2 | 45:2n:35:ARG:NH1 | 2.55 | 0.40 |
| 33:2b:63:MET:HG3 | 33:2b:225:ALA:HB1 | 2.02 | 0.40 |
| 33:2b:95:GLN:HB2 | 33:2b:148:TYR:CD1 | 2.56 | 0.40 |
| 33:2b:98:LEU:HD13 | 33:2b:108:ILE:HD12 | 2.02 | 0.40 |
| 33:2b:146:GLN:O | 33:2b:150:SER:HB3 | 2.22 | 0.40 |
| 34:2c:22:TRP:HZ3 | 34:2c:24:ALA:HB2 | 1.85 | 0.40 |
| 36:2e:7:GLU:N | 36:2e:35:GLY:O | 2.39 | 0.40 |
| 36:2e:139:LEU:HA | 36:2e:142:LEU:HD12 | 2.04 | 0.40 |
| 37:2f:37:VAL:HG13 | 37:2f:65:VAL:HG12 | 2.02 | 0.40 |
| 41:2j:40:LEU:HB2 | 41:2j:69:ASN:CB | 2.46 | 0.40 |
| 45:2n:14:PRO:HG3 | 45:2n:20:ALA:HB2 | 2.03 | 0.40 |
| 55:2x:23:C:H2' | 55:2x:24:U:H6 | 1.82 | 0.40 |
| 54:2y:48:C:C2 | 54:2y:59:U:H1' | 2.56 | 0.40 |
| 54:2y:63:G:H2' | 54:2y:64:A:O4' | 2.22 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1A:86:C:H4' | 1:1A:104:U:H1' | 2.03 | 0.40 |
| 1:1A:1164:G:H2' | 1:1A:1165:U:C6 | 2.57 | 0.40 |
| 1:1A:1923:U:H2' | 1:1A:1924:C:C6 | 2.55 | 0.40 |
| 1:1A:2031:A:C6 | 1:1A:2498:C:H1' | 2.57 | 0.40 |
| 1:1A:2065:C:H2' | 1:1A:2066:C:C6 | 2.56 | 0.40 |
| 7:1H:3:ARG:NH1 | 7:1H:5:GLY:H | 2.20 | 0.40 |
| 24:12:1:MET:HE2 | 24:12:6:VAL:HG22 | 2.03 | 0.40 |
| 25:13:6:VAL:HG13 | 25:13:54:VAL:CG1 | 2.50 | 0.40 |
| 28:16:9:LEU:HD11 | 28:16:34:LEU:HD12 | 2.04 | 0.40 |
| 32:1a:229:U:H2' | 32:1a:230:G:C8 | 2.56 | 0.40 |
| 32:1a:625:G:H2' | 32:1a:626:U:C6 | 2.57 | 0.40 |
| 32:1a:946:A:O2' | 32:1a:1333:A:N3 | 2.45 | 0.40 |
| 32:1a:1044:A:C5 | 32:1a:1045:C:H1' | 2.56 | 0.40 |
| 32:1a:1263:C:H2' | 32:1a:1264:C:C6 | 2.55 | 0.40 |
| 32:1a:1333:A:H2' | 32:1a:1334:G:O4' | 2.22 | 0.40 |
| 34:1c:119:ARG:HE | 34:1c:140:ARG:CZ | 2.34 | 0.40 |
| 54:1w:35:A:H2' | 54:1w:36:A:O4' | 2.22 | 0.40 |
| 54:1y:35:A:H8 | 54:1y:35:A:OP2 | 2.04 | 0.40 |
| 1:2A:384:U:H2' | 1:2A:385:C:H6 | 1.86 | 0.40 |
| 1:2A:797:C:OP1 | 5:2F:60:SER:OG | 2.37 | 0.40 |
| 1:2A:863:A:P | 12:2Q:22:LYS:HG3 | 2.61 | 0.40 |
| 1:2A:1019:U:OP1 | 1:2A:1035:U:O2' | 2.30 | 0.40 |
| 1:2A:1541:G:H3' | 1:2A:1542:A:H8 | 1.86 | 0.40 |
| 1:2A:1786:A:H1' | 1:2A:1938:A:N6 | 2.37 | 0.40 |
| 1:2A:2843:G:H1 | 1:2A:2874:C:H42 | 1.69 | 0.40 |
| 4:2E:169:ASN:HB2 | 4:2E:203:LYS:HG3 | 2.03 | 0.40 |
| 15:2T:11:GLU:OE1 | 15:2T:57:PHE:HB3 | 2.21 | 0.40 |
| 15:2T:82:LEU:HA | 15:2T:82:LEU:HD23 | 1.82 | 0.40 |
| 24:22:12:GLU:O | 24:22:16:LEU:HG | 2.22 | 0.40 |
| 27:25:16:ARG:HG3 | 27:25:17:ASP:N | 2.37 | 0.40 |
| 32:2a:284:G:H2' | 32:2a:285:G:H8 | 1.84 | 0.40 |
| 32:2a:690:G:O6 | 42:2k:55:LYS:NZ | 2.54 | 0.40 |
| 32:2a:1169:A:H2' | 32:2a:1170:A:C8 | 2.57 | 0.40 |
| 32:2a:1225:A:H2' | 32:2a:1226:C:C5 | 2.56 | 0.40 |
| 32:2a:1275:A:H3' | 32:2a:1276:G:C8 | 2.53 | 0.40 |
| 33:2b:133:LYS:HE3 | 33:2b:133:LYS:HB2 | 1.89 | 0.40 |
| 35:2d:3:ARG:NH1 | 35:2d:5:ILE:HG13 | 2.36 | 0.40 |
| 36:2e:89:ILE:HD12 | 36:2e:89:ILE:HA | 1.83 | 0.40 |
| 37:2f:82:ARG:HB2 | 37:2f:85:VAL:HG23 | 2.02 | 0.40 |
| 1:1A:214:G:O2' | 1:1A:216:A:O2' | 2.31 | 0.40 |
| 2:1B:14:U:OP2 | 2:1B:70:C:O2' | 2.39 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 11:1P:111:ARG:HB3 | 11:1P:128:HIS:CG | 2.56 | 0.40 |
| 11:1P:120:ALA:HB2 | 11:1P:137:LYS:HB3 | 2.03 | 0.40 |
| 32:1a:115:G:H4' | 32:1a:116:A:O5' | 2.21 | 0.40 |
| 32:1a:1284:C:H3' | 32:1a:1285:A:H8 | 1.86 | 0.40 |
| 33:1b:62:ALA:HB3 | 33:1b:225:ALA:HB3 | 2.03 | 0.40 |
| 33:1b:115:LEU:HD21 | 33:1b:153:ARG:HH11 | 1.86 | 0.40 |
| 38:1g:28:ASN:HD21 | 38:1g:36:LYS:NZ | 2.19 | 0.40 |
| 41:1j:39:PRO:HA | 41:1j:70:ARG:HD3 | 2.03 | 0.40 |
| 47:1p:60:LEU:HD12 | 47:1p:60:LEU:HA | 1.90 | 0.40 |
| 1:2A:918:A:C5 | 1:2A:919:G:H1' | 2.57 | 0.40 |
| 1:2A:1372:U:H2' | 1:2A:1373:A:O4' | 2.21 | 0.40 |
| 1:2A:1915:5MU:H2' | 1:2A:1916:A:O4' | 2.21 | 0.40 |
| 1:2A:1987:G:H2' | 1:2A:1988:C:C6 | 2.56 | 0.40 |
| 1:2A:2050:C:N4 | 1:2A:2051:A:N1 | 2.70 | 0.40 |
| 3:2D:17:THR:HG1 | 3:2D:205:VAL:H | 1.64 | 0.40 |
| 19:2X:5:TYR:CZ | 24:22:30:ARG:HD2 | 2.57 | 0.40 |
| 21:2Z:71:VAL:HG22 | 21:2Z:88:PHE:CE1 | 2.57 | 0.40 |
| 32:2a:427:U:O2' | 32:2a:541:G:OP1 | 2.27 | 0.40 |
| 32:2a:495:A:H1' | 32:2a:496:A:H5" | 2.04 | 0.40 |
| 32:2a:875:C:H1' | 39:2h:15:ASN:HD21 | 1.86 | 0.40 |
| 32:2a:1347:G:H8 | 40:2i:107:ARG:HB2 | 1.85 | 0.40 |
| 32:2a:1353:G:C2 | 32:2a:1370:G:C2 | 3.09 | 0.40 |
| 35:2d:116:GLN:O | 35:2d:120:LEU:HG | 2.21 | 0.40 |
| 43:2l:59:ARG:HA | 43:2l:65:GLU:HA | 2.02 | 0.40 |
| 48:2q:40:LYS:HD3 | 48:2q:42:TYR:OH | 2.22 | 0.40 |
| 51:2t:43:LEU:HD13 | 51:2t:51:GLU:HB3 | 2.04 | 0.40 |
| 54:2y:9:A:O5' | 54:2y:46:7MG:N2 | 2.36 | 0.40 |

There are no symmetry-related clashes.

## 5.3 Torsion angles (i)

### 5.3.1 Protein backbone (i)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 3 | 1D | 273/276 (99%) | 261 (96%) | 11 (4%) | 1 (0%) | 30 | 51 |
| 3 | 2D | 273/276 (99%) | 261 (96%) | 11 (4%) | 1 (0%) | 30 | 51 |
| 4 | 1E | 202/206 (98%) | 194 (96%) | 7 (4%) | 1 (0%) | 24 | 46 |
| 4 | 2E | 202/206 (98%) | 195 (96%) | 6 (3%) | 1 (0%) | 24 | 46 |
| 5 | 1F | 201/210 (96%) | 193 (96%) | 7 (4%) | 1 (0%) | 24 | 46 |
| 5 | 2F | 201/210 (96%) | 197 (98%) | 1 (0%) | 3 (2%) | 8 | 18 |
| 6 | 1G | 179/182 (98%) | 168 (94%) | 10 (6%) | 1 (1%) | 21 | 42 |
| 6 | 2G | 179/182 (98%) | 159 (89%) | 18 (10%) | 2 (1%) | 11 | 25 |
| 7 | 1H | 172/180 (96%) | 163 (95%) | 8 (5%) | 1 (1%) | 21 | 42 |
| 7 | 2H | 172/180 (96%) | 160 (93%) | 10 (6%) | 2 (1%) | 10 | 23 |
| 8 | 1I | 144/148 (97%) | 137 (95%) | 7 (5%) | 0 | 100 | 100 |
| 8 | 2I | 144/148 (97%) | 134 (93%) | 10 (7%) | 0 | 100 | 100 |
| 9 | 1N | 138/140 (99%) | 135 (98%) | 3 (2%) | 0 | 100 | 100 |
| 9 | 2N | 138/140 (99%) | 133 (96%) | 5 (4%) | 0 | 100 | 100 |
| 10 | 1O | 120/122 (98%) | 116 (97%) | 4 (3%) | 0 | 100 | 100 |
| 10 | 2O | 120/122 (98%) | 114 (95%) | 6 (5%) | 0 | 100 | 100 |
| 11 | 1P | 147/150 (98%) | 139 (95%) | 8 (5%) | 0 | 100 | 100 |
| 11 | 2P | 147/150 (98%) | 141 (96%) | 6 (4%) | 0 | 100 | 100 |
| 12 | 1Q | 139/141 (99%) | 129 (93%) | 10 (7%) | 0 | 100 | 100 |
| 12 | 2Q | 139/141 (99%) | 132 (95%) | 7 (5%) | 0 | 100 | 100 |
| 13 | 1R | 116/118 (98%) | 111 (96%) | 5 (4%) | 0 | 100 | 100 |
| 13 | 2R | 116/118 (98%) | 112 (97%) | 4 (3%) | 0 | 100 | 100 |
| 14 | 1S | 108/112 (96%) | 103 (95%) | 5 (5%) | 0 | 100 | 100 |
| 14 | 2S | 108/112 (96%) | 102 (94%) | 6 (6%) | 0 | 100 | 100 |
| 15 | 1T | 129/146 (88%) | 122 (95%) | 7 (5%) | 0 | 100 | 100 |
| 15 | 2T | 129/146 (88%) | 124 (96%) | 5 (4%) | 0 | 100 | 100 |
| 16 | 1U | 114/118 (97%) | 114 (100%) | 0 | 0 | 100 | 100 |
| 16 | 2U | 114/118 (97%) | 113 (99%) | 1 (1%) | 0 | 100 | 100 |
| 17 | 1V | 99/101 (98%) | 93 (94%) | 5 (5%) | 1 (1%) | 12 | 28 |
| 17 | 2V | 99/101 (98%) | 94 (95%) | 4 (4%) | 1 (1%) | 12 | 28 |
| 18 | 1W | 110/113 (97%) | 108 (98%) | 2 (2%) | 0 | 100 | 100 |
| 18 | 2W | 110/113 (97%) | 108 (98%) | 2 (2%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 19 | 1X | 93/96 (97%) | 90 (97%) | 3 (3%) | 0 | 100 | 100 |
| 19 | 2X | 93/96 (97%) | 89 (96%) | 4 (4%) | 0 | 100 | 100 |
| 20 | 1Y | 105/110 (96%) | 101 (96%) | 4 (4%) | 0 | 100 | 100 |
| 20 | 2Y | 105/110 (96%) | 102 (97%) | 3 (3%) | 0 | 100 | 100 |
| 21 | 1Z | 148/206 (72%) | 140 (95%) | 8 (5%) | 0 | 100 | 100 |
| 21 | 2Z | 156/206 (76%) | 142 (91%) | 14 (9%) | 0 | 100 | 100 |
| 22 | 10 | 81/85 (95%) | 80 (99%) | 1 (1%) | 0 | 100 | 100 |
| 22 | 20 | 81/85 (95%) | 77 (95%) | 4 (5%) | 0 | 100 | 100 |
| 23 | 11 | 95/98 (97%) | 93 (98%) | 1 (1%) | 1 (1%) | 11 | 25 |
| 23 | 21 | 95/98 (97%) | 93 (98%) | 2 (2%) | 0 | 100 | 100 |
| 24 | 12 | 68/72 (94%) | 67 (98%) | 1 (2%) | 0 | 100 | 100 |
| 24 | 22 | 68/72 (94%) | 67 (98%) | 1 (2%) | 0 | 100 | 100 |
| 25 | 13 | 57/60 (95%) | 55 (96%) | 2 (4%) | 0 | 100 | 100 |
| 25 | 23 | 57/60 (95%) | 55 (96%) | 2 (4%) | 0 | 100 | 100 |
| 26 | 14 | 67/71 (94%) | 57 (85%) | 7 (10%) | 3 (4%) | 2 | 2 |
| 26 | 24 | 67/71 (94%) | 54 (81%) | 11 (16%) | 2 (3%) | 3 | 6 |
| 27 | 15 | 57/60 (95%) | 56 (98%) | 1 (2%) | 0 | 100 | 100 |
| 27 | 25 | 57/60 (95%) | 54 (95%) | 3 (5%) | 0 | 100 | 100 |
| 28 | 16 | 51/54 (94%) | 50 (98%) | 1 (2%) | 0 | 100 | 100 |
| 28 | 26 | 51/54 (94%) | 51 (100%) | 0 | 0 | 100 | 100 |
| 29 | 17 | 46/49 (94%) | 46 (100%) | 0 | 0 | 100 | 100 |
| 29 | 27 | 46/49 (94%) | 44 (96%) | 2 (4%) | 0 | 100 | 100 |
| 30 | 18 | 62/65 (95%) | 62 (100%) | 0 | 0 | 100 | 100 |
| 30 | 28 | 62/65 (95%) | 61 (98%) | 1 (2%) | 0 | 100 | 100 |
| 31 | 19 | 35/37 (95%) | 35 (100%) | 0 | 0 | 100 | 100 |
| 31 | 29 | 35/37 (95%) | 34 (97%) | 1 (3%) | 0 | 100 | 100 |
| 33 | 1b | 229/256 (90%) | 202 (88%) | 20 (9%) | 7 (3%) | 3 | 5 |
| 33 | 2b | 229/256 (90%) | 203 (89%) | 20 (9%) | 6 (3%) | 4 | 7 |
| 34 | 1c | 204/239 (85%) | 187 (92%) | 15 (7%) | 2 (1%) | 12 | 28 |
| 34 | 2c | 204/239 (85%) | 187 (92%) | 15 (7%) | 2 (1%) | 12 | 28 |
| 35 | 1d | 206/209 (99%) | 198 (96%) | 7 (3%) | 1 (0%) | 24 | 46 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| 35 | 2d | 206/209 (99%) | 193 (94%) | 11 (5%) | 2 (1%) | 12 28 |
| 36 | 1e | 146/162 (90%) | 140 (96%) | 5 (3%) | 1 (1%) | 18 38 |
| 36 | 2e | 146/162 (90%) | 141 (97%) | 5 (3%) | 0 | 100 100 |
| 37 | 1f | 98/101 (97%) | 95 (97%) | 3 (3%) | 0 | 100 100 |
| 37 | 2f | 98/101 (97%) | 96 (98%) | 2 (2%) | 0 | 100 100 |
| 38 | 1g | 153/156 (98%) | 144 (94%) | 7 (5%) | 2 (1%) | 9 21 |
| 38 | 2g | 153/156 (98%) | 140 (92%) | 11 (7%) | 2 (1%) | 9 21 |
| 39 | 1h | 135/138 (98%) | 132 (98%) | 3 (2%) | 0 | 100 100 |
| 39 | 2h | 135/138 (98%) | 130 (96%) | 5 (4%) | 0 | 100 100 |
| 40 | 1i | 125/128 (98%) | 112 (90%) | 13 (10%) | 0 | 100 100 |
| 40 | 2i | 125/128 (98%) | 109 (87%) | 16 (13%) | 0 | 100 100 |
| 41 | 1j | 95/105 (90%) | 85 (90%) | 6 (6%) | 4 (4%) | 2 3 |
| 41 | 2j | 94/105 (90%) | 81 (86%) | 6 (6%) | 7 (7%) | 1 1 |
| 42 | 1k | 112/129 (87%) | 104 (93%) | 6 (5%) | 2 (2%) | 6 14 |
| 42 | 2k | 112/129 (87%) | 104 (93%) | 6 (5%) | 2 (2%) | 6 14 |
| 43 | 1l | 119/132 (90%) | 112 (94%) | 6 (5%) | 1 (1%) | 16 34 |
| 43 | 2l | 119/132 (90%) | 112 (94%) | 7 (6%) | 0 | 100 100 |
| 44 | 1m | 121/126 (96%) | 112 (93%) | 9 (7%) | 0 | 100 100 |
| 44 | 2m | 120/126 (95%) | 111 (92%) | 9 (8%) | 0 | 100 100 |
| 45 | 1n | 58/61 (95%) | 56 (97%) | 2 (3%) | 0 | 100 100 |
| 45 | 2n | 58/61 (95%) | 54 (93%) | 4 (7%) | 0 | 100 100 |
| 46 | 1o | 86/89 (97%) | 84 (98%) | 2 (2%) | 0 | 100 100 |
| 46 | 2o | 86/89 (97%) | 84 (98%) | 2 (2%) | 0 | 100 100 |
| 47 | 1p | 80/88 (91%) | 74 (92%) | 6 (8%) | 0 | 100 100 |
| 47 | 2p | 80/88 (91%) | 77 (96%) | 3 (4%) | 0 | 100 100 |
| 48 | 1q | 97/105 (92%) | 94 (97%) | 2 (2%) | 1 (1%) | 12 28 |
| 48 | 2q | 97/105 (92%) | 93 (96%) | 3 (3%) | 1 (1%) | 12 28 |
| 49 | 1r | 66/88 (75%) | 64 (97%) | 2 (3%) | 0 | 100 100 |
| 49 | 2r | 66/88 (75%) | 64 (97%) | 2 (3%) | 0 | 100 100 |
| 50 | 1s | 81/93 (87%) | 72 (89%) | 9 (11%) | 0 | 100 100 |
| 50 | 2s | 81/93 (87%) | 72 (89%) | 8 (10%) | 1 (1%) | 10 23 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| 51 | 1t | 94/106 (89%) | 86 (92%) | 5 (5%) | 3 (3%) | 3 5 |
| 51 | 2t | 94/106 (89%) | 85 (90%) | 6 (6%) | 3 (3%) | 3 5 |
| 52 | 1u | 21/27 (78%) | 20 (95%) | 1 (5%) | 0 | 100 100 |
| 52 | 2u | 21/27 (78%) | 20 (95%) | 1 (5%) | 0 | 100 100 |
| All | All | 11370/12128 (94%) | 10749 (94%) | 549 (5%) | 72 (1%) | 21 42 |

All (72) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 5 | 1F | 130 | ALA |
| 7 | 1H | 126 | PRO |
| 23 | 11 | 3 | LYS |
| 26 | 14 | 58 | ARG |
| 33 | 1b | 10 | LEU |
| 33 | 1b | 22 | LYS |
| 7 | 2H | 126 | PRO |
| 26 | 24 | 55 | ARG |
| 26 | 24 | 65 | ASP |
| 33 | 2b | 10 | LEU |
| 41 | 2j | 75 | ILE |
| 51 | 2t | 10 | LEU |
| 33 | 1b | 9 | GLU |
| 41 | 1j | 55 | LYS |
| 41 | 1j | 75 | ILE |
| 35 | 2d | 181 | MET |
| 38 | 2g | 7 | ALA |
| 41 | 2j | 33 | GLN |
| 42 | 2k | 49 | GLY |
| 3 | 1D | 3 | VAL |
| 6 | 1G | 43 | LEU |
| 26 | 14 | 65 | ASP |
| 35 | 1d | 5 | ILE |
| 48 | 1q | 33 | GLY |
| 51 | 1t | 10 | LEU |
| 51 | 1t | 97 | ALA |
| 34 | 2c | 156 | ARG |
| 41 | 2j | 29 | ARG |
| 41 | 2j | 78 | ASN |
| 41 | 2j | 79 | ARG |
| 4 | 1E | 52 | LEU |
| 33 | 1b | 20 | GLU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 33 | 1b | 125 | PRO |
| 34 | 1c | 107 | GLN |
| 38 | 1g | 114 | ARG |
| 41 | 1j | 33 | GLN |
| 41 | 1j | 78 | ASN |
| 4 | 2E | 52 | LEU |
| 5 | 2F | 130 | ALA |
| 7 | 2H | 47 | GLU |
| 17 | 2V | 79 | VAL |
| 33 | 2b | 16 | HIS |
| 33 | 2b | 20 | GLU |
| 34 | 2c | 85 | ARG |
| 51 | 2t | 97 | ALA |
| 17 | 1V | 79 | VAL |
| 33 | 1b | 17 | PHE |
| 33 | 1b | 37 | ASN |
| 38 | 1g | 80 | VAL |
| 43 | 1l | 91 | LYS |
| 3 | 2D | 3 | VAL |
| 5 | 2F | 26 | ALA |
| 6 | 2G | 49 | ASP |
| 6 | 2G | 52 | ILE |
| 33 | 2b | 17 | PHE |
| 35 | 2d | 5 | ILE |
| 38 | 2g | 80 | VAL |
| 48 | 2q | 68 | ARG |
| 51 | 2t | 47 | GLY |
| 34 | 1c | 66 | VAL |
| 51 | 1t | 47 | GLY |
| 5 | 2F | 89 | VAL |
| 33 | 2b | 9 | GLU |
| 50 | 2s | 9 | VAL |
| 26 | 14 | 64 | GLY |
| 42 | 1k | 105 | VAL |
| 33 | 2b | 127 | ILE |
| 42 | 2k | 105 | VAL |
| 36 | 1e | 69 | VAL |
| 41 | 2j | 24 | VAL |
| 41 | 2j | 39 | PRO |
| 42 | 1k | 49 | GLY |

### 5.3.2 Protein sidechains (i)

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 3 | 1D | 215/218 (99%) | 198 (92%) | 17 (8%) | 11 26 |
| 3 | 2D | 215/218 (99%) | 201 (94%) | 14 (6%) | 15 35 |
| 4 | 1E | 164/166 (99%) | 148 (90%) | 16 (10%) | 7 17 |
| 4 | 2E | 164/166 (99%) | 155 (94%) | 9 (6%) | 19 41 |
| 5 | 1F | 160/166 (96%) | 146 (91%) | 14 (9%) | 9 21 |
| 5 | 2F | 159/166 (96%) | 148 (93%) | 11 (7%) | 14 32 |
| 6 | 1G | 143/156 (92%) | 134 (94%) | 9 (6%) | 16 36 |
| 6 | 2G | 143/156 (92%) | 129 (90%) | 14 (10%) | 7 17 |
| 7 | 1H | 144/148 (97%) | 136 (94%) | 8 (6%) | 19 40 |
| 7 | 2H | 144/148 (97%) | 138 (96%) | 6 (4%) | 26 52 |
| 8 | 1I | 113/124 (91%) | 107 (95%) | 6 (5%) | 20 43 |
| 8 | 2I | 105/124 (85%) | 95 (90%) | 10 (10%) | 8 18 |
| 9 | 1N | 118/119 (99%) | 108 (92%) | 10 (8%) | 10 22 |
| 9 | 2N | 118/119 (99%) | 110 (93%) | 8 (7%) | 14 32 |
| 10 | 1O | 100/100 (100%) | 96 (96%) | 4 (4%) | 28 55 |
| 10 | 2O | 100/100 (100%) | 97 (97%) | 3 (3%) | 36 64 |
| 11 | 1P | 115/116 (99%) | 109 (95%) | 6 (5%) | 21 44 |
| 11 | 2P | 115/116 (99%) | 110 (96%) | 5 (4%) | 26 51 |
| 12 | 1Q | 111/111 (100%) | 106 (96%) | 5 (4%) | 24 50 |
| 12 | 2Q | 111/111 (100%) | 107 (96%) | 4 (4%) | 31 58 |
| 13 | 1R | 101/101 (100%) | 88 (87%) | 13 (13%) | 4 8 |
| 13 | 2R | 101/101 (100%) | 90 (89%) | 11 (11%) | 6 13 |
| 14 | 1S | 86/88 (98%) | 82 (95%) | 4 (5%) | 23 48 |
| 14 | 2S | 85/88 (97%) | 83 (98%) | 2 (2%) | 43 70 |
| 15 | 1T | 115/127 (91%) | 111 (96%) | 4 (4%) | 32 59 |
| 15 | 2T | 113/127 (89%) | 112 (99%) | 1 (1%) | 70 87 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 16 | 1U | 93/94 (99%) | 90 (97%) | 3 (3%) | 34 62 |
| 16 | 2U | 93/94 (99%) | 89 (96%) | 4 (4%) | 26 51 |
| 17 | 1V | 80/82 (98%) | 70 (88%) | 10 (12%) | 4 9 |
| 17 | 2V | 80/82 (98%) | 70 (88%) | 10 (12%) | 4 9 |
| 18 | 1W | 90/92 (98%) | 81 (90%) | 9 (10%) | 7 16 |
| 18 | 2W | 90/92 (98%) | 84 (93%) | 6 (7%) | 15 33 |
| 19 | 1X | 77/78 (99%) | 73 (95%) | 4 (5%) | 21 44 |
| 19 | 2X | 77/78 (99%) | 75 (97%) | 2 (3%) | 40 68 |
| 20 | 1Y | 85/91 (93%) | 78 (92%) | 7 (8%) | 10 24 |
| 20 | 2Y | 85/91 (93%) | 76 (89%) | 9 (11%) | 6 14 |
| 21 | 1Z | 135/179 (75%) | 124 (92%) | 11 (8%) | 11 24 |
| 21 | 2Z | 137/179 (76%) | 131 (96%) | 6 (4%) | 25 50 |
| 22 | 10 | 65/67 (97%) | 63 (97%) | 2 (3%) | 35 63 |
| 22 | 20 | 65/67 (97%) | 64 (98%) | 1 (2%) | 57 80 |
| 23 | 11 | 80/83 (96%) | 76 (95%) | 4 (5%) | 22 46 |
| 23 | 21 | 80/83 (96%) | 77 (96%) | 3 (4%) | 29 56 |
| 24 | 12 | 65/67 (97%) | 62 (95%) | 3 (5%) | 24 49 |
| 24 | 22 | 65/67 (97%) | 65 (100%) | 0 | 100 100 |
| 25 | 13 | 51/52 (98%) | 48 (94%) | 3 (6%) | 18 38 |
| 25 | 23 | 50/52 (96%) | 48 (96%) | 2 (4%) | 28 55 |
| 26 | 14 | 59/63 (94%) | 53 (90%) | 6 (10%) | 7 15 |
| 26 | 24 | 53/63 (84%) | 52 (98%) | 1 (2%) | 50 75 |
| 27 | 15 | 50/52 (96%) | 47 (94%) | 3 (6%) | 17 37 |
| 27 | 25 | 50/52 (96%) | 47 (94%) | 3 (6%) | 17 37 |
| 28 | 16 | 51/52 (98%) | 49 (96%) | 2 (4%) | 28 55 |
| 28 | 26 | 50/52 (96%) | 47 (94%) | 3 (6%) | 17 37 |
| 29 | 17 | 41/42 (98%) | 36 (88%) | 5 (12%) | 5 10 |
| 29 | 27 | 41/42 (98%) | 36 (88%) | 5 (12%) | 5 10 |
| 30 | 18 | 54/55 (98%) | 49 (91%) | 5 (9%) | 8 18 |
| 30 | 28 | 54/55 (98%) | 52 (96%) | 2 (4%) | 30 57 |
| 31 | 19 | 34/34 (100%) | 33 (97%) | 1 (3%) | 37 65 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 31 | 29 | 34/34 (100%) | 30 (88%) | 4 (12%) | 5 10 |
| 33 | 1b | 192/220 (87%) | 183 (95%) | 9 (5%) | 23 48 |
| 33 | 2b | 187/220 (85%) | 177 (95%) | 10 (5%) | 20 43 |
| 34 | 1c | 142/188 (76%) | 135 (95%) | 7 (5%) | 22 47 |
| 34 | 2c | 140/188 (74%) | 133 (95%) | 7 (5%) | 22 46 |
| 35 | 1d | 169/181 (93%) | 157 (93%) | 12 (7%) | 13 31 |
| 35 | 2d | 173/181 (96%) | 159 (92%) | 14 (8%) | 11 24 |
| 36 | 1e | 113/123 (92%) | 103 (91%) | 10 (9%) | 9 21 |
| 36 | 2e | 114/123 (93%) | 110 (96%) | 4 (4%) | 32 59 |
| 37 | 1f | 84/90 (93%) | 79 (94%) | 5 (6%) | 17 37 |
| 37 | 2f | 85/90 (94%) | 82 (96%) | 3 (4%) | 32 59 |
| 38 | 1g | 119/127 (94%) | 113 (95%) | 6 (5%) | 22 46 |
| 38 | 2g | 120/127 (94%) | 116 (97%) | 4 (3%) | 33 61 |
| 39 | 1h | 114/119 (96%) | 104 (91%) | 10 (9%) | 9 21 |
| 39 | 2h | 114/119 (96%) | 107 (94%) | 7 (6%) | 17 37 |
| 40 | 1i | 90/99 (91%) | 86 (96%) | 4 (4%) | 25 50 |
| 40 | 2i | 89/99 (90%) | 81 (91%) | 8 (9%) | 9 20 |
| 41 | 1j | 66/92 (72%) | 63 (96%) | 3 (4%) | 24 50 |
| 41 | 2j | 69/92 (75%) | 66 (96%) | 3 (4%) | 26 51 |
| 42 | 1k | 82/99 (83%) | 80 (98%) | 2 (2%) | 43 70 |
| 42 | 2k | 83/99 (84%) | 81 (98%) | 2 (2%) | 43 70 |
| 43 | 1l | 96/108 (89%) | 91 (95%) | 5 (5%) | 21 44 |
| 43 | 2l | 96/108 (89%) | 92 (96%) | 4 (4%) | 26 52 |
| 44 | 1m | 93/101 (92%) | 90 (97%) | 3 (3%) | 34 62 |
| 44 | 2m | 92/101 (91%) | 87 (95%) | 5 (5%) | 20 42 |
| 45 | 1n | 49/50 (98%) | 44 (90%) | 5 (10%) | 7 15 |
| 45 | 2n | 49/50 (98%) | 42 (86%) | 7 (14%) | 3 6 |
| 46 | 1o | 78/80 (98%) | 76 (97%) | 2 (3%) | 40 68 |
| 46 | 2o | 78/80 (98%) | 77 (99%) | 1 (1%) | 61 82 |
| 47 | 1p | 69/74 (93%) | 66 (96%) | 3 (4%) | 26 51 |
| 47 | 2p | 68/74 (92%) | 61 (90%) | 7 (10%) | 7 15 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 48 | 1q | 94/97 (97%) | 90 (96%) | 4 (4%) | 26 51 |
| 48 | 2q | 94/97 (97%) | 94 (100%) | 0 | 100 100 |
| 49 | 1r | 59/77 (77%) | 55 (93%) | 4 (7%) | 14 32 |
| 49 | 2r | 59/77 (77%) | 55 (93%) | 4 (7%) | 14 32 |
| 50 | 1s | 69/80 (86%) | 68 (99%) | 1 (1%) | 59 81 |
| 50 | 2s | 67/80 (84%) | 63 (94%) | 4 (6%) | 17 37 |
| 51 | 1t | 70/82 (85%) | 65 (93%) | 5 (7%) | 13 31 |
| 51 | 2t | 70/82 (85%) | 69 (99%) | 1 (1%) | 59 81 |
| 52 | 1u | 18/22 (82%) | 17 (94%) | 1 (6%) | 19 40 |
| 52 | 2u | 18/22 (82%) | 18 (100%) | 0 | 100 100 |
| All | All | 9303/10064 (92%) | 8754 (94%) | 549 (6%) | 18 38 |

All (549) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | 1D | 14 | ARG |
| 3 | 1D | 22 | SER |
| 3 | 1D | 32 | SER |
| 3 | 1D | 37 | LEU |
| 3 | 1D | 94 | LEU |
| 3 | 1D | 113 | VAL |
| 3 | 1D | 142 | VAL |
| 3 | 1D | 155 | LEU |
| 3 | 1D | 157 | ARG |
| 3 | 1D | 162 | SER |
| 3 | 1D | 168 | ARG |
| 3 | 1D | 193 | VAL |
| 3 | 1D | 211 | ARG |
| 3 | 1D | 217 | ARG |
| 3 | 1D | 221 | VAL |
| 3 | 1D | 229 | VAL |
| 3 | 1D | 242 | ARG |
| 4 | 1E | 9 | VAL |
| 4 | 1E | 21 | VAL |
| 4 | 1E | 24 | THR |
| 4 | 1E | 34 | VAL |
| 4 | 1E | 47 | VAL |
| 4 | 1E | 73 | GLU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 4 | 1E | 75 | VAL |
| 4 | 1E | 77 | ILE |
| 4 | 1E | 78 | LEU |
| 4 | 1E | 90 | THR |
| 4 | 1E | 111 | ARG |
| 4 | 1E | 116 | VAL |
| 4 | 1E | 170 | LEU |
| 4 | 1E | 175 | VAL |
| 4 | 1E | 181 | LEU |
| 4 | 1E | 184 | VAL |
| 5 | 1F | 24 | LEU |
| 5 | 1F | 33 | LEU |
| 5 | 1F | 44 | ARG |
| 5 | 1F | 53 | THR |
| 5 | 1F | 57 | VAL |
| 5 | 1F | 88 | VAL |
| 5 | 1F | 106 | ARG |
| 5 | 1F | 132 | VAL |
| 5 | 1F | 140 | LEU |
| 5 | 1F | 162 | LEU |
| 5 | 1F | 170 | LEU |
| 5 | 1F | 183 | VAL |
| 5 | 1F | 192 | LEU |
| 5 | 1F | 201 | VAL |
| 6 | 1G | 3 | LEU |
| 6 | 1G | 5 | VAL |
| 6 | 1G | 43 | LEU |
| 6 | 1G | 49 | ASP |
| 6 | 1G | 70 | VAL |
| 6 | 1G | 82 | LEU |
| 6 | 1G | 140 | ILE |
| 6 | 1G | 159 | VAL |
| 6 | 1G | 175 | LEU |
| 7 | 1H | 15 | VAL |
| 7 | 1H | 23 | ARG |
| 7 | 1H | 24 | VAL |
| 7 | 1H | 51 | ARG |
| 7 | 1H | 71 | LEU |
| 7 | 1H | 84 | SER |
| 7 | 1H | 122 | THR |
| 7 | 1H | 124 | GLU |
| 8 | 1I | 9 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 8 | 1I | 38 | LEU |
| 8 | 1I | 92 | VAL |
| 8 | 1I | 109 | ILE |
| 8 | 1I | 116 | LEU |
| 8 | 1I | 129 | THR |
| 9 | 1N | 14 | VAL |
| 9 | 1N | 28 | THR |
| 9 | 1N | 32 | THR |
| 9 | 1N | 33 | LEU |
| 9 | 1N | 34 | LEU |
| 9 | 1N | 46 | VAL |
| 9 | 1N | 62 | VAL |
| 9 | 1N | 73 | THR |
| 9 | 1N | 99 | LEU |
| 9 | 1N | 121 | LYS |
| 10 | 1O | 9 | GLU |
| 10 | 1O | 10 | VAL |
| 10 | 1O | 35 | VAL |
| 10 | 1O | 98 | VAL |
| 11 | 1P | 3 | LEU |
| 11 | 1P | 83 | VAL |
| 11 | 1P | 95 | VAL |
| 11 | 1P | 101 | VAL |
| 11 | 1P | 125 | VAL |
| 11 | 1P | 147 | LEU |
| 12 | 1Q | 6 | ARG |
| 12 | 1Q | 7 | MET |
| 12 | 1Q | 35 | VAL |
| 12 | 1Q | 75 | THR |
| 12 | 1Q | 101 | ARG |
| 13 | 1R | 15 | SER |
| 13 | 1R | 29 | LEU |
| 13 | 1R | 33 | ARG |
| 13 | 1R | 36 | THR |
| 13 | 1R | 44 | LEU |
| 13 | 1R | 54 | LEU |
| 13 | 1R | 65 | LEU |
| 13 | 1R | 67 | LEU |
| 13 | 1R | 91 | GLN |
| 13 | 1R | 96 | ARG |
| 13 | 1R | 100 | LEU |
| 13 | 1R | 111 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 13 | 1R | 114 | VAL |
| 14 | 1S | 14 | VAL |
| 14 | 1S | 17 | ARG |
| 14 | 1S | 69 | VAL |
| 14 | 1S | 110 | LEU |
| 15 | 1T | 28 | VAL |
| 15 | 1T | 89 | VAL |
| 15 | 1T | 96 | ARG |
| 15 | 1T | 128 | GLU |
| 16 | 1U | 59 | ARG |
| 16 | 1U | 83 | LEU |
| 16 | 1U | 95 | LEU |
| 17 | 1V | 1 | MET |
| 17 | 1V | 46 | VAL |
| 17 | 1V | 51 | VAL |
| 17 | 1V | 52 | VAL |
| 17 | 1V | 61 | VAL |
| 17 | 1V | 62 | LEU |
| 17 | 1V | 72 | VAL |
| 17 | 1V | 73 | SER |
| 17 | 1V | 79 | VAL |
| 17 | 1V | 82 | ARG |
| 18 | 1W | 6 | ILE |
| 18 | 1W | 11 | ARG |
| 18 | 1W | 15 | ARG |
| 18 | 1W | 17 | VAL |
| 18 | 1W | 19 | LEU |
| 18 | 1W | 23 | LEU |
| 18 | 1W | 95 | ILE |
| 18 | 1W | 100 | THR |
| 18 | 1W | 107 | LEU |
| 19 | 1X | 35 | THR |
| 19 | 1X | 38 | GLU |
| 19 | 1X | 72 | LYS |
| 19 | 1X | 81 | VAL |
| 20 | 1Y | 7 | VAL |
| 20 | 1Y | 31 | LEU |
| 20 | 1Y | 63 | LYS |
| 20 | 1Y | 64 | GLU |
| 20 | 1Y | 72 | VAL |
| 20 | 1Y | 97 | ARG |
| 20 | 1Y | 99 | CYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 21 | 1Z | 41 | LEU |
| 21 | 1Z | 42 | VAL |
| 21 | 1Z | 53 | ILE |
| 21 | 1Z | 61 | LEU |
| 21 | 1Z | 91 | LEU |
| 21 | 1Z | 126 | VAL |
| 21 | 1Z | 136 | PHE |
| 21 | 1Z | 137 | ILE |
| 21 | 1Z | 154 | ASP |
| 21 | 1Z | 161 | VAL |
| 21 | 1Z | 170 | THR |
| 22 | 10 | 39 | ARG |
| 22 | 10 | 74 | ARG |
| 23 | 11 | 11 | ARG |
| 23 | 11 | 30 | VAL |
| 23 | 11 | 80 | LEU |
| 23 | 11 | 95 | LEU |
| 24 | 12 | 3 | LEU |
| 24 | 12 | 30 | ARG |
| 24 | 12 | 41 | ILE |
| 25 | 13 | 23 | LEU |
| 25 | 13 | 34 | GLU |
| 25 | 13 | 60 | GLU |
| 26 | 14 | 31 | ILE |
| 26 | 14 | 49 | PHE |
| 26 | 14 | 53 | GLU |
| 26 | 14 | 56 | VAL |
| 26 | 14 | 58 | ARG |
| 26 | 14 | 63 | TYR |
| 27 | 15 | 6 | VAL |
| 27 | 15 | 16 | ARG |
| 27 | 15 | 29 | THR |
| 28 | 16 | 9 | LEU |
| 28 | 16 | 48 | VAL |
| 29 | 17 | 9 | ARG |
| 29 | 17 | 29 | LYS |
| 29 | 17 | 39 | ARG |
| 29 | 17 | 43 | THR |
| 29 | 17 | 46 | VAL |
| 30 | 18 | 14 | VAL |
| 30 | 18 | 23 | VAL |
| 30 | 18 | 29 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 30 | 18 | 30 | ARG |
| 30 | 18 | 32 | LEU |
| 31 | 19 | 4 | ARG |
| 33 | 1b | 80 | ILE |
| 33 | 1b | 93 | VAL |
| 33 | 1b | 107 | THR |
| 33 | 1b | 112 | VAL |
| 33 | 1b | 115 | LEU |
| 33 | 1b | 121 | LEU |
| 33 | 1b | 142 | LEU |
| 33 | 1b | 160 | ASP |
| 33 | 1b | 162 | ILE |
| 34 | 1c | 3 | ASN |
| 34 | 1c | 57 | ILE |
| 34 | 1c | 70 | VAL |
| 34 | 1c | 89 | GLU |
| 34 | 1c | 112 | SER |
| 34 | 1c | 116 | VAL |
| 34 | 1c | 196 | LEU |
| 35 | 1d | 5 | ILE |
| 35 | 1d | 8 | VAL |
| 35 | 1d | 10 | ARG |
| 35 | 1d | 49 | ARG |
| 35 | 1d | 53 | ASP |
| 35 | 1d | 56 | VAL |
| 35 | 1d | 135 | LEU |
| 35 | 1d | 140 | VAL |
| 35 | 1d | 144 | ASP |
| 35 | 1d | 175 | SER |
| 35 | 1d | 182 | LYS |
| 35 | 1d | 194 | LEU |
| 36 | 1e | 16 | THR |
| 36 | 1e | 20 | GLN |
| 36 | 1e | 41 | VAL |
| 36 | 1e | 51 | VAL |
| 36 | 1e | 64 | ARG |
| 36 | 1e | 71 | LEU |
| 36 | 1e | 81 | GLU |
| 36 | 1e | 91 | LEU |
| 36 | 1e | 120 | THR |
| 36 | 1e | 131 | ILE |
| 37 | 1f | 17 | SER |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 37 | 1f | 19 | LEU |
| 37 | 1f | 25 | ILE |
| 37 | 1f | 55 | ASP |
| 37 | 1f | 72 | VAL |
| 38 | 1g | 6 | ARG |
| 38 | 1g | 9 | VAL |
| 38 | 1g | 24 | THR |
| 38 | 1g | 50 | ILE |
| 38 | 1g | 79 | ARG |
| 38 | 1g | 98 | SER |
| 39 | 1h | 13 | ILE |
| 39 | 1h | 25 | ASP |
| 39 | 1h | 26 | VAL |
| 39 | 1h | 51 | VAL |
| 39 | 1h | 52 | ASP |
| 39 | 1h | 63 | LEU |
| 39 | 1h | 82 | HIS |
| 39 | 1h | 104 | ARG |
| 39 | 1h | 112 | LEU |
| 39 | 1h | 137 | VAL |
| 40 | 1i | 64 | THR |
| 40 | 1i | 86 | VAL |
| 40 | 1i | 108 | VAL |
| 40 | 1i | 128 | ARG |
| 41 | 1j | 19 | SER |
| 41 | 1j | 81 | THR |
| 41 | 1j | 92 | THR |
| 42 | 1k | 48 | ILE |
| 42 | 1k | 120 | ARG |
| 43 | 1l | 18 | VAL |
| 43 | 1l | 27 | LEU |
| 43 | 1l | 33 | ARG |
| 43 | 1l | 57 | LYS |
| 43 | 1l | 83 | VAL |
| 44 | 1m | 19 | LEU |
| 44 | 1m | 43 | THR |
| 44 | 1m | 70 | LEU |
| 45 | 1n | 6 | LEU |
| 45 | 1n | 13 | THR |
| 45 | 1n | 18 | VAL |
| 45 | 1n | 22 | THR |
| 45 | 1n | 33 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 46 | 1o | 5 | LYS |
| 46 | 1o | 66 | LEU |
| 47 | 1p | 20 | VAL |
| 47 | 1p | 21 | VAL |
| 47 | 1p | 62 | VAL |
| 48 | 1q | 6 | LEU |
| 48 | 1q | 9 | VAL |
| 48 | 1q | 35 | VAL |
| 48 | 1q | 63 | ARG |
| 49 | 1r | 35 | ARG |
| 49 | 1r | 37 | VAL |
| 49 | 1r | 47 | THR |
| 49 | 1r | 76 | LEU |
| 50 | 1s | 12 | ASP |
| 51 | 1t | 10 | LEU |
| 51 | 1t | 13 | LEU |
| 51 | 1t | 20 | LEU |
| 51 | 1t | 31 | SER |
| 51 | 1t | 84 | LEU |
| 52 | 1u | 17 | THR |
| 3 | 2D | 14 | ARG |
| 3 | 2D | 54 | ARG |
| 3 | 2D | 94 | LEU |
| 3 | 2D | 99 | ASP |
| 3 | 2D | 113 | VAL |
| 3 | 2D | 116 | GLN |
| 3 | 2D | 138 | VAL |
| 3 | 2D | 141 | VAL |
| 3 | 2D | 142 | VAL |
| 3 | 2D | 157 | ARG |
| 3 | 2D | 169 | GLU |
| 3 | 2D | 204 | ILE |
| 3 | 2D | 211 | ARG |
| 3 | 2D | 221 | VAL |
| 4 | 2E | 7 | VAL |
| 4 | 2E | 9 | VAL |
| 4 | 2E | 12 | THR |
| 4 | 2E | 21 | VAL |
| 4 | 2E | 38 | THR |
| 4 | 2E | 75 | VAL |
| 4 | 2E | 116 | VAL |
| 4 | 2E | 175 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 4 | 2E | 181 | LEU |
| 5 | 2F | 12 | LEU |
| 5 | 2F | 57 | VAL |
| 5 | 2F | 70 | THR |
| 5 | 2F | 88 | VAL |
| 5 | 2F | 106 | ARG |
| 5 | 2F | 132 | VAL |
| 5 | 2F | 170 | LEU |
| 5 | 2F | 183 | VAL |
| 5 | 2F | 192 | LEU |
| 5 | 2F | 195 | ASP |
| 5 | 2F | 201 | VAL |
| 6 | 2G | 9 | ARG |
| 6 | 2G | 28 | VAL |
| 6 | 2G | 31 | VAL |
| 6 | 2G | 43 | LEU |
| 6 | 2G | 49 | ASP |
| 6 | 2G | 70 | VAL |
| 6 | 2G | 79 | ASN |
| 6 | 2G | 92 | VAL |
| 6 | 2G | 97 | ASP |
| 6 | 2G | 109 | VAL |
| 6 | 2G | 130 | ASN |
| 6 | 2G | 140 | ILE |
| 6 | 2G | 145 | THR |
| 6 | 2G | 159 | VAL |
| 7 | 2H | 15 | VAL |
| 7 | 2H | 70 | THR |
| 7 | 2H | 71 | LEU |
| 7 | 2H | 134 | SER |
| 7 | 2H | 139 | GLN |
| 7 | 2H | 148 | ILE |
| 8 | 2I | 3 | VAL |
| 8 | 2I | 31 | LEU |
| 8 | 2I | 38 | LEU |
| 8 | 2I | 47 | LEU |
| 8 | 2I | 77 | LEU |
| 8 | 2I | 92 | VAL |
| 8 | 2I | 123 | LEU |
| 8 | 2I | 127 | VAL |
| 8 | 2I | 142 | VAL |
| 8 | 2I | 144 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 9 | 2N | 9 | VAL |
| 9 | 2N | 14 | VAL |
| 9 | 2N | 33 | LEU |
| 9 | 2N | 34 | LEU |
| 9 | 2N | 46 | VAL |
| 9 | 2N | 62 | VAL |
| 9 | 2N | 67 | LEU |
| 9 | 2N | 99 | LEU |
| 10 | 2O | 63 | VAL |
| 10 | 2O | 69 | ILE |
| 10 | 2O | 98 | VAL |
| 11 | 2P | 95 | VAL |
| 11 | 2P | 105 | LEU |
| 11 | 2P | 131 | SER |
| 11 | 2P | 133 | SER |
| 11 | 2P | 148 | LEU |
| 12 | 2Q | 1 | MET |
| 12 | 2Q | 2 | LEU |
| 12 | 2Q | 38 | GLU |
| 12 | 2Q | 75 | THR |
| 13 | 2R | 24 | GLN |
| 13 | 2R | 29 | LEU |
| 13 | 2R | 33 | ARG |
| 13 | 2R | 36 | THR |
| 13 | 2R | 44 | LEU |
| 13 | 2R | 54 | LEU |
| 13 | 2R | 65 | LEU |
| 13 | 2R | 91 | GLN |
| 13 | 2R | 96 | ARG |
| 13 | 2R | 111 | LEU |
| 13 | 2R | 114 | VAL |
| 14 | 2S | 8 | GLU |
| 14 | 2S | 48 | LEU |
| 15 | 2T | 96 | ARG |
| 16 | 2U | 8 | VAL |
| 16 | 2U | 55 | ARG |
| 16 | 2U | 95 | LEU |
| 16 | 2U | 100 | VAL |
| 17 | 2V | 14 | VAL |
| 17 | 2V | 52 | VAL |
| 17 | 2V | 57 | VAL |
| 17 | 2V | 61 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 17 | 2V | 62 | LEU |
| 17 | 2V | 72 | VAL |
| 17 | 2V | 79 | VAL |
| 17 | 2V | 82 | ARG |
| 17 | 2V | 95 | LEU |
| 17 | 2V | 98 | GLU |
| 18 | 2W | 11 | ARG |
| 18 | 2W | 15 | ARG |
| 18 | 2W | 17 | VAL |
| 18 | 2W | 23 | LEU |
| 18 | 2W | 39 | THR |
| 18 | 2W | 107 | LEU |
| 19 | 2X | 62 | LYS |
| 19 | 2X | 81 | VAL |
| 20 | 2Y | 19 | LYS |
| 20 | 2Y | 21 | LYS |
| 20 | 2Y | 55 | TYR |
| 20 | 2Y | 61 | ILE |
| 20 | 2Y | 72 | VAL |
| 20 | 2Y | 88 | LYS |
| 20 | 2Y | 90 | LEU |
| 20 | 2Y | 99 | CYS |
| 20 | 2Y | 107 | ASP |
| 21 | 2Z | 42 | VAL |
| 21 | 2Z | 96 | VAL |
| 21 | 2Z | 126 | VAL |
| 21 | 2Z | 154 | ASP |
| 21 | 2Z | 155 | LEU |
| 21 | 2Z | 171 | ILE |
| 22 | 20 | 14 | ARG |
| 23 | 21 | 4 | VAL |
| 23 | 21 | 35 | THR |
| 23 | 21 | 38 | SER |
| 25 | 23 | 30 | ARG |
| 25 | 23 | 57 | GLU |
| 26 | 24 | 50 | VAL |
| 27 | 25 | 6 | VAL |
| 27 | 25 | 29 | THR |
| 27 | 25 | 58 | LEU |
| 28 | 26 | 9 | LEU |
| 28 | 26 | 25 | LYS |
| 28 | 26 | 48 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 29 | 27 | 39 | ARG |
| 29 | 27 | 41 | ARG |
| 29 | 27 | 43 | THR |
| 29 | 27 | 46 | VAL |
| 29 | 27 | 48 | LYS |
| 30 | 28 | 14 | VAL |
| 30 | 28 | 41 | ILE |
| 31 | 29 | 4 | ARG |
| 31 | 29 | 7 | VAL |
| 31 | 29 | 17 | ILE |
| 31 | 29 | 26 | ILE |
| 33 | 2b | 93 | VAL |
| 33 | 2b | 111 | ARG |
| 33 | 2b | 112 | VAL |
| 33 | 2b | 115 | LEU |
| 33 | 2b | 124 | SER |
| 33 | 2b | 127 | ILE |
| 33 | 2b | 154 | LEU |
| 33 | 2b | 189 | ASP |
| 33 | 2b | 195 | ASP |
| 33 | 2b | 213 | LEU |
| 34 | 2c | 3 | ASN |
| 34 | 2c | 59 | ARG |
| 34 | 2c | 68 | VAL |
| 34 | 2c | 103 | VAL |
| 34 | 2c | 115 | LEU |
| 34 | 2c | 154 | SER |
| 34 | 2c | 196 | LEU |
| 35 | 2d | 8 | VAL |
| 35 | 2d | 10 | ARG |
| 35 | 2d | 17 | VAL |
| 35 | 2d | 19 | LEU |
| 35 | 2d | 31 | CYS |
| 35 | 2d | 34 | GLU |
| 35 | 2d | 83 | SER |
| 35 | 2d | 108 | LEU |
| 35 | 2d | 112 | VAL |
| 35 | 2d | 119 | GLN |
| 35 | 2d | 135 | LEU |
| 35 | 2d | 170 | VAL |
| 35 | 2d | 194 | LEU |
| 35 | 2d | 205 | GLU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 36 | 2e | 41 | VAL |
| 36 | 2e | 53 | LEU |
| 36 | 2e | 83 | GLU |
| 36 | 2e | 149 | GLU |
| 37 | 2f | 61 | LEU |
| 37 | 2f | 72 | VAL |
| 37 | 2f | 81 | ILE |
| 38 | 2g | 52 | GLU |
| 38 | 2g | 61 | VAL |
| 38 | 2g | 79 | ARG |
| 38 | 2g | 113 | GLU |
| 39 | 2h | 2 | LEU |
| 39 | 2h | 8 | ASP |
| 39 | 2h | 25 | ASP |
| 39 | 2h | 51 | VAL |
| 39 | 2h | 69 | ARG |
| 39 | 2h | 114 | THR |
| 39 | 2h | 137 | VAL |
| 40 | 2i | 23 | ASN |
| 40 | 2i | 27 | THR |
| 40 | 2i | 64 | THR |
| 40 | 2i | 81 | ILE |
| 40 | 2i | 102 | LEU |
| 40 | 2i | 107 | ARG |
| 40 | 2i | 108 | VAL |
| 40 | 2i | 128 | ARG |
| 41 | 2j | 16 | LEU |
| 41 | 2j | 72 | VAL |
| 41 | 2j | 81 | THR |
| 42 | 2k | 48 | ILE |
| 42 | 2k | 109 | VAL |
| 43 | 2l | 18 | VAL |
| 43 | 2l | 27 | LEU |
| 43 | 2l | 113 | ARG |
| 43 | 2l | 117 | ARG |
| 44 | 2m | 3 | ARG |
| 44 | 2m | 15 | VAL |
| 44 | 2m | 60 | VAL |
| 44 | 2m | 103 | THR |
| 44 | 2m | 117 | VAL |
| 45 | 2n | 3 | ARG |
| 45 | 2n | 6 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 45 | 2n | 7 | ILE |
| 45 | 2n | 18 | VAL |
| 45 | 2n | 22 | THR |
| 45 | 2n | 31 | ARG |
| 45 | 2n | 33 | VAL |
| 46 | 2o | 39 | LEU |
| 47 | 2p | 2 | VAL |
| 47 | 2p | 20 | VAL |
| 47 | 2p | 21 | VAL |
| 47 | 2p | 44 | THR |
| 47 | 2p | 60 | LEU |
| 47 | 2p | 62 | VAL |
| 47 | 2p | 67 | THR |
| 49 | 2r | 21 | LYS |
| 49 | 2r | 47 | THR |
| 49 | 2r | 76 | LEU |
| 49 | 2r | 85 | LEU |
| 50 | 2s | 5 | LEU |
| 50 | 2s | 33 | THR |
| 50 | 2s | 77 | THR |
| 50 | 2s | 83 | HIS |
| 51 | 2t | 51 | GLU |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (115) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | 1D | 87 | ASN |
| 3 | 1D | 166 | GLN |
| 4 | 1E | 48 | GLN |
| 4 | 1E | 121 | ASN |
| 5 | 1F | 69 | HIS |
| 5 | 1F | 203 | GLN |
| 5 | 1F | 204 | ASN |
| 6 | 1G | 26 | GLN |
| 6 | 1G | 108 | ASN |
| 8 | 1I | 11 | ASN |
| 9 | 1N | 69 | GLN |
| 12 | 1Q | 113 | GLN |
| 12 | 1Q | 123 | HIS |
| 13 | 1R | 31 | HIS |
| 13 | 1R | 61 | HIS |
| 13 | 1R | 71 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 15 | 1T | 58 | ASN |
| 16 | 1U | 72 | HIS |
| 19 | 1X | 31 | HIS |
| 19 | 1X | 82 | GLN |
| 20 | 1Y | 6 | HIS |
| 21 | 1Z | 54 | HIS |
| 22 | 10 | 29 | GLN |
| 24 | 12 | 46 | GLN |
| 24 | 12 | 56 | GLN |
| 26 | 14 | 47 | GLN |
| 28 | 16 | 20 | ASN |
| 33 | 1b | 78 | GLN |
| 34 | 1c | 6 | HIS |
| 34 | 1c | 104 | GLN |
| 34 | 1c | 108 | ASN |
| 34 | 1c | 162 | GLN |
| 35 | 1d | 74 | GLN |
| 35 | 1d | 77 | ASN |
| 35 | 1d | 116 | GLN |
| 35 | 1d | 123 | HIS |
| 35 | 1d | 125 | HIS |
| 36 | 1e | 78 | HIS |
| 37 | 1f | 100 | ASN |
| 38 | 1g | 28 | ASN |
| 38 | 1g | 148 | ASN |
| 40 | 1i | 3 | GLN |
| 40 | 1i | 73 | GLN |
| 41 | 1j | 21 | GLN |
| 41 | 1j | 56 | HIS |
| 43 | 1l | 80 | HIS |
| 43 | 1l | 99 | HIS |
| 44 | 1m | 62 | ASN |
| 46 | 1o | 46 | HIS |
| 47 | 1p | 16 | HIS |
| 50 | 1s | 57 | HIS |
| 50 | 1s | 69 | HIS |
| 51 | 1t | 16 | HIS |
| 3 | 2D | 116 | GLN |
| 5 | 2F | 69 | HIS |
| 5 | 2F | 75 | HIS |
| 5 | 2F | 204 | ASN |
| 8 | 2I | 104 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 8 | 2I | 105 | HIS |
| 8 | 2I | 139 | GLN |
| 9 | 2N | 128 | HIS |
| 11 | 2P | 35 | HIS |
| 12 | 2Q | 89 | ASN |
| 13 | 2R | 13 | HIS |
| 13 | 2R | 31 | HIS |
| 13 | 2R | 71 | GLN |
| 15 | 2T | 58 | ASN |
| 15 | 2T | 90 | GLN |
| 16 | 2U | 81 | HIS |
| 16 | 2U | 94 | ASN |
| 17 | 2V | 80 | GLN |
| 18 | 2W | 62 | HIS |
| 19 | 2X | 31 | HIS |
| 19 | 2X | 82 | GLN |
| 20 | 2Y | 43 | ASN |
| 21 | 2Z | 73 | GLN |
| 22 | 20 | 29 | GLN |
| 24 | 22 | 56 | GLN |
| 24 | 22 | 65 | ASN |
| 26 | 24 | 46 | GLN |
| 33 | 2b | 40 | HIS |
| 33 | 2b | 78 | GLN |
| 33 | 2b | 94 | ASN |
| 34 | 2c | 108 | ASN |
| 34 | 2c | 139 | GLN |
| 34 | 2c | 176 | HIS |
| 35 | 2d | 74 | GLN |
| 35 | 2d | 77 | ASN |
| 35 | 2d | 116 | GLN |
| 35 | 2d | 125 | HIS |
| 36 | 2e | 78 | HIS |
| 37 | 2f | 73 | ASN |
| 37 | 2f | 100 | ASN |
| 38 | 2g | 13 | GLN |
| 38 | 2g | 28 | ASN |
| 38 | 2g | 37 | ASN |
| 38 | 2g | 86 | GLN |
| 38 | 2g | 109 | ASN |
| 40 | 2i | 3 | GLN |
| 40 | 2i | 58 | HIS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | 2j | 56 | HIS |
| 42 | 2k | 22 | HIS |
| 42 | 2k | 117 | ASN |
| 43 | 2l | 99 | HIS |
| 46 | 2o | 50 | HIS |
| 46 | 2o | 62 | GLN |
| 47 | 2p | 16 | HIS |
| 48 | 2q | 45 | HIS |
| 49 | 2r | 63 | GLN |
| 50 | 2s | 23 | ASN |
| 50 | 2s | 47 | HIS |
| 50 | 2s | 57 | HIS |
| 50 | 2s | 69 | HIS |
| 50 | 2s | 83 | HIS |
| 51 | 2t | 42 | GLN |

### 5.3.3 RNA

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|---|---|---|---|---|
| 1 | 1A | 2864/2915 (98%) | 431 (15%) | 29 (1%) |
| 1 | 2A | 2791/2915 (95%) | 482 (17%) | 24 (0%) |
| 2 | 1B | 120/121 (99%) | 11 (9%) | 1 (0%) |
| 2 | 2B | 118/121 (97%) | 33 (27%) | 0 |
| 32 | 1a | 1497/1521 (98%) | 240 (16%) | 0 |
| 32 | 2a | 1501/1521 (98%) | 286 (19%) | 0 |
| 53 | 1v | 12/24 (50%) | 2 (16%) | 0 |
| 53 | 2v | 12/24 (50%) | 4 (33%) | 0 |
| 54 | 1w | 72/76 (94%) | 23 (31%) | 0 |
| 54 | 1y | 72/76 (94%) | 19 (26%) | 0 |
| 54 | 2w | 69/76 (90%) | 22 (31%) | 0 |
| 54 | 2y | 70/76 (92%) | 21 (30%) | 0 |
| 55 | 1x | 75/77 (97%) | 10 (13%) | 0 |
| 55 | 2x | 75/77 (97%) | 13 (17%) | 0 |
| All | All | 9348/9620 (97%) | 1597 (17%) | 54 (0%) |

All (1597) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 1A | 9 | U |
| 1 | 1A | 12 | U |
| 1 | 1A | 13 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 1A | 27 | G |
| 1 | 1A | 34 | C |
| 1 | 1A | 36 | G |
| 1 | 1A | 45 | C |
| 1 | 1A | 51 | G |
| 1 | 1A | 55 | G |
| 1 | 1A | 58 | G |
| 1 | 1A | 71 | A |
| 1 | 1A | 72 | U |
| 1 | 1A | 74 | A |
| 1 | 1A | 75 | G |
| 1 | 1A | 84 | A |
| 1 | 1A | 95 | G |
| 1 | 1A | 102 | G |
| 1 | 1A | 118 | A |
| 1 | 1A | 119 | A |
| 1 | 1A | 120 | U |
| 1 | 1A | 125 | G |
| 1 | 1A | 136 | G |
| 1 | 1A | 139(A) | G |
| 1 | 1A | 182 | A |
| 1 | 1A | 196 | A |
| 1 | 1A | 199 | A |
| 1 | 1A | 200 | U |
| 1 | 1A | 205 | G |
| 1 | 1A | 215 | G |
| 1 | 1A | 216 | A |
| 1 | 1A | 222 | A |
| 1 | 1A | 225 | A |
| 1 | 1A | 228 | A |
| 1 | 1A | 229 | A |
| 1 | 1A | 232 | G |
| 1 | 1A | 248 | G |
| 1 | 1A | 269 | U |
| 1 | 1A | 271(E) | U |
| 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 | 271(S) | G |
| 1 | 1A | 271(U) | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 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 | 352 | G |
| 1 | 1A | 363 | G |
| 1 | 1A | 380 | U |
| 1 | 1A | 386 | G |
| 1 | 1A | 396 | G |
| 1 | 1A | 405 | U |
| 1 | 1A | 411 | G |
| 1 | 1A | 412 | A |
| 1 | 1A | 421 | U |
| 1 | 1A | 428 | A |
| 1 | 1A | 444 | C |
| 1 | 1A | 448 | U |
| 1 | 1A | 457 | A |
| 1 | 1A | 481 | G |
| 1 | 1A | 504 | U |
| 1 | 1A | 505 | A |
| 1 | 1A | 509 | C |
| 1 | 1A | 510 | C |
| 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 | 563 | G |
| 1 | 1A | 573 | G |
| 1 | 1A | 574 | C |
| 1 | 1A | 575 | A |
| 1 | 1A | 587 | C |
| 1 | 1A | 603 | A |
| 1 | 1A | 604 | G |
| 1 | 1A | 607 | U |
| 1 | 1A | 614(B) | G |
| 1 | 1A | 615 | G |
| 1 | 1A | 621 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 1A | 627 | A |
| 1 | 1A | 637 | A |
| 1 | 1A | 645 | C |
| 1 | 1A | 646 | A |
| 1 | 1A | 652(E) | G |
| 1 | 1A | 652(T) | C |
| 1 | 1A | 669 | G |
| 1 | 1A | 686 | G |
| 1 | 1A | 730 | C |
| 1 | 1A | 740 | U |
| 1 | 1A | 765 | G |
| 1 | 1A | 775 | G |
| 1 | 1A | 776 | G |
| 1 | 1A | 782 | A |
| 1 | 1A | 784 | A |
| 1 | 1A | 785 | G |
| 1 | 1A | 790 | C |
| 1 | 1A | 792 | G |
| 1 | 1A | 805 | G |
| 1 | 1A | 812 | C |
| 1 | 1A | 819 | A |
| 1 | 1A | 827 | U |
| 1 | 1A | 828 | U |
| 1 | 1A | 854 | G |
| 1 | 1A | 859 | G |
| 1 | 1A | 866 | A |
| 1 | 1A | 877 | U |
| 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 | 890 | A |
| 1 | 1A | 895 | U |
| 1 | 1A | 896 | A |
| 1 | 1A | 897 | C |
| 1 | 1A | 898 | C |
| 1 | 1A | 907 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 1A | 910 | A |
| 1 | 1A | 932 | G |
| 1 | 1A | 945 | A |
| 1 | 1A | 946 | G |
| 1 | 1A | 953 | A |
| 1 | 1A | 958 | U |
| 1 | 1A | 959 | A |
| 1 | 1A | 961 | C |
| 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 | 1026 | U |
| 1 | 1A | 1033 | U |
| 1 | 1A | 1038 | C |
| 1 | 1A | 1041 | C |
| 1 | 1A | 1044 | G |
| 1 | 1A | 1045 | A |
| 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 | 1063 | G |
| 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 | 1077 | A |
| 1 | 1A | 1078 | U |
| 1 | 1A | 1079 | C |
| 1 | 1A | 1082 | U |
| 1 | 1A | 1083 | U |
| 1 | 1A | 1084 | A |
| 1 | 1A | 1088 | A |
| 1 | 1A | 1089 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 1A | 1090 | U |
| 1 | 1A | 1091 | G |
| 1 | 1A | 1093 | G |
| 1 | 1A | 1094 | U |
| 1 | 1A | 1101 | U |
| 1 | 1A | 1102 | C |
| 1 | 1A | 1103 | A |
| 1 | 1A | 1110 | G |
| 1 | 1A | 1111 | A |
| 1 | 1A | 1112 | G |
| 1 | 1A | 1115 | G |
| 1 | 1A | 1116 | C |
| 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 | 1220 | A |
| 1 | 1A | 1244 | G |
| 1 | 1A | 1247 | A |
| 1 | 1A | 1250 | G |
| 1 | 1A | 1253 | A |
| 1 | 1A | 1256 | G |
| 1 | 1A | 1271 | G |
| 1 | 1A | 1272 | A |
| 1 | 1A | 1273 | U |
| 1 | 1A | 1275 | A |
| 1 | 1A | 1276 | A |
| 1 | 1A | 1300 | U |
| 1 | 1A | 1301 | A |
| 1 | 1A | 1303 | G |
| 1 | 1A | 1313 | U |
| 1 | 1A | 1352 | U |
| 1 | 1A | 1359 | A |
| 1 | 1A | 1360 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 1A | 1365 | A |
| 1 | 1A | 1380 | G |
| 1 | 1A | 1384 | A |
| 1 | 1A | 1385 | G |
| 1 | 1A | 1386 | C |
| 1 | 1A | 1416 | G |
| 1 | 1A | 1417 | C |
| 1 | 1A | 1421 | G |
| 1 | 1A | 1428 | C |
| 1 | 1A | 1439 | A |
| 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 | 1509 | C |
| 1 | 1A | 1509(A) | A |
| 1 | 1A | 1558 | A |
| 1 | 1A | 1559 | G |
| 1 | 1A | 1566 | A |
| 1 | 1A | 1569 | A |
| 1 | 1A | 1578 | U |
| 1 | 1A | 1581 | G |
| 1 | 1A | 1584 | C |
| 1 | 1A | 1586 | A |
| 1 | 1A | 1608 | A |
| 1 | 1A | 1610 | A |
| 1 | 1A | 1648 | C |
| 1 | 1A | 1654 | A |
| 1 | 1A | 1664 | A |
| 1 | 1A | 1669 | A |
| 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 | 1746 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 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 | 1786 | A |
| 1 | 1A | 1791 | A |
| 1 | 1A | 1800 | C |
| 1 | 1A | 1801 | G |
| 1 | 1A | 1816 | G |
| 1 | 1A | 1847 | A |
| 1 | 1A | 1858 | G |
| 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 | 1915 | 5MU |
| 1 | 1A | 1929 | G |
| 1 | 1A | 1930 | G |
| 1 | 1A | 1937 | A |
| 1 | 1A | 1938 | A |
| 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 | 1993 | U |
| 1 | 1A | 1997 | G |
| 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 |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 1A | 2060 | A |
| 1 | 1A | 2061 | G |
| 1 | 1A | 2069 | G |
| 1 | 1A | 2110 | G |
| 1 | 1A | 2111 | C |
| 1 | 1A | 2113 | U |
| 1 | 1A | 2118 | U |
| 1 | 1A | 2119 | A |
| 1 | 1A | 2121 | G |
| 1 | 1A | 2126 | A |
| 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 | 2140 | C |
| 1 | 1A | 2141 | G |
| 1 | 1A | 2142 | C |
| 1 | 1A | 2144 | U |
| 1 | 1A | 2147 | G |
| 1 | 1A | 2150 | U |
| 1 | 1A | 2151 | G |
| 1 | 1A | 2157 | G |
| 1 | 1A | 2158 | A |
| 1 | 1A | 2159 | G |
| 1 | 1A | 2162 | G |
| 1 | 1A | 2165 | G |
| 1 | 1A | 2166 | G |
| 1 | 1A | 2168 | G |
| 1 | 1A | 2171 | A |
| 1 | 1A | 2172 | U |
| 1 | 1A | 2173 | A |
| 1 | 1A | 2181 | G |
| 1 | 1A | 2182 | G |
| 1 | 1A | 2184 | G |
| 1 | 1A | 2192 | G |
| 1 | 1A | 2198 | A |
| 1 | 1A | 2206 | G |
| 1 | 1A | 2207 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 1A | 2208 | A |
| 1 | 1A | 2219 | G |
| 1 | 1A | 2225 | A |
| 1 | 1A | 2238 | G |
| 1 | 1A | 2239 | G |
| 1 | 1A | 2268 | A |
| 1 | 1A | 2269 | A |
| 1 | 1A | 2273 | A |
| 1 | 1A | 2283 | C |
| 1 | 1A | 2287 | A |
| 1 | 1A | 2305 | A |
| 1 | 1A | 2308 | G |
| 1 | 1A | 2309 | A |
| 1 | 1A | 2320 | A |
| 1 | 1A | 2325 | G |
| 1 | 1A | 2334 | G |
| 1 | 1A | 2336 | A |
| 1 | 1A | 2347 | C |
| 1 | 1A | 2361 | A |
| 1 | 1A | 2372 | G |
| 1 | 1A | 2383 | G |
| 1 | 1A | 2385 | C |
| 1 | 1A | 2396 | G |
| 1 | 1A | 2400 | G |
| 1 | 1A | 2406 | U |
| 1 | 1A | 2408 | U |
| 1 | 1A | 2410 | G |
| 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 | 2448 | A |
| 1 | 1A | 2449 | U |
| 1 | 1A | 2474 | C |
| 1 | 1A | 2476 | A |
| 1 | 1A | 2484 | G |
| 1 | 1A | 2491 | U |
| 1 | 1A | 2498 | C |
| 1 | 1A | 2502 | G |
| 1 | 1A | 2505 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 1A | 2518 | A |
| 1 | 1A | 2520 | C |
| 1 | 1A | 2529 | G |
| 1 | 1A | 2554 | U |
| 1 | 1A | 2566 | A |
| 1 | 1A | 2567 | G |
| 1 | 1A | 2573 | C |
| 1 | 1A | 2602 | A |
| 1 | 1A | 2609 | U |
| 1 | 1A | 2611 | U |
| 1 | 1A | 2612 | C |
| 1 | 1A | 2629 | A |
| 1 | 1A | 2630 | G |
| 1 | 1A | 2654 | A |
| 1 | 1A | 2689 | U |
| 1 | 1A | 2690 | C |
| 1 | 1A | 2691 | C |
| 1 | 1A | 2702 | U |
| 1 | 1A | 2703 | C |
| 1 | 1A | 2712(A) | A |
| 1 | 1A | 2713 | A |
| 1 | 1A | 2714 | G |
| 1 | 1A | 2726 | U |
| 1 | 1A | 2733 | A |
| 1 | 1A | 2757 | A |
| 1 | 1A | 2758 | A |
| 1 | 1A | 2761 | G |
| 1 | 1A | 2764 | A |
| 1 | 1A | 2765 | A |
| 1 | 1A | 2766 | G |
| 1 | 1A | 2769 | C |
| 1 | 1A | 2778 | A |
| 1 | 1A | 2790 | A |
| 1 | 1A | 2791 | C |
| 1 | 1A | 2793 | G |
| 1 | 1A | 2794 | C |
| 1 | 1A | 2802 | G |
| 1 | 1A | 2805 | G |
| 1 | 1A | 2818 | G |
| 1 | 1A | 2820 | A |
| 1 | 1A | 2821 | A |
| 1 | 1A | 2834 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 1A | 2835 | A |
| 1 | 1A | 2858 | C |
| 1 | 1A | 2872 | G |
| 1 | 1A | 2873 | A |
| 1 | 1A | 2876 | G |
| 1 | 1A | 2880 | C |
| 1 | 1A | 2892 | A |
| 1 | 1A | 2894 | G |
| 2 | 1B | 2 | C |
| 2 | 1B | 12 | C |
| 2 | 1B | 21 | G |
| 2 | 1B | 25 | A |
| 2 | 1B | 35 | U |
| 2 | 1B | 50 | G |
| 2 | 1B | 56 | G |
| 2 | 1B | 73 | A |
| 2 | 1B | 85 | G |
| 2 | 1B | 109 | C |
| 2 | 1B | 110 | G |
| 32 | 1a | 7 | G |
| 32 | 1a | 9 | G |
| 32 | 1a | 32 | A |
| 32 | 1a | 33 | A |
| 32 | 1a | 39 | G |
| 32 | 1a | 47 | C |
| 32 | 1a | 48 | C |
| 32 | 1a | 50 | A |
| 32 | 1a | 51 | A |
| 32 | 1a | 52 | G |
| 32 | 1a | 61 | G |
| 32 | 1a | 65 | U |
| 32 | 1a | 91 | C |
| 32 | 1a | 98 | G |
| 32 | 1a | 116 | A |
| 32 | 1a | 120 | A |
| 32 | 1a | 121 | C |
| 32 | 1a | 131 | C |
| 32 | 1a | 163 | C |
| 32 | 1a | 174 | C |
| 32 | 1a | 180 | U |
| 32 | 1a | 183 | G |
| 32 | 1a | 189(D) | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 32 | 1a | 189(F) | U |
| 32 | 1a | 189(G) | G |
| 32 | 1a | 189(J) | G |
| 32 | 1a | 195 | A |
| 32 | 1a | 197 | A |
| 32 | 1a | 199 | G |
| 32 | 1a | 201 | C |
| 32 | 1a | 202 | U |
| 32 | 1a | 203 | U |
| 32 | 1a | 204 | U |
| 32 | 1a | 216 | G |
| 32 | 1a | 217 | C |
| 32 | 1a | 219 | C |
| 32 | 1a | 222 | U |
| 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 | 321 | A |
| 32 | 1a | 328 | C |
| 32 | 1a | 332 | G |
| 32 | 1a | 344 | A |
| 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 | 384 | G |
| 32 | 1a | 397 | A |
| 32 | 1a | 398 | C |
| 32 | 1a | 406 | G |
| 32 | 1a | 412 | A |
| 32 | 1a | 423 | G |
| 32 | 1a | 424 | G |
| 32 | 1a | 429 | U |
| 32 | 1a | 439 | A |
| 32 | 1a | 452 | A |
| 32 | 1a | 453 | A |
| 32 | 1a | 461 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 32 | 1a | 470 | C |
| 32 | 1a | 471 | G |
| 32 | 1a | 485 | G |
| 32 | 1a | 496 | A |
| 32 | 1a | 498 | U |
| 32 | 1a | 505 | G |
| 32 | 1a | 509 | A |
| 32 | 1a | 510 | A |
| 32 | 1a | 511 | C |
| 32 | 1a | 518 | C |
| 32 | 1a | 528 | C |
| 32 | 1a | 531 | U |
| 32 | 1a | 532 | A |
| 32 | 1a | 547 | A |
| 32 | 1a | 559 | A |
| 32 | 1a | 561 | U |
| 32 | 1a | 568 | G |
| 32 | 1a | 572 | A |
| 32 | 1a | 573 | A |
| 32 | 1a | 576 | G |
| 32 | 1a | 577 | G |
| 32 | 1a | 596 | C |
| 32 | 1a | 629 | G |
| 32 | 1a | 630 | G |
| 32 | 1a | 653 | A |
| 32 | 1a | 665 | A |
| 32 | 1a | 686 | U |
| 32 | 1a | 687 | A |
| 32 | 1a | 688 | G |
| 32 | 1a | 695 | A |
| 32 | 1a | 723 | U |
| 32 | 1a | 731 | G |
| 32 | 1a | 749 | C |
| 32 | 1a | 755 | G |
| 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 |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 32 | 1a | 828 | A |
| 32 | 1a | 840 | C |
| 32 | 1a | 841 | U |
| 32 | 1a | 851 | G |
| 32 | 1a | 853 | G |
| 32 | 1a | 859 | A |
| 32 | 1a | 870 | U |
| 32 | 1a | 872 | A |
| 32 | 1a | 902 | G |
| 32 | 1a | 914 | A |
| 32 | 1a | 926 | G |
| 32 | 1a | 927 | G |
| 32 | 1a | 932 | C |
| 32 | 1a | 934 | C |
| 32 | 1a | 955 | U |
| 32 | 1a | 960 | U |
| 32 | 1a | 961 | U |
| 32 | 1a | 968 | A |
| 32 | 1a | 969 | A |
| 32 | 1a | 971 | G |
| 32 | 1a | 974 | A |
| 32 | 1a | 975 | A |
| 32 | 1a | 976 | G |
| 32 | 1a | 977 | A |
| 32 | 1a | 982 | U |
| 32 | 1a | 992 | U |
| 32 | 1a | 993 | G |
| 32 | 1a | 997 | U |
| 32 | 1a | 1000 | U |
| 32 | 1a | 1003 | G |
| 32 | 1a | 1005 | A |
| 32 | 1a | 1006 | C |
| 32 | 1a | 1009 | 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 | 1029 | C |
| 32 | 1a | 1030(A) | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 32 | 1a | 1030(B) | C |
| 32 | 1a | 1030(C) | G |
| 32 | 1a | 1031 | G |
| 32 | 1a | 1032 | G |
| 32 | 1a | 1033 | G |
| 32 | 1a | 1039 | C |
| 32 | 1a | 1045 | C |
| 32 | 1a | 1054 | C |
| 32 | 1a | 1065 | U |
| 32 | 1a | 1066 | C |
| 32 | 1a | 1068 | G |
| 32 | 1a | 1070 | U |
| 32 | 1a | 1081 | G |
| 32 | 1a | 1087 | G |
| 32 | 1a | 1094 | G |
| 32 | 1a | 1095 | U |
| 32 | 1a | 1101 | A |
| 32 | 1a | 1104 | G |
| 32 | 1a | 1108 | G |
| 32 | 1a | 1121 | U |
| 32 | 1a | 1125 | U |
| 32 | 1a | 1132 | C |
| 32 | 1a | 1134 | G |
| 32 | 1a | 1136 | U |
| 32 | 1a | 1137 | C |
| 32 | 1a | 1138 | G |
| 32 | 1a | 1139 | G |
| 32 | 1a | 1140 | C |
| 32 | 1a | 1146 | A |
| 32 | 1a | 1152 | A |
| 32 | 1a | 1156 | G |
| 32 | 1a | 1157 | A |
| 32 | 1a | 1159 | U |
| 32 | 1a | 1160 | G |
| 32 | 1a | 1166 | G |
| 32 | 1a | 1184 | G |
| 32 | 1a | 1193 | G |
| 32 | 1a | 1196 | U |
| 32 | 1a | 1197 | G |
| 32 | 1a | 1202 | G |
| 32 | 1a | 1212 | U |
| 32 | 1a | 1213 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 32 | 1a | 1222 | G |
| 32 | 1a | 1226 | C |
| 32 | 1a | 1227 | A |
| 32 | 1a | 1236 | A |
| 32 | 1a | 1238 | A |
| 32 | 1a | 1246 | C |
| 32 | 1a | 1256 | A |
| 32 | 1a | 1257 | U |
| 32 | 1a | 1260 | C |
| 32 | 1a | 1270 | C |
| 32 | 1a | 1275 | A |
| 32 | 1a | 1276 | G |
| 32 | 1a | 1278 | U |
| 32 | 1a | 1279 | A |
| 32 | 1a | 1280 | A |
| 32 | 1a | 1286 | A |
| 32 | 1a | 1287 | A |
| 32 | 1a | 1299 | A |
| 32 | 1a | 1300 | G |
| 32 | 1a | 1302 | U |
| 32 | 1a | 1320 | C |
| 32 | 1a | 1338 | G |
| 32 | 1a | 1346 | A |
| 32 | 1a | 1347 | G |
| 32 | 1a | 1353 | G |
| 32 | 1a | 1363 | C |
| 32 | 1a | 1363(A) | A |
| 32 | 1a | 1368 | G |
| 32 | 1a | 1370 | G |
| 32 | 1a | 1378 | C |
| 32 | 1a | 1394 | A |
| 32 | 1a | 1397 | C |
| 32 | 1a | 1419 | G |
| 32 | 1a | 1442 | G |
| 32 | 1a | 1442(A) | G |
| 32 | 1a | 1446 | U |
| 32 | 1a | 1452 | C |
| 32 | 1a | 1456 | G |
| 32 | 1a | 1487 | G |
| 32 | 1a | 1492 | A |
| 32 | 1a | 1494 | G |
| 32 | 1a | 1503 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 32 | 1a | 1504 | G |
| 32 | 1a | 1506 | U |
| 32 | 1a | 1517 | G |
| 32 | 1a | 1519 | MA6 |
| 32 | 1a | 1520 | G |
| 32 | 1a | 1529 | G |
| 32 | 1a | 1530 | G |
| 53 | 1v | 13 | A |
| 53 | 1v | 24 | A |
| 54 | 1w | 2 | C |
| 54 | 1w | 3 | C |
| 54 | 1w | 6 | G |
| 54 | 1w | 7 | A |
| 54 | 1w | 8 | 4SU |
| 54 | 1w | 9 | A |
| 54 | 1w | 14 | A |
| 54 | 1w | 19 | G |
| 54 | 1w | 20 | U |
| 54 | 1w | 23 | A |
| 54 | 1w | 24 | G |
| 54 | 1w | 25 | C |
| 54 | 1w | 45 | U |
| 54 | 1w | 46 | 7MG |
| 54 | 1w | 47 | U |
| 54 | 1w | 48 | C |
| 54 | 1w | 50 | U |
| 54 | 1w | 63 | G |
| 54 | 1w | 68 | C |
| 54 | 1w | 70 | G |
| 54 | 1w | 71 | G |
| 54 | 1w | 73 | A |
| 54 | 1w | 74 | C |
| 55 | 1x | 6 | G |
| 55 | 1x | 9 | G |
| 55 | 1x | 14 | A |
| 55 | 1x | 19 | G |
| 55 | 1x | 21 | A |
| 55 | 1x | 22 | G |
| 55 | 1x | 47 | U |
| 55 | 1x | 63 | G |
| 55 | 1x | 64 | G |
| 55 | 1x | 76 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 54 | 1y | 6 | G |
| 54 | 1y | 8 | 4SU |
| 54 | 1y | 9 | A |
| 54 | 1y | 11 | C |
| 54 | 1y | 13 | C |
| 54 | 1y | 14 | A |
| 54 | 1y | 19 | G |
| 54 | 1y | 20 | U |
| 54 | 1y | 21 | A |
| 54 | 1y | 22 | G |
| 54 | 1y | 35 | A |
| 54 | 1y | 44 | G |
| 54 | 1y | 45 | U |
| 54 | 1y | 46 | 7MG |
| 54 | 1y | 47 | U |
| 54 | 1y | 57 | G |
| 54 | 1y | 59 | U |
| 54 | 1y | 61 | C |
| 54 | 1y | 70 | G |
| 1 | 2A | 10 | G |
| 1 | 2A | 11 | G |
| 1 | 2A | 15 | G |
| 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 | 83 | G |
| 1 | 2A | 84 | A |
| 1 | 2A | 90 | U |
| 1 | 2A | 95 | G |
| 1 | 2A | 96 | G |
| 1 | 2A | 100 | G |
| 1 | 2A | 102 | G |
| 1 | 2A | 118 | A |
| 1 | 2A | 120 | U |
| 1 | 2A | 131 | G |
| 1 | 2A | 141 | A |
| 1 | 2A | 154(A) | C |
| 1 | 2A | 157 | U |
| 1 | 2A | 173 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 2A | 181 | A |
| 1 | 2A | 196 | A |
| 1 | 2A | 199 | A |
| 1 | 2A | 205 | G |
| 1 | 2A | 214 | G |
| 1 | 2A | 215 | G |
| 1 | 2A | 216 | A |
| 1 | 2A | 221 | A |
| 1 | 2A | 222 | A |
| 1 | 2A | 225 | A |
| 1 | 2A | 228 | A |
| 1 | 2A | 229 | A |
| 1 | 2A | 233 | A |
| 1 | 2A | 248 | G |
| 1 | 2A | 249 | C |
| 1 | 2A | 266 | G |
| 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 | 277 | C |
| 1 | 2A | 278 | A |
| 1 | 2A | 294 | A |
| 1 | 2A | 304 | G |
| 1 | 2A | 311 | A |
| 1 | 2A | 324 | A |
| 1 | 2A | 327 | G |
| 1 | 2A | 329 | G |
| 1 | 2A | 330 | A |
| 1 | 2A | 342 | G |
| 1 | 2A | 352 | G |
| 1 | 2A | 362 | U |
| 1 | 2A | 363 | G |
| 1 | 2A | 363(B) | G |
| 1 | 2A | 363(D) | G |
| 1 | 2A | 386 | G |
| 1 | 2A | 389 | G |
| 1 | 2A | 396 | G |
| 1 | 2A | 411 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 2A | 412 | A |
| 1 | 2A | 422 | A |
| 1 | 2A | 435 | C |
| 1 | 2A | 444 | C |
| 1 | 2A | 454 | A |
| 1 | 2A | 455 | C |
| 1 | 2A | 457 | A |
| 1 | 2A | 481 | G |
| 1 | 2A | 505 | A |
| 1 | 2A | 508 | G |
| 1 | 2A | 509 | C |
| 1 | 2A | 528 | A |
| 1 | 2A | 529 | A |
| 1 | 2A | 531 | C |
| 1 | 2A | 532 | A |
| 1 | 2A | 533 | G |
| 1 | 2A | 545 | 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 | 595 | C |
| 1 | 2A | 599 | G |
| 1 | 2A | 603 | A |
| 1 | 2A | 604 | G |
| 1 | 2A | 607 | U |
| 1 | 2A | 614(A) | U |
| 1 | 2A | 614(B) | G |
| 1 | 2A | 615 | G |
| 1 | 2A | 616 | G |
| 1 | 2A | 627 | A |
| 1 | 2A | 637 | A |
| 1 | 2A | 645 | C |
| 1 | 2A | 652(B) | A |
| 1 | 2A | 652(U) | G |
| 1 | 2A | 653 | A |
| 1 | 2A | 661 | C |
| 1 | 2A | 669 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 2A | 686 | G |
| 1 | 2A | 701 | G |
| 1 | 2A | 712 | G |
| 1 | 2A | 717 | G |
| 1 | 2A | 726 | G |
| 1 | 2A | 730 | C |
| 1 | 2A | 753 | C |
| 1 | 2A | 771 | G |
| 1 | 2A | 775 | G |
| 1 | 2A | 776 | G |
| 1 | 2A | 778 | G |
| 1 | 2A | 782 | A |
| 1 | 2A | 783 | A |
| 1 | 2A | 784 | A |
| 1 | 2A | 785 | G |
| 1 | 2A | 790 | C |
| 1 | 2A | 792 | G |
| 1 | 2A | 805 | G |
| 1 | 2A | 806 | C |
| 1 | 2A | 811 | U |
| 1 | 2A | 812 | C |
| 1 | 2A | 819 | A |
| 1 | 2A | 827 | U |
| 1 | 2A | 828 | U |
| 1 | 2A | 832 | G |
| 1 | 2A | 847 | U |
| 1 | 2A | 854 | G |
| 1 | 2A | 856 | C |
| 1 | 2A | 857 | C |
| 1 | 2A | 859 | G |
| 1 | 2A | 866 | A |
| 1 | 2A | 869 | G |
| 1 | 2A | 873 | G |
| 1 | 2A | 874 | G |
| 1 | 2A | 875 | G |
| 1 | 2A | 879 | G |
| 1 | 2A | 880 | G |
| 1 | 2A | 884 | C |
| 1 | 2A | 886 | C |
| 1 | 2A | 887 | A |
| 1 | 2A | 888 | C |
| 1 | 2A | 889 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 2A | 890 | A |
| 1 | 2A | 892 | G |
| 1 | 2A | 893 | C |
| 1 | 2A | 894 | C |
| 1 | 2A | 895 | U |
| 1 | 2A | 896 | A |
| 1 | 2A | 900 | A |
| 1 | 2A | 901 | A |
| 1 | 2A | 910 | A |
| 1 | 2A | 914 | C |
| 1 | 2A | 917 | A |
| 1 | 2A | 932 | G |
| 1 | 2A | 933 | A |
| 1 | 2A | 936 | C |
| 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 | 979 | G |
| 1 | 2A | 980 | A |
| 1 | 2A | 983 | A |
| 1 | 2A | 996 | A |
| 1 | 2A | 997 | G |
| 1 | 2A | 1012 | U |
| 1 | 2A | 1013 | C |
| 1 | 2A | 1017 | G |
| 1 | 2A | 1020 | A |
| 1 | 2A | 1022 | G |
| 1 | 2A | 1025 | G |
| 1 | 2A | 1027 | A |
| 1 | 2A | 1033 | U |
| 1 | 2A | 1038 | C |
| 1 | 2A | 1039 | G |
| 1 | 2A | 1043 | C |
| 1 | 2A | 1114 | G |
| 1 | 2A | 1116 | C |
| 1 | 2A | 1130 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 2A | 1135 | C |
| 1 | 2A | 1136 | G |
| 1 | 2A | 1139 | G |
| 1 | 2A | 1166 | C |
| 1 | 2A | 1167 | U |
| 1 | 2A | 1171 | G |
| 1 | 2A | 1188 | U |
| 1 | 2A | 1195 | G |
| 1 | 2A | 1206 | G |
| 1 | 2A | 1210 | A |
| 1 | 2A | 1211 | U |
| 1 | 2A | 1220 | A |
| 1 | 2A | 1229 | G |
| 1 | 2A | 1237 | A |
| 1 | 2A | 1248 | G |
| 1 | 2A | 1253 | A |
| 1 | 2A | 1256 | G |
| 1 | 2A | 1271 | G |
| 1 | 2A | 1272 | A |
| 1 | 2A | 1273 | U |
| 1 | 2A | 1284 | A |
| 1 | 2A | 1287 | A |
| 1 | 2A | 1300 | U |
| 1 | 2A | 1301 | A |
| 1 | 2A | 1309 | G |
| 1 | 2A | 1314 | C |
| 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 | 1373 | A |
| 1 | 2A | 1376 | 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 |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 2A | 1421 | G |
| 1 | 2A | 1427 | A |
| 1 | 2A | 1428 | C |
| 1 | 2A | 1437 | C |
| 1 | 2A | 1444 | G |
| 1 | 2A | 1445 | A |
| 1 | 2A | 1449 | A |
| 1 | 2A | 1450 | G |
| 1 | 2A | 1460 | A |
| 1 | 2A | 1463 | C |
| 1 | 2A | 1467 | C |
| 1 | 2A | 1471 | A |
| 1 | 2A | 1478 | G |
| 1 | 2A | 1482 | G |
| 1 | 2A | 1490 | A |
| 1 | 2A | 1493 | C |
| 1 | 2A | 1494 | A |
| 1 | 2A | 1496 | A |
| 1 | 2A | 1497 | U |
| 1 | 2A | 1508 | A |
| 1 | 2A | 1509 | C |
| 1 | 2A | 1509(A) | A |
| 1 | 2A | 1525 | G |
| 1 | 2A | 1531 | C |
| 1 | 2A | 1532 | C |
| 1 | 2A | 1533 | G |
| 1 | 2A | 1537 | G |
| 1 | 2A | 1543 | C |
| 1 | 2A | 1544 | A |
| 1 | 2A | 1547 | C |
| 1 | 2A | 1558 | A |
| 1 | 2A | 1566 | A |
| 1 | 2A | 1569 | A |
| 1 | 2A | 1578 | U |
| 1 | 2A | 1579 | A |
| 1 | 2A | 1580 | A |
| 1 | 2A | 1584 | C |
| 1 | 2A | 1586 | A |
| 1 | 2A | 1608 | A |
| 1 | 2A | 1609 | A |
| 1 | 2A | 1610 | A |
| 1 | 2A | 1640 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 2A | 1648 | C |
| 1 | 2A | 1654 | A |
| 1 | 2A | 1663 | C |
| 1 | 2A | 1674 | G |
| 1 | 2A | 1696 | G |
| 1 | 2A | 1700 | A |
| 1 | 2A | 1701 | A |
| 1 | 2A | 1703 | G |
| 1 | 2A | 1721 | G |
| 1 | 2A | 1722 | A |
| 1 | 2A | 1739 | U |
| 1 | 2A | 1740 | G |
| 1 | 2A | 1746 | G |
| 1 | 2A | 1756 | G |
| 1 | 2A | 1758 | G |
| 1 | 2A | 1762 | A |
| 1 | 2A | 1763 | G |
| 1 | 2A | 1764 | G |
| 1 | 2A | 1773 | A |
| 1 | 2A | 1780 | A |
| 1 | 2A | 1782 | C |
| 1 | 2A | 1786 | A |
| 1 | 2A | 1791 | A |
| 1 | 2A | 1800 | C |
| 1 | 2A | 1801 | G |
| 1 | 2A | 1811 | G |
| 1 | 2A | 1812 | A |
| 1 | 2A | 1816 | G |
| 1 | 2A | 1835 | G |
| 1 | 2A | 1847 | A |
| 1 | 2A | 1848 | 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 | 1936 | A |
| 1 | 2A | 1938 | A |
| 1 | 2A | 1955 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 2A | 1963 | U |
| 1 | 2A | 1967 | C |
| 1 | 2A | 1970 | A |
| 1 | 2A | 1971 | A |
| 1 | 2A | 1972 | A |
| 1 | 2A | 1992 | G |
| 1 | 2A | 1993 | U |
| 1 | 2A | 1997 | G |
| 1 | 2A | 2020 | A |
| 1 | 2A | 2023 | G |
| 1 | 2A | 2027 | G |
| 1 | 2A | 2031 | A |
| 1 | 2A | 2032 | G |
| 1 | 2A | 2033 | A |
| 1 | 2A | 2043 | C |
| 1 | 2A | 2050 | 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 | 2096 | U |
| 1 | 2A | 2103 | C |
| 1 | 2A | 2111 | C |
| 1 | 2A | 2113 | U |
| 1 | 2A | 2116 | G |
| 1 | 2A | 2117 | A |
| 1 | 2A | 2119 | A |
| 1 | 2A | 2120 | G |
| 1 | 2A | 2122 | U |
| 1 | 2A | 2124 | G |
| 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 |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 2A | 2137 | C |
| 1 | 2A | 2138 | C |
| 1 | 2A | 2140 | C |
| 1 | 2A | 2142 | C |
| 1 | 2A | 2146 | C |
| 1 | 2A | 2148 | G |
| 1 | 2A | 2150 | U |
| 1 | 2A | 2153 | G |
| 1 | 2A | 2157 | G |
| 1 | 2A | 2158 | A |
| 1 | 2A | 2161 | C |
| 1 | 2A | 2166 | G |
| 1 | 2A | 2167 | U |
| 1 | 2A | 2168 | G |
| 1 | 2A | 2169 | A |
| 1 | 2A | 2172 | U |
| 1 | 2A | 2174 | C |
| 1 | 2A | 2178 | C |
| 1 | 2A | 2180 | U |
| 1 | 2A | 2185 | C |
| 1 | 2A | 2189 | U |
| 1 | 2A | 2192 | G |
| 1 | 2A | 2198 | A |
| 1 | 2A | 2206 | G |
| 1 | 2A | 2207 | G |
| 1 | 2A | 2208 | A |
| 1 | 2A | 2225 | A |
| 1 | 2A | 2239 | G |
| 1 | 2A | 2273 | A |
| 1 | 2A | 2275 | C |
| 1 | 2A | 2278 | A |
| 1 | 2A | 2283 | C |
| 1 | 2A | 2287 | A |
| 1 | 2A | 2289 | G |
| 1 | 2A | 2294 | C |
| 1 | 2A | 2305 | A |
| 1 | 2A | 2308 | G |
| 1 | 2A | 2311 | A |
| 1 | 2A | 2319 | G |
| 1 | 2A | 2320 | A |
| 1 | 2A | 2325 | G |
| 1 | 2A | 2327 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 2A | 2334 | G |
| 1 | 2A | 2336 | A |
| 1 | 2A | 2347 | C |
| 1 | 2A | 2350 | C |
| 1 | 2A | 2352 | A |
| 1 | 2A | 2353 | G |
| 1 | 2A | 2361 | A |
| 1 | 2A | 2376 | A |
| 1 | 2A | 2377 | A |
| 1 | 2A | 2383 | G |
| 1 | 2A | 2385 | C |
| 1 | 2A | 2403 | C |
| 1 | 2A | 2406 | U |
| 1 | 2A | 2410 | G |
| 1 | 2A | 2425 | A |
| 1 | 2A | 2429 | G |
| 1 | 2A | 2430 | A |
| 1 | 2A | 2435 | A |
| 1 | 2A | 2439 | A |
| 1 | 2A | 2441 | C |
| 1 | 2A | 2445 | G |
| 1 | 2A | 2448 | A |
| 1 | 2A | 2468 | G |
| 1 | 2A | 2474 | C |
| 1 | 2A | 2476 | A |
| 1 | 2A | 2477 | C |
| 1 | 2A | 2478 | A |
| 1 | 2A | 2480 | C |
| 1 | 2A | 2487 | G |
| 1 | 2A | 2490 | G |
| 1 | 2A | 2491 | U |
| 1 | 2A | 2502 | G |
| 1 | 2A | 2505 | G |
| 1 | 2A | 2506 | U |
| 1 | 2A | 2507 | C |
| 1 | 2A | 2518 | A |
| 1 | 2A | 2520 | C |
| 1 | 2A | 2554 | U |
| 1 | 2A | 2566 | A |
| 1 | 2A | 2567 | G |
| 1 | 2A | 2586 | C |
| 1 | 2A | 2602 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 2A | 2609 | U |
| 1 | 2A | 2610 | C |
| 1 | 2A | 2611 | U |
| 1 | 2A | 2612 | C |
| 1 | 2A | 2623 | G |
| 1 | 2A | 2629 | A |
| 1 | 2A | 2630 | G |
| 1 | 2A | 2654 | A |
| 1 | 2A | 2662 | A |
| 1 | 2A | 2689 | U |
| 1 | 2A | 2690 | C |
| 1 | 2A | 2691 | C |
| 1 | 2A | 2712(A) | A |
| 1 | 2A | 2713 | A |
| 1 | 2A | 2714 | G |
| 1 | 2A | 2718 | G |
| 1 | 2A | 2726 | U |
| 1 | 2A | 2733 | A |
| 1 | 2A | 2751 | G |
| 1 | 2A | 2758 | A |
| 1 | 2A | 2759 | G |
| 1 | 2A | 2764 | A |
| 1 | 2A | 2765 | A |
| 1 | 2A | 2766 | G |
| 1 | 2A | 2778 | A |
| 1 | 2A | 2779 | U |
| 1 | 2A | 2780 | G |
| 1 | 2A | 2789 | C |
| 1 | 2A | 2802 | G |
| 1 | 2A | 2818 | G |
| 1 | 2A | 2820 | A |
| 1 | 2A | 2821 | A |
| 1 | 2A | 2833 | G |
| 1 | 2A | 2835 | A |
| 1 | 2A | 2850 | A |
| 1 | 2A | 2872 | G |
| 1 | 2A | 2880 | C |
| 1 | 2A | 2894 | G |
| 1 | 2A | 2897 | U |
| 2 | 2B | 2 | C |
| 2 | 2B | 4 | C |
| 2 | 2B | 5 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | 2B | 8 | U |
| 2 | 2B | 13 | A |
| 2 | 2B | 19 | G |
| 2 | 2B | 20 | C |
| 2 | 2B | 25 | A |
| 2 | 2B | 30 | C |
| 2 | 2B | 34 | U |
| 2 | 2B | 42 | C |
| 2 | 2B | 52 | A |
| 2 | 2B | 53 | A |
| 2 | 2B | 56 | G |
| 2 | 2B | 63 | G |
| 2 | 2B | 64 | C |
| 2 | 2B | 65 | C |
| 2 | 2B | 66 | A |
| 2 | 2B | 67 | G |
| 2 | 2B | 72 | G |
| 2 | 2B | 73 | A |
| 2 | 2B | 74 | U |
| 2 | 2B | 75 | G |
| 2 | 2B | 85 | G |
| 2 | 2B | 94 | C |
| 2 | 2B | 106 | G |
| 2 | 2B | 108 | U |
| 2 | 2B | 110 | G |
| 2 | 2B | 111 | G |
| 2 | 2B | 114 | C |
| 2 | 2B | 116 | G |
| 2 | 2B | 119 | G |
| 2 | 2B | 120 | A |
| 32 | 2a | 6 | 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 | 66 | G |
| 32 | 2a | 73 | G |
| 32 | 2a | 79 | G |
| 32 | 2a | 88 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 32 | 2a | 89 | C |
| 32 | 2a | 101 | A |
| 32 | 2a | 105 | G |
| 32 | 2a | 116 | A |
| 32 | 2a | 117 | G |
| 32 | 2a | 121 | C |
| 32 | 2a | 124 | G |
| 32 | 2a | 131 | C |
| 32 | 2a | 142 | G |
| 32 | 2a | 144 | G |
| 32 | 2a | 146 | G |
| 32 | 2a | 159 | G |
| 32 | 2a | 163 | C |
| 32 | 2a | 174 | C |
| 32 | 2a | 180 | U |
| 32 | 2a | 182 | U |
| 32 | 2a | 184 | G |
| 32 | 2a | 189(E) | U |
| 32 | 2a | 189(F) | U |
| 32 | 2a | 195 | A |
| 32 | 2a | 197 | A |
| 32 | 2a | 201 | C |
| 32 | 2a | 202 | U |
| 32 | 2a | 203 | U |
| 32 | 2a | 204 | U |
| 32 | 2a | 216 | G |
| 32 | 2a | 247 | G |
| 32 | 2a | 251 | G |
| 32 | 2a | 258 | G |
| 32 | 2a | 266 | G |
| 32 | 2a | 267 | C |
| 32 | 2a | 269 | C |
| 32 | 2a | 281 | G |
| 32 | 2a | 289 | G |
| 32 | 2a | 318 | G |
| 32 | 2a | 321 | A |
| 32 | 2a | 328 | C |
| 32 | 2a | 332 | G |
| 32 | 2a | 350 | G |
| 32 | 2a | 351 | G |
| 32 | 2a | 352 | C |
| 32 | 2a | 353 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 32 | 2a | 354 | G |
| 32 | 2a | 367 | U |
| 32 | 2a | 372 | C |
| 32 | 2a | 373 | A |
| 32 | 2a | 397 | A |
| 32 | 2a | 398 | C |
| 32 | 2a | 406 | G |
| 32 | 2a | 412 | A |
| 32 | 2a | 415 | A |
| 32 | 2a | 421 | U |
| 32 | 2a | 423 | G |
| 32 | 2a | 429 | U |
| 32 | 2a | 430 | A |
| 32 | 2a | 441 | A |
| 32 | 2a | 442 | C |
| 32 | 2a | 452 | A |
| 32 | 2a | 461 | A |
| 32 | 2a | 470 | C |
| 32 | 2a | 484 | G |
| 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 | 517 | G |
| 32 | 2a | 518 | C |
| 32 | 2a | 528 | C |
| 32 | 2a | 531 | U |
| 32 | 2a | 532 | A |
| 32 | 2a | 547 | A |
| 32 | 2a | 559 | A |
| 32 | 2a | 560 | U |
| 32 | 2a | 561 | U |
| 32 | 2a | 564 | C |
| 32 | 2a | 572 | A |
| 32 | 2a | 573 | A |
| 32 | 2a | 574 | A |
| 32 | 2a | 576 | G |
| 32 | 2a | 577 | G |
| 32 | 2a | 596 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 32 | 2a | 598 | U |
| 32 | 2a | 618 | C |
| 32 | 2a | 630 | G |
| 32 | 2a | 653 | A |
| 32 | 2a | 657 | G |
| 32 | 2a | 665 | A |
| 32 | 2a | 687 | A |
| 32 | 2a | 688 | G |
| 32 | 2a | 694 | A |
| 32 | 2a | 695 | A |
| 32 | 2a | 703 | G |
| 32 | 2a | 721 | G |
| 32 | 2a | 723 | U |
| 32 | 2a | 724 | G |
| 32 | 2a | 731 | G |
| 32 | 2a | 749 | C |
| 32 | 2a | 755 | G |
| 32 | 2a | 777 | A |
| 32 | 2a | 792 | A |
| 32 | 2a | 793 | U |
| 32 | 2a | 794 | A |
| 32 | 2a | 815 | A |
| 32 | 2a | 817 | C |
| 32 | 2a | 821 | G |
| 32 | 2a | 828 | A |
| 32 | 2a | 834 | C |
| 32 | 2a | 840 | C |
| 32 | 2a | 841 | U |
| 32 | 2a | 851 | G |
| 32 | 2a | 853 | G |
| 32 | 2a | 859 | A |
| 32 | 2a | 874 | G |
| 32 | 2a | 880 | C |
| 32 | 2a | 885 | G |
| 32 | 2a | 902 | G |
| 32 | 2a | 914 | A |
| 32 | 2a | 926 | G |
| 32 | 2a | 927 | G |
| 32 | 2a | 932 | C |
| 32 | 2a | 934 | C |
| 32 | 2a | 935 | A |
| 32 | 2a | 959 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 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 | 983 | A |
| 32 | 2a | 984 | C |
| 32 | 2a | 989 | C |
| 32 | 2a | 992 | U |
| 32 | 2a | 993 | G |
| 32 | 2a | 995 | C |
| 32 | 2a | 997 | U |
| 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 | 1011 | G |
| 32 | 2a | 1013 | G |
| 32 | 2a | 1017 | G |
| 32 | 2a | 1021 | G |
| 32 | 2a | 1022 | G |
| 32 | 2a | 1023 | G |
| 32 | 2a | 1025 | U |
| 32 | 2a | 1026 | G |
| 32 | 2a | 1027 | C |
| 32 | 2a | 1029 | C |
| 32 | 2a | 1030(A) | G |
| 32 | 2a | 1030(B) | C |
| 32 | 2a | 1030(D) | A |
| 32 | 2a | 1031 | G |
| 32 | 2a | 1033 | G |
| 32 | 2a | 1035 | A |
| 32 | 2a | 1038 | C |
| 32 | 2a | 1039 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 32 | 2a | 1040 | U |
| 32 | 2a | 1044 | A |
| 32 | 2a | 1045 | C |
| 32 | 2a | 1046 | A |
| 32 | 2a | 1051 | C |
| 32 | 2a | 1053 | G |
| 32 | 2a | 1064 | G |
| 32 | 2a | 1065 | U |
| 32 | 2a | 1066 | C |
| 32 | 2a | 1068 | G |
| 32 | 2a | 1077 | G |
| 32 | 2a | 1079 | G |
| 32 | 2a | 1081 | G |
| 32 | 2a | 1094 | G |
| 32 | 2a | 1095 | U |
| 32 | 2a | 1101 | A |
| 32 | 2a | 1103 | C |
| 32 | 2a | 1113 | C |
| 32 | 2a | 1115 | C |
| 32 | 2a | 1116 | C |
| 32 | 2a | 1117 | G |
| 32 | 2a | 1122 | U |
| 32 | 2a | 1125 | U |
| 32 | 2a | 1129 | C |
| 32 | 2a | 1130 | A |
| 32 | 2a | 1136 | U |
| 32 | 2a | 1137 | C |
| 32 | 2a | 1138 | G |
| 32 | 2a | 1139 | G |
| 32 | 2a | 1145 | C |
| 32 | 2a | 1146 | A |
| 32 | 2a | 1152 | A |
| 32 | 2a | 1157 | A |
| 32 | 2a | 1159 | U |
| 32 | 2a | 1160 | G |
| 32 | 2a | 1171 | G |
| 32 | 2a | 1172 | C |
| 32 | 2a | 1182 | G |
| 32 | 2a | 1183 | A |
| 32 | 2a | 1184 | G |
| 32 | 2a | 1189 | C |
| 32 | 2a | 1196 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 32 | 2a | 1197 | G |
| 32 | 2a | 1202 | G |
| 32 | 2a | 1209 | C |
| 32 | 2a | 1211 | U |
| 32 | 2a | 1212 | U |
| 32 | 2a | 1213 | A |
| 32 | 2a | 1228 | C |
| 32 | 2a | 1233 | G |
| 32 | 2a | 1236 | A |
| 32 | 2a | 1238 | A |
| 32 | 2a | 1240 | U |
| 32 | 2a | 1241 | G |
| 32 | 2a | 1248 | A |
| 32 | 2a | 1255 | G |
| 32 | 2a | 1256 | A |
| 32 | 2a | 1257 | U |
| 32 | 2a | 1260 | C |
| 32 | 2a | 1264 | C |
| 32 | 2a | 1270 | C |
| 32 | 2a | 1273 | G |
| 32 | 2a | 1275 | A |
| 32 | 2a | 1276 | G |
| 32 | 2a | 1278 | U |
| 32 | 2a | 1279 | A |
| 32 | 2a | 1280 | A |
| 32 | 2a | 1285 | A |
| 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 | 1312 | G |
| 32 | 2a | 1319 | A |
| 32 | 2a | 1320 | C |
| 32 | 2a | 1347 | G |
| 32 | 2a | 1363 | C |
| 32 | 2a | 1364 | U |
| 32 | 2a | 1368 | G |
| 32 | 2a | 1370 | G |
| 32 | 2a | 1397 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 32 | 2a | 1402 | 4OC |
| 32 | 2a | 1419 | G |
| 32 | 2a | 1442 | G |
| 32 | 2a | 1442(A) | G |
| 32 | 2a | 1442(B) | A |
| 32 | 2a | 1447 | A |
| 32 | 2a | 1452 | C |
| 32 | 2a | 1456 | G |
| 32 | 2a | 1492 | A |
| 32 | 2a | 1494 | G |
| 32 | 2a | 1496 | C |
| 32 | 2a | 1497 | G |
| 32 | 2a | 1503 | A |
| 32 | 2a | 1504 | G |
| 32 | 2a | 1506 | U |
| 32 | 2a | 1517 | G |
| 32 | 2a | 1519 | MA6 |
| 32 | 2a | 1520 | G |
| 32 | 2a | 1529 | G |
| 32 | 2a | 1530 | G |
| 32 | 2a | 1531 | A |
| 32 | 2a | 1532 | U |
| 53 | 2v | 13 | A |
| 53 | 2v | 14 | A |
| 53 | 2v | 18 | G |
| 53 | 2v | 24 | A |
| 54 | 2w | 3 | C |
| 54 | 2w | 4 | C |
| 54 | 2w | 5 | G |
| 54 | 2w | 13 | C |
| 54 | 2w | 14 | A |
| 54 | 2w | 19 | G |
| 54 | 2w | 22 | G |
| 54 | 2w | 29 | G |
| 54 | 2w | 36 | A |
| 54 | 2w | 38 | A |
| 54 | 2w | 46 | 7MG |
| 54 | 2w | 47 | U |
| 54 | 2w | 48 | C |
| 54 | 2w | 56 | C |
| 54 | 2w | 59 | U |
| 54 | 2w | 62 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 54 | 2w | 63 | G |
| 54 | 2w | 65 | G |
| 54 | 2w | 68 | C |
| 54 | 2w | 69 | G |
| 54 | 2w | 72 | C |
| 54 | 2w | 74 | C |
| 55 | 2x | 9 | G |
| 55 | 2x | 18 | G |
| 55 | 2x | 21 | A |
| 55 | 2x | 22 | G |
| 55 | 2x | 46 | G |
| 55 | 2x | 47 | U |
| 55 | 2x | 48 | C |
| 55 | 2x | 52 | G |
| 55 | 2x | 56 | C |
| 55 | 2x | 63 | G |
| 55 | 2x | 67 | C |
| 55 | 2x | 68 | C |
| 55 | 2x | 76 | A |
| 54 | 2y | 5 | G |
| 54 | 2y | 6 | G |
| 54 | 2y | 8 | 4SU |
| 54 | 2y | 11 | C |
| 54 | 2y | 12 | U |
| 54 | 2y | 13 | C |
| 54 | 2y | 19 | G |
| 54 | 2y | 35 | A |
| 54 | 2y | 41 | C |
| 54 | 2y | 44 | G |
| 54 | 2y | 45 | U |
| 54 | 2y | 46 | 7MG |
| 54 | 2y | 48 | C |
| 54 | 2y | 52 | G |
| 54 | 2y | 53 | G |
| 54 | 2y | 57 | G |
| 54 | 2y | 59 | U |
| 54 | 2y | 61 | C |
| 54 | 2y | 65 | G |
| 54 | 2y | 70 | G |
| 54 | 2y | 73 | A |

All (54) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 1A | 90 | U |
| 1 | 1A | 195 | A |
| 1 | 1A | 196 | A |
| 1 | 1A | 266 | G |
| 1 | 1A | 271(K) | U |
| 1 | 1A | 278 | A |
| 1 | 1A | 548 | A |
| 1 | 1A | 746 | A |
| 1 | 1A | 895 | U |
| 1 | 1A | 1047 | G |
| 1 | 1A | 1065 | U |
| 1 | 1A | 1067 | A |
| 1 | 1A | 1174 | A |
| 1 | 1A | 1176 | G |
| 1 | 1A | 1210 | A |
| 1 | 1A | 1275 | A |
| 1 | 1A | 1379 | A |
| 1 | 1A | 1420 | U |
| 1 | 1A | 1442 | G |
| 1 | 1A | 1508 | A |
| 1 | 1A | 1653 | G |
| 1 | 1A | 2134 | A |
| 1 | 1A | 2170 | A |
| 1 | 1A | 2181 | G |
| 1 | 1A | 2183 | C |
| 1 | 1A | 2406 | U |
| 1 | 1A | 2430 | A |
| 1 | 1A | 2689 | U |
| 1 | 1A | 2756 | U |
| 2 | 1B | 1 | U |
| 1 | 2A | 34 | C |
| 1 | 2A | 228 | A |
| 1 | 2A | 266 | G |
| 1 | 2A | 271(K) | U |
| 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 | 900 | A |
| 1 | 2A | 1210 | A |
| 1 | 2A | 1379 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 2A | 1420 | U |
| 1 | 2A | 1442 | G |
| 1 | 2A | 1493 | C |
| 1 | 2A | 1530 | C |
| 1 | 2A | 1653 | G |
| 1 | 2A | 1913 | A |
| 1 | 2A | 1992 | G |
| 1 | 2A | 2119 | A |
| 1 | 2A | 2126 | A |
| 1 | 2A | 2351 | G |
| 1 | 2A | 2689 | U |

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

84 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 | $\#\|Z\| > 2$ |
| 54 | PSU | 2y | 55 | 54 | 18,21,22 | 1.34 | 2 (11%) | 21,30,33 | 2.03 | 4 (19%) |
| 1 | 5MC | 2A | 1942 | 1 | 19,22,23 | 1.65 | 3 (15%) | 26,32,35 | 1.11 | 2 (7%) |
| 1 | 2MA | 1A | 2503 | 56,1 | 22,25,26 | 1.49 | 5 (22%) | 32,37,40 | 2.26 | 9 (28%) |
| 32 | PSU | 1a | 516 | 32 | 18,21,22 | 1.37 | 2 (11%) | 21,30,33 | 1.96 | 3 (14%) |
| 1 | PSU | 2A | 1917 | 1 | 18,21,22 | 1.36 | 2 (11%) | 21,30,33 | 2.05 | 4 (19%) |
| 54 | 7MG | 1w | 46 | 54 | 23,26,27 | 1.42 | 4 (17%) | 27,39,42 | 2.55 | 8 (29%) |
| 1 | 4OC | 1A | 1920 | 1 | 19,22,24 | 0.80 | 0 | 25,31,35 | 0.95 | 1 (4%) |
| 1 | 2MU | 2A | 2552 | 56,1 | 19,22,24 | 1.30 | 3 (15%) | 25,31,36 | 1.88 | 6 (24%) |
| 1 | PSU | 1A | 1917 | 1 | 18,21,22 | 1.36 | 2 (11%) | 21,30,33 | 2.02 | 4 (19%) |
| 54 | PSU | 2y | 32 | 54 | 18,21,22 | 1.37 | 2 (11%) | 21,30,33 | 2.02 | 4 (19%) |
| 55 | 5MU | 1x | 54 | 56,55 | 19,22,23 | 1.42 | 5 (26%) | 27,32,35 | 1.98 | 6 (22%) |
| 1 | OMG | 2A | 2251 | 56,1,55 | 23,26,27 | 1.21 | 3 (13%) | 32,38,41 | 1.97 | 6 (18%) |
| 54 | PSU | 2y | 39 | 54 | 18,21,22 | 1.34 | 2 (11%) | 21,30,33 | 2.00 | 4 (19%) |
| 32 | 7MG | 1a | 527 | 56,32 | 23,26,27 | 1.36 | 4 (17%) | 27,39,42 | 2.61 | 7 (25%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 32 | 7MG | 2a | 527 | 56,32 | 23,26,27 | 1.33 | 3 (13%) | 27,39,42 | 2.62 | 7 (25%) |
| 1 | 5MC | 1A | 1942 | 1 | 19,22,23 | 1.60 | 3 (15%) | 26,32,35 | 1.12 | 2 (7%) |
| 1 | PSU | 2A | 2605 | 1 | 18,21,22 | 1.38 | 3 (16%) | 21,30,33 | 2.03 | 4 (19%) |
| 54 | 4SU | 1w | 8 | 54 | 18,21,22 | 1.81 | 5 (27%) | 25,30,33 | 1.89 | 5 (20%) |
| 43 | 0TD | 1l | 92 | 43 | 8,9,10 | 4.56 | 1 (12%) | 6,11,13 | 4.80 | 3 (50%) |
| 54 | 7MG | 1y | 46 | 54 | 23,26,27 | 1.34 | 4 (17%) | 27,39,42 | 2.62 | 7 (25%) |
| 54 | PSU | 2w | 39 | 54 | 18,21,22 | 1.37 | 2 (11%) | 21,30,33 | 1.84 | 3 (14%) |
| 54 | PSU | 1y | 55 | 54 | 18,21,22 | 1.35 | 2 (11%) | 21,30,33 | 2.03 | 3 (14%) |
| 1 | 2MA | 2A | 2503 | 56,1 | 22,25,26 | 1.50 | 4 (18%) | 32,37,40 | 2.27 | 7 (21%) |
| 32 | 5MC | 1a | 1407 | 32 | 19,22,23 | 1.65 | 3 (15%) | 26,32,35 | 1.14 | 2 (7%) |
| 54 | 5MU | 1w | 54 | 54 | 19,22,23 | 1.37 | 6 (31%) | 27,32,35 | 2.17 | 7 (25%) |
| 32 | MA6 | 1a | 1518 | 32 | 23,26,27 | 1.51 | 4 (17%) | 33,38,41 | 2.31 | 13 (39%) |
| 55 | 4SU | 2x | 8 | 56,55 | 18,21,22 | 2.04 | 5 (27%) | 25,30,33 | 1.79 | 7 (28%) |
| 1 | PSU | 2A | 1911 | 1 | 18,21,22 | 1.36 | 2 (11%) | 21,30,33 | 2.00 | 3 (14%) |
| 32 | 5MC | 1a | 967 | 32 | 19,22,23 | 1.62 | 3 (15%) | 26,32,35 | 1.14 | 2 (7%) |
| 32 | 5MC | 2a | 1404 | 32 | 19,22,23 | 1.74 | 3 (15%) | 26,32,35 | 1.19 | 3 (11%) |
| 32 | MA6 | 2a | 1518 | 32 | 23,26,27 | 1.57 | 5 (21%) | 33,38,41 | 2.28 | 12 (36%) |
| 54 | PSU | 2w | 32 | 54 | 18,21,22 | 1.35 | 2 (11%) | 21,30,33 | 1.99 | 3 (14%) |
| 32 | UR3 | 1a | 1498 | 32 | 19,22,23 | 1.02 | 1 (5%) | 26,32,35 | 1.73 | 3 (11%) |
| 54 | MIA | 2y | 37 | 54 | 21,24,32 | 1.59 | 4 (19%) | 30,35,47 | 2.05 | 7 (23%) |
| 1 | 4OC | 2A | 1920 | 1 | 19,22,24 | 0.78 | 0 | 25,31,35 | 0.90 | 1 (4%) |
| 54 | 7MG | 2y | 46 | 54 | 23,26,27 | 1.34 | 3 (13%) | 27,39,42 | 2.74 | 6 (22%) |
| 32 | 5MC | 2a | 1407 | 32 | 19,22,23 | 1.56 | 3 (15%) | 26,32,35 | 1.11 | 3 (11%) |
| 1 | 2MU | 1A | 2552 | 56,1 | 19,22,24 | 1.19 | 2 (10%) | 25,31,36 | 2.00 | 6 (24%) |
| 54 | 5MU | 2y | 54 | 54 | 19,22,23 | 1.44 | 6 (31%) | 27,32,35 | 1.85 | 7 (25%) |
| 54 | PSU | 1w | 32 | 54 | 18,21,22 | 1.37 | 2 (11%) | 21,30,33 | 1.94 | 3 (14%) |
| 32 | M2G | 1a | 966 | 32 | 24,27,28 | 1.30 | 3 (12%) | 33,40,43 | 1.82 | 5 (15%) |
| 32 | 5MC | 2a | 967 | 32 | 19,22,23 | 1.71 | 3 (15%) | 26,32,35 | 1.13 | 3 (11%) |
| 32 | M2G | 2a | 966 | 32 | 24,27,28 | 1.31 | 4 (16%) | 33,40,43 | 1.87 | 6 (18%) |
| 55 | PSU | 2x | 55 | 55 | 18,21,22 | 1.38 | 2 (11%) | 21,30,33 | 2.03 | 4 (19%) |
| 1 | 5MU | 2A | 1939 | 56,1 | 19,22,23 | 1.42 | 6 (31%) | 27,32,35 | 2.23 | 6 (22%) |
| 32 | PSU | 2a | 516 | 32 | 18,21,22 | 1.38 | 2 (11%) | 21,30,33 | 1.91 | 3 (14%) |
| 55 | 5MU | 2x | 54 | 55 | 19,22,23 | 1.41 | 6 (31%) | 27,32,35 | 2.03 | 6 (22%) |
| 54 | 4SU | 2w | 8 | 54 | 18,21,22 | 1.80 | 4 (22%) | 25,30,33 | 2.67 | 6 (24%) |
| 55 | 5MC | 1x | 32 | 55 | 19,22,23 | 1.72 | 3 (15%) | 26,32,35 | 1.22 | 2 (7%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 54 | 4SU | 1y | 8 | 54 | 18,21,22 | 1.76 | 4 (22%) | 25,30,33 | 2.01 | 4 (16%) |
| 54 | PSU | 1w | 55 | 54 | 18,21,22 | 1.43 | 2 (11%) | 21,30,33 | 2.11 | 3 (14%) |
| 54 | MIA | 2w | 37 | 54 | 24,27,32 | 2.05 | 5 (20%) | 32,39,47 | 2.42 | 10 (31%) |
| 32 | 5MC | 2a | 1400 | 32 | 19,22,23 | 1.64 | 3 (15%) | 26,32,35 | 1.10 | 2 (7%) |
| 55 | 5MC | 2x | 32 | 55 | 19,22,23 | 1.69 | 3 (15%) | 26,32,35 | 1.16 | 3 (11%) |
| 32 | MA6 | 1a | 1519 | 32 | 23,26,27 | 1.56 | 4 (17%) | 33,38,41 | 2.31 | 13 (39%) |
| 55 | PSU | 1x | 55 | 56,55 | 18,21,22 | 1.37 | 2 (11%) | 21,30,33 | 2.02 | 4 (19%) |
| 32 | MA6 | 2a | 1519 | 32 | 23,26,27 | 1.59 | 4 (17%) | 33,38,41 | 2.28 | 11 (33%) |
| 32 | UR3 | 2a | 1498 | 32 | 19,22,23 | 1.04 | 2 (10%) | 26,32,35 | 1.78 | 3 (11%) |
| 54 | 7MG | 2w | 46 | 54 | 23,26,27 | 1.36 | 4 (17%) | 27,39,42 | 2.56 | 7 (25%) |
| 1 | 5MC | 2A | 1962 | 56,1 | 19,22,23 | 1.65 | 3 (15%) | 26,32,35 | 1.11 | 2 (7%) |
| 32 | 5MC | 1a | 1400 | 32 | 19,22,23 | 1.68 | 3 (15%) | 26,32,35 | 1.13 | 3 (11%) |
| 54 | PSU | 2w | 55 | 54 | 18,21,22 | 1.39 | 2 (11%) | 21,30,33 | 2.02 | 3 (14%) |
| 54 | 5MU | 2w | 54 | 54 | 19,22,23 | 1.37 | 5 (26%) | 27,32,35 | 1.86 | 7 (25%) |
| 54 | PSU | 1y | 39 | 54 | 18,21,22 | 1.33 | 2 (11%) | 21,30,33 | 2.07 | 4 (19%) |
| 1 | 5MC | 1A | 1962 | 56,1 | 19,22,23 | 1.63 | 3 (15%) | 26,32,35 | 1.10 | 2 (7%) |
| 54 | 4SU | 2y | 8 | 54 | 18,21,22 | 1.87 | 5 (27%) | 25,30,33 | 2.03 | 5 (20%) |
| 54 | 5MU | 1y | 54 | 54 | 19,22,23 | 1.41 | 5 (26%) | 27,32,35 | 2.13 | 6 (22%) |
| 1 | 5MU | 1A | 1939 | 56,1 | 19,22,23 | 1.40 | 6 (31%) | 27,32,35 | 2.15 | 6 (22%) |
| 32 | 2MG | 1a | 1207 | 32 | 23,26,27 | 1.25 | 4 (17%) | 33,38,41 | 2.15 | 6 (18%) |
| 32 | 2MG | 2a | 1207 | 32 | 23,26,27 | 1.24 | 3 (13%) | 33,38,41 | 2.18 | 7 (21%) |
| 54 | PSU | 1w | 39 | 54 | 18,21,22 | 1.37 | 2 (11%) | 21,30,33 | 2.01 | 4 (19%) |
| 1 | OMG | 1A | 2251 | 56,1,55 | 23,26,27 | 1.17 | 3 (13%) | 32,38,41 | 1.98 | 6 (18%) |
| 54 | MIA | 1y | 37 | 54 | 21,24,32 | 1.59 | 4 (19%) | 30,35,47 | 2.00 | 8 (26%) |
| 32 | 4OC | 1a | 1402 | 32 | 20,23,24 | 0.77 | 0 | 25,32,35 | 0.95 | 1 (4%) |
| 43 | 0TD | 2l | 92 | 43 | 8,9,10 | 4.51 | 1 (12%) | 6,11,13 | 3.45 | 3 (50%) |
| 1 | PSU | 1A | 1911 | 1 | 18,21,22 | 1.39 | 2 (11%) | 21,30,33 | 2.07 | 4 (19%) |
| 1 | PSU | 1A | 2605 | 56,1 | 18,21,22 | 1.37 | 2 (11%) | 21,30,33 | 1.92 | 3 (14%) |
| 54 | MIA | 1w | 37 | 54 | 28,31,32 | 2.33 | 6 (21%) | 38,44,47 | 2.73 | 13 (34%) |
| 54 | PSU | 1y | 32 | 54 | 18,21,22 | 1.37 | 2 (11%) | 21,30,33 | 1.99 | 3 (14%) |
| 1 | 5MU | 2A | 1915 | 1 | 19,22,23 | 1.44 | 5 (26%) | 27,32,35 | 2.06 | 6 (22%) |
| 55 | 4SU | 1x | 8 | 55 | 18,21,22 | 2.15 | 6 (33%) | 25,30,33 | 1.61 | 5 (20%) |
| 32 | 5MC | 1a | 1404 | 32 | 19,22,23 | 1.71 | 3 (15%) | 26,32,35 | 1.14 | 3 (11%) |
| 32 | 4OC | 2a | 1402 | 56,32 | 20,23,24 | 0.77 | 0 | 25,32,35 | 0.97 | 1 (4%) |
| 1 | 5MU | 1A | 1915 | 1 | 19,22,23 | 1.44 | 5 (26%) | 27,32,35 | 2.08 | 6 (22%) |

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 |
|---|---|---|---|---|---|---|---|
| 54 | PSU | 2y | 55 | 54 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | 5MC | 2A | 1942 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | 2MA | 1A | 2503 | 56,1 | - | 1/7/25/26 | 0/3/3/3 |
| 32 | PSU | 1a | 516 | 32 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | PSU | 2A | 1917 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 54 | 7MG | 1w | 46 | 54 | - | 2/7/37/38 | 0/3/3/3 |
| 1 | 4OC | 1A | 1920 | 1 | - | 1/9/27/30 | 0/2/2/2 |
| 1 | 2MU | 2A | 2552 | 56,1 | - | 0/9/27/28 | 0/2/2/2 |
| 1 | PSU | 1A | 1917 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 54 | PSU | 2y | 32 | 54 | - | 0/7/25/26 | 0/2/2/2 |
| 55 | 5MU | 1x | 54 | 56,55 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | OMG | 2A | 2251 | 56,1,55 | - | 1/9/27/28 | 0/3/3/3 |
| 54 | PSU | 2y | 39 | 54 | - | 0/7/25/26 | 0/2/2/2 |
| 32 | 7MG | 1a | 527 | 56,32 | - | 3/7/37/38 | 0/3/3/3 |
| 32 | 7MG | 2a | 527 | 56,32 | - | 1/7/37/38 | 0/3/3/3 |
| 1 | 5MC | 1A | 1942 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | PSU | 2A | 2605 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 54 | 4SU | 1w | 8 | 54 | - | 0/7/25/26 | 0/2/2/2 |
| 43 | 0TD | 1l | 92 | 43 | - | 1/7/12/14 | - |
| 54 | 7MG | 1y | 46 | 54 | - | 3/7/37/38 | 0/3/3/3 |
| 54 | PSU | 2w | 39 | 54 | - | 2/7/25/26 | 0/2/2/2 |
| 54 | PSU | 1y | 55 | 54 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | 2MA | 2A | 2503 | 56,1 | - | 0/7/25/26 | 0/3/3/3 |
| 32 | 5MC | 1a | 1407 | 32 | - | 0/7/25/26 | 0/2/2/2 |
| 54 | 5MU | 1w | 54 | 54 | - | 0/7/25/26 | 0/2/2/2 |
| 32 | MA6 | 1a | 1518 | 32 | - | 2/11/29/30 | 0/3/3/3 |
| 55 | 4SU | 2x | 8 | 56,55 | - | 1/7/25/26 | 0/2/2/2 |
| 1 | PSU | 2A | 1911 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 32 | 5MC | 1a | 967 | 32 | - | 1/7/25/26 | 0/2/2/2 |
| 32 | 5MC | 2a | 1404 | 32 | - | 0/7/25/26 | 0/2/2/2 |
| 32 | MA6 | 2a | 1518 | 32 | - | 2/11/29/30 | 0/3/3/3 |
| 54 | PSU | 2w | 32 | 54 | - | 0/7/25/26 | 0/2/2/2 |
| 32 | UR3 | 1a | 1498 | 32 | - | 0/7/25/26 | 0/2/2/2 |
| 54 | MIA | 2y | 37 | 54 | - | 0/7/25/34 | 0/3/3/3 |
| 1 | 4OC | 2A | 1920 | 1 | - | 0/9/27/30 | 0/2/2/2 |
| 54 | 7MG | 2y | 46 | 54 | - | 3/7/37/38 | 0/3/3/3 |
| 32 | 5MC | 2a | 1407 | 32 | - | 0/7/25/26 | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 1 | 2MU | 1A | 2552 | 56,1 | - | 0/9/27/28 | 0/2/2/2 |
| 54 | 5MU | 2y | 54 | 54 | - | 0/7/25/26 | 0/2/2/2 |
| 54 | PSU | 1w | 32 | 54 | - | 0/7/25/26 | 0/2/2/2 |
| 32 | M2G | 1a | 966 | 32 | - | 0/11/29/30 | 0/3/3/3 |
| 32 | 5MC | 2a | 967 | 32 | - | 0/7/25/26 | 0/2/2/2 |
| 32 | M2G | 2a | 966 | 32 | - | 0/11/29/30 | 0/3/3/3 |
| 55 | PSU | 2x | 55 | 55 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | 5MU | 2A | 1939 | 56,1 | - | 0/7/25/26 | 0/2/2/2 |
| 32 | PSU | 2a | 516 | 32 | - | 0/7/25/26 | 0/2/2/2 |
| 55 | 5MU | 2x | 54 | 55 | - | 0/7/25/26 | 0/2/2/2 |
| 54 | 4SU | 2w | 8 | 54 | - | 0/7/25/26 | 0/2/2/2 |
| 55 | 5MC | 1x | 32 | 55 | - | 0/7/25/26 | 0/2/2/2 |
| 54 | 4SU | 1y | 8 | 54 | - | 3/7/25/26 | 0/2/2/2 |
| 54 | PSU | 1w | 55 | 54 | - | 0/7/25/26 | 0/2/2/2 |
| 54 | MIA | 2w | 37 | 54 | - | 0/11/29/34 | 0/3/3/3 |
| 32 | 5MC | 2a | 1400 | 32 | - | 1/7/25/26 | 0/2/2/2 |
| 55 | 5MC | 2x | 32 | 55 | - | 0/7/25/26 | 0/2/2/2 |
| 32 | MA6 | 1a | 1519 | 32 | - | 4/11/29/30 | 0/3/3/3 |
| 55 | PSU | 1x | 55 | 56,55 | - | 0/7/25/26 | 0/2/2/2 |
| 32 | MA6 | 2a | 1519 | 32 | - | 6/11/29/30 | 0/3/3/3 |
| 32 | UR3 | 2a | 1498 | 32 | - | 0/7/25/26 | 0/2/2/2 |
| 54 | 7MG | 2w | 46 | 54 | - | 2/7/37/38 | 0/3/3/3 |
| 1 | 5MC | 2A | 1962 | 56,1 | - | 0/7/25/26 | 0/2/2/2 |
| 32 | 5MC | 1a | 1400 | 32 | - | 2/7/25/26 | 0/2/2/2 |
| 54 | PSU | 2w | 55 | 54 | - | 0/7/25/26 | 0/2/2/2 |
| 54 | 5MU | 2w | 54 | 54 | - | 0/7/25/26 | 0/2/2/2 |
| 54 | PSU | 1y | 39 | 54 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | 5MC | 1A | 1962 | 56,1 | - | 0/7/25/26 | 0/2/2/2 |
| 54 | 4SU | 2y | 8 | 54 | - | 2/7/25/26 | 0/2/2/2 |
| 54 | 5MU | 1y | 54 | 54 | - | 1/7/25/26 | 0/2/2/2 |
| 1 | 5MU | 1A | 1939 | 56,1 | - | 0/7/25/26 | 0/2/2/2 |
| 32 | 2MG | 1a | 1207 | 32 | - | 0/9/27/28 | 0/3/3/3 |
| 32 | 2MG | 2a | 1207 | 32 | - | 0/9/27/28 | 0/3/3/3 |
| 54 | PSU | 1w | 39 | 54 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | OMG | 1A | 2251 | 56,1,55 | - | 0/9/27/28 | 0/3/3/3 |
| 54 | MIA | 1y | 37 | 54 | - | 0/7/25/34 | 0/3/3/3 |
| 32 | 4OC | 1a | 1402 | 32 | - | 2/9/29/30 | 0/2/2/2 |
| 43 | 0TD | 2l | 92 | 43 | - | 2/7/12/14 | - |
| 1 | PSU | 1A | 1911 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | PSU | 1A | 2605 | 56,1 | - | 0/7/25/26 | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 54 | MIA | 1w | 37 | 54 | - | 1/15/33/34 | 0/3/3/3 |
| 54 | PSU | 1y | 32 | 54 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | 5MU | 2A | 1915 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 55 | 4SU | 1x | 8 | 55 | - | 0/7/25/26 | 0/2/2/2 |
| 32 | 5MC | 1a | 1404 | 32 | - | 0/7/25/26 | 0/2/2/2 |
| 32 | 4OC | 2a | 1402 | 56,32 | - | 2/9/29/30 | 0/2/2/2 |
| 1 | 5MU | 1A | 1915 | 1 | - | 2/7/25/26 | 0/2/2/2 |

All (268) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 43 | 1l | 92 | 0TD | CB-SB | -12.49 | 1.69 | 1.82 |
| 43 | 2l | 92 | 0TD | CB-SB | -12.35 | 1.69 | 1.82 |
| 54 | 1w | 37 | MIA | C13-C14 | 6.84 | 1.52 | 1.32 |
| 54 | 1w | 37 | MIA | C2-S10 | -6.74 | 1.70 | 1.75 |
| 54 | 2w | 37 | MIA | C2-S10 | -6.47 | 1.70 | 1.75 |
| 32 | 2a | 1404 | 5MC | C5-C4 | 6.33 | 1.48 | 1.44 |
| 32 | 2a | 967 | 5MC | C5-C4 | 6.25 | 1.48 | 1.44 |
| 55 | 1x | 32 | 5MC | C5-C4 | 6.25 | 1.48 | 1.44 |
| 32 | 1a | 1404 | 5MC | C5-C4 | 6.24 | 1.48 | 1.44 |
| 55 | 2x | 32 | 5MC | C5-C4 | 6.11 | 1.48 | 1.44 |
| 32 | 1a | 1400 | 5MC | C5-C4 | 6.06 | 1.48 | 1.44 |
| 32 | 1a | 1407 | 5MC | C5-C4 | 6.05 | 1.48 | 1.44 |
| 1 | 1A | 1962 | 5MC | C5-C4 | 6.03 | 1.48 | 1.44 |
| 1 | 2A | 1962 | 5MC | C5-C4 | 6.03 | 1.48 | 1.44 |
| 1 | 2A | 1942 | 5MC | C5-C4 | 5.95 | 1.48 | 1.44 |
| 32 | 2a | 1400 | 5MC | C5-C4 | 5.93 | 1.48 | 1.44 |
| 32 | 1a | 967 | 5MC | C5-C4 | 5.81 | 1.48 | 1.44 |
| 1 | 1A | 1942 | 5MC | C5-C4 | 5.72 | 1.48 | 1.44 |
| 32 | 2a | 1407 | 5MC | C5-C4 | 5.57 | 1.48 | 1.44 |
| 32 | 2a | 1519 | MA6 | C5-C4 | 5.01 | 1.48 | 1.39 |
| 54 | 2w | 37 | MIA | C5-C4 | 4.99 | 1.48 | 1.39 |
| 54 | 2w | 8 | 4SU | C4-S4 | -4.99 | 1.59 | 1.68 |
| 54 | 2y | 8 | 4SU | C4-S4 | -4.95 | 1.59 | 1.68 |
| 54 | 2y | 37 | MIA | C5-C4 | 4.94 | 1.47 | 1.39 |
| 55 | 2x | 8 | 4SU | C4-S4 | -4.94 | 1.59 | 1.68 |
| 54 | 1y | 37 | MIA | C5-C4 | 4.91 | 1.47 | 1.39 |
| 32 | 2a | 1518 | MA6 | C5-C4 | 4.90 | 1.47 | 1.39 |
| 54 | 1w | 37 | MIA | C5-C4 | 4.90 | 1.47 | 1.39 |
| 55 | 1x | 8 | 4SU | C4-S4 | -4.81 | 1.60 | 1.68 |
| 32 | 1a | 1519 | MA6 | C5-C4 | 4.73 | 1.47 | 1.39 |
| 32 | 1a | 1518 | MA6 | C5-C4 | 4.71 | 1.47 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 54 | 1w | 8 | 4SU | C4-S4 | -4.71 | 1.60 | 1.68 |
| 54 | 1y | 8 | 4SU | C4-S4 | -4.71 | 1.60 | 1.68 |
| 55 | 1x | 8 | 4SU | C4-N3 | -4.65 | 1.32 | 1.37 |
| 1 | 1A | 2503 | 2MA | C5-C4 | 4.59 | 1.47 | 1.39 |
| 1 | 2A | 2503 | 2MA | C5-C4 | 4.53 | 1.47 | 1.39 |
| 55 | 2x | 8 | 4SU | C4-N3 | -4.35 | 1.33 | 1.37 |
| 54 | 1w | 55 | PSU | C6-C5 | 3.88 | 1.39 | 1.35 |
| 54 | 2w | 55 | PSU | C6-C5 | 3.77 | 1.39 | 1.35 |
| 54 | 2y | 32 | PSU | C6-C5 | 3.77 | 1.39 | 1.35 |
| 54 | 2w | 39 | PSU | C6-C5 | 3.72 | 1.39 | 1.35 |
| 54 | 1y | 32 | PSU | C6-C5 | 3.70 | 1.39 | 1.35 |
| 55 | 2x | 55 | PSU | C6-C5 | 3.67 | 1.39 | 1.35 |
| 32 | 2a | 516 | PSU | C6-C5 | 3.58 | 1.39 | 1.35 |
| 55 | 1x | 55 | PSU | C6-C5 | 3.54 | 1.39 | 1.35 |
| 54 | 2y | 55 | PSU | C6-C5 | 3.54 | 1.39 | 1.35 |
| 54 | 2w | 32 | PSU | C6-C5 | 3.53 | 1.39 | 1.35 |
| 54 | 2y | 46 | 7MG | C5-C4 | 3.52 | 1.48 | 1.37 |
| 54 | 1y | 55 | PSU | C6-C5 | 3.51 | 1.39 | 1.35 |
| 1 | 2A | 1917 | PSU | C6-C5 | 3.49 | 1.39 | 1.35 |
| 1 | 2A | 1911 | PSU | C6-C5 | 3.48 | 1.39 | 1.35 |
| 54 | 1y | 39 | PSU | C6-C5 | 3.48 | 1.39 | 1.35 |
| 1 | 2A | 2605 | PSU | C6-C5 | 3.45 | 1.39 | 1.35 |
| 54 | 1w | 46 | 7MG | C4-N9 | -3.44 | 1.33 | 1.37 |
| 54 | 1y | 46 | 7MG | C5-C4 | 3.44 | 1.48 | 1.37 |
| 54 | 1w | 32 | PSU | C6-C5 | 3.42 | 1.39 | 1.35 |
| 54 | 1w | 39 | PSU | C6-C5 | 3.42 | 1.39 | 1.35 |
| 1 | 1A | 1917 | PSU | C6-C5 | 3.40 | 1.39 | 1.35 |
| 54 | 2y | 8 | 4SU | C4-N3 | -3.39 | 1.34 | 1.37 |
| 54 | 1w | 46 | 7MG | C5-C4 | 3.39 | 1.48 | 1.37 |
| 1 | 1A | 2605 | PSU | C6-C5 | 3.39 | 1.39 | 1.35 |
| 54 | 2y | 39 | PSU | C6-C5 | 3.37 | 1.39 | 1.35 |
| 32 | 1a | 516 | PSU | C6-C5 | 3.36 | 1.39 | 1.35 |
| 55 | 1x | 8 | 4SU | C5-C4 | -3.36 | 1.38 | 1.42 |
| 54 | 2w | 46 | 7MG | C4-N9 | -3.35 | 1.33 | 1.37 |
| 1 | 1A | 1911 | PSU | C6-C5 | 3.34 | 1.39 | 1.35 |
| 32 | 2a | 527 | 7MG | C5-C4 | 3.34 | 1.47 | 1.37 |
| 55 | 1x | 8 | 4SU | C2-N3 | -3.34 | 1.32 | 1.38 |
| 32 | 1a | 527 | 7MG | C5-C4 | 3.33 | 1.47 | 1.37 |
| 54 | 2w | 46 | 7MG | C5-C4 | 3.32 | 1.47 | 1.37 |
| 54 | 1w | 8 | 4SU | C4-N3 | -3.24 | 1.34 | 1.37 |
| 32 | 1a | 527 | 7MG | C4-N9 | -3.21 | 1.33 | 1.37 |
| 32 | 2a | 1207 | 2MG | C5-C4 | 3.19 | 1.47 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 32 | 2a | 1519 | MA6 | C5-C6 | 3.17 | 1.49 | 1.41 |
| 32 | 2a | 966 | M2G | C5-C4 | 3.16 | 1.47 | 1.38 |
| 1 | 2A | 2251 | OMG | C5-C4 | 3.16 | 1.47 | 1.38 |
| 32 | 2a | 1518 | MA6 | C5-C6 | 3.14 | 1.49 | 1.41 |
| 54 | 1y | 8 | 4SU | C4-N3 | -3.14 | 1.34 | 1.37 |
| 32 | 1a | 1207 | 2MG | C5-C4 | 3.10 | 1.47 | 1.38 |
| 32 | 1a | 966 | M2G | C5-C4 | 3.10 | 1.47 | 1.38 |
| 55 | 2x | 8 | 4SU | C5-C4 | -3.09 | 1.38 | 1.42 |
| 1 | 1A | 2251 | OMG | C5-C4 | 3.09 | 1.47 | 1.38 |
| 32 | 2a | 1404 | 5MC | C6-C5 | 3.06 | 1.39 | 1.34 |
| 32 | 1a | 1519 | MA6 | C5-C6 | 3.02 | 1.49 | 1.41 |
| 55 | 1x | 32 | 5MC | C6-C5 | 3.00 | 1.39 | 1.34 |
| 32 | 1a | 1518 | MA6 | C5-C6 | 2.99 | 1.49 | 1.41 |
| 32 | 2a | 966 | M2G | C2-N2 | 2.98 | 1.40 | 1.35 |
| 1 | 2A | 1915 | 5MU | C6-C5 | 2.97 | 1.39 | 1.34 |
| 1 | 1A | 1915 | 5MU | C6-C5 | 2.96 | 1.39 | 1.34 |
| 55 | 2x | 32 | 5MC | C6-C5 | 2.92 | 1.39 | 1.34 |
| 32 | 1a | 1404 | 5MC | C6-C5 | 2.92 | 1.39 | 1.34 |
| 54 | 2w | 8 | 4SU | C5-C4 | -2.92 | 1.39 | 1.42 |
| 32 | 2a | 967 | 5MC | C6-C5 | 2.91 | 1.39 | 1.34 |
| 54 | 1w | 37 | MIA | C5-C6 | 2.89 | 1.48 | 1.41 |
| 1 | 2A | 1939 | 5MU | C6-C5 | 2.88 | 1.39 | 1.34 |
| 32 | 1a | 966 | M2G | C2-N2 | 2.88 | 1.40 | 1.35 |
| 54 | 1y | 54 | 5MU | C6-C5 | 2.88 | 1.39 | 1.34 |
| 32 | 1a | 1400 | 5MC | C6-C5 | 2.87 | 1.39 | 1.34 |
| 54 | 2w | 8 | 4SU | C4-N3 | -2.87 | 1.34 | 1.37 |
| 54 | 2w | 37 | MIA | C5-C6 | 2.86 | 1.48 | 1.41 |
| 54 | 1y | 37 | MIA | C5-C6 | 2.85 | 1.48 | 1.41 |
| 55 | 2x | 54 | 5MU | C6-C5 | 2.85 | 1.39 | 1.34 |
| 1 | 2A | 2552 | 2MU | C4-N3 | -2.84 | 1.33 | 1.38 |
| 1 | 2A | 1942 | 5MC | C6-C5 | 2.83 | 1.39 | 1.34 |
| 1 | 1A | 1939 | 5MU | C6-C5 | 2.83 | 1.39 | 1.34 |
| 1 | 1A | 1942 | 5MC | C6-C5 | 2.81 | 1.39 | 1.34 |
| 54 | 2y | 37 | MIA | C5-C6 | 2.80 | 1.48 | 1.41 |
| 32 | 2a | 1400 | 5MC | C6-C5 | 2.79 | 1.39 | 1.34 |
| 55 | 2x | 8 | 4SU | C2-N3 | -2.79 | 1.33 | 1.38 |
| 55 | 1x | 54 | 5MU | C6-C5 | 2.78 | 1.39 | 1.34 |
| 1 | 1A | 2605 | PSU | C4-N3 | -2.75 | 1.33 | 1.38 |
| 54 | 2w | 54 | 5MU | C6-C5 | 2.74 | 1.39 | 1.34 |
| 32 | 1a | 1407 | 5MC | C6-C5 | 2.74 | 1.39 | 1.34 |
| 1 | 1A | 1911 | PSU | C4-N3 | -2.73 | 1.33 | 1.38 |
| 54 | 2y | 54 | 5MU | C6-C5 | 2.71 | 1.39 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | 2A | 2605 | PSU | C4-N3 | -2.70 | 1.33 | 1.38 |
| 1 | 2A | 1939 | 5MU | C4-N3 | -2.70 | 1.33 | 1.38 |
| 32 | 2a | 527 | 7MG | C4-N9 | -2.68 | 1.34 | 1.37 |
| 54 | 2y | 8 | 4SU | C5-C4 | -2.67 | 1.39 | 1.42 |
| 32 | 2a | 1407 | 5MC | C6-C5 | 2.66 | 1.38 | 1.34 |
| 1 | 1A | 2503 | 2MA | C5-C6 | 2.66 | 1.48 | 1.41 |
| 54 | 1w | 39 | PSU | C4-N3 | -2.66 | 1.33 | 1.38 |
| 1 | 2A | 1962 | 5MC | C6-C5 | 2.65 | 1.38 | 1.34 |
| 1 | 1A | 1939 | 5MU | C4-N3 | -2.64 | 1.33 | 1.38 |
| 1 | 2A | 2503 | 2MA | C5-C6 | 2.64 | 1.48 | 1.41 |
| 54 | 1w | 8 | 4SU | C5-C4 | -2.64 | 1.39 | 1.42 |
| 1 | 1A | 1915 | 5MU | C4-N3 | -2.63 | 1.33 | 1.38 |
| 55 | 1x | 54 | 5MU | C4-N3 | -2.63 | 1.33 | 1.38 |
| 54 | 2y | 55 | PSU | C4-N3 | -2.62 | 1.33 | 1.38 |
| 1 | 1A | 1917 | PSU | C4-N3 | -2.61 | 1.34 | 1.38 |
| 55 | 2x | 54 | 5MU | C4-N3 | -2.61 | 1.34 | 1.38 |
| 1 | 2A | 1911 | PSU | C4-N3 | -2.61 | 1.34 | 1.38 |
| 32 | 1a | 966 | M2G | C6-N1 | -2.60 | 1.34 | 1.38 |
| 54 | 2w | 54 | 5MU | C4-N3 | -2.59 | 1.34 | 1.38 |
| 1 | 1A | 2552 | 2MU | C4-N3 | -2.59 | 1.34 | 1.38 |
| 54 | 2y | 54 | 5MU | C4-N3 | -2.58 | 1.34 | 1.38 |
| 54 | 1w | 54 | 5MU | C6-C5 | 2.58 | 1.38 | 1.34 |
| 1 | 1A | 1915 | 5MU | C2-N1 | 2.58 | 1.42 | 1.38 |
| 32 | 1a | 967 | 5MC | C6-C5 | 2.58 | 1.38 | 1.34 |
| 54 | 2w | 39 | PSU | C4-N3 | -2.57 | 1.34 | 1.38 |
| 1 | 2A | 1917 | PSU | C4-N3 | -2.57 | 1.34 | 1.38 |
| 1 | 2A | 2251 | OMG | C6-N1 | -2.57 | 1.34 | 1.38 |
| 54 | 1y | 8 | 4SU | C5-C4 | -2.56 | 1.39 | 1.42 |
| 54 | 2y | 39 | PSU | C4-N3 | -2.56 | 1.34 | 1.38 |
| 1 | 2A | 1915 | 5MU | C4-C5 | 2.55 | 1.49 | 1.44 |
| 1 | 1A | 1962 | 5MC | C6-C5 | 2.54 | 1.38 | 1.34 |
| 1 | 2A | 1915 | 5MU | C4-N3 | -2.54 | 1.34 | 1.38 |
| 54 | 1w | 32 | PSU | C4-N3 | -2.53 | 1.34 | 1.38 |
| 54 | 1w | 55 | PSU | C4-N3 | -2.53 | 1.34 | 1.38 |
| 54 | 2w | 8 | 4SU | C2-N1 | 2.53 | 1.42 | 1.38 |
| 54 | 1y | 54 | 5MU | C4-N3 | -2.51 | 1.34 | 1.38 |
| 32 | 1a | 516 | PSU | C4-N3 | -2.51 | 1.34 | 1.38 |
| 54 | 1w | 54 | 5MU | C4-C5 | 2.50 | 1.48 | 1.44 |
| 55 | 2x | 55 | PSU | C4-N3 | -2.49 | 1.34 | 1.38 |
| 32 | 1a | 1207 | 2MG | C6-N1 | -2.48 | 1.34 | 1.38 |
| 54 | 2w | 55 | PSU | C4-N3 | -2.47 | 1.34 | 1.38 |
| 54 | 2y | 54 | 5MU | C2-N1 | 2.47 | 1.42 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 55 | 1x | 55 | PSU | C4-N3 | -2.47 | 1.34 | 1.38 |
| 54 | 1y | 32 | PSU | C4-N3 | -2.47 | 1.34 | 1.38 |
| 54 | 1y | 46 | 7MG | C4-N9 | -2.46 | 1.34 | 1.37 |
| 54 | 2y | 46 | 7MG | C6-N1 | -2.46 | 1.34 | 1.38 |
| 54 | 1w | 46 | 7MG | C6-N1 | -2.46 | 1.34 | 1.38 |
| 54 | 1y | 37 | MIA | C8-N7 | 2.46 | 1.36 | 1.31 |
| 54 | 1y | 39 | PSU | C4-N3 | -2.45 | 1.34 | 1.38 |
| 54 | 1y | 55 | PSU | C4-N3 | -2.45 | 1.34 | 1.38 |
| 1 | 2A | 2552 | 2MU | C5-C4 | 2.43 | 1.49 | 1.43 |
| 54 | 2w | 32 | PSU | C4-N3 | -2.42 | 1.34 | 1.38 |
| 55 | 2x | 54 | 5MU | C4-C5 | 2.42 | 1.48 | 1.44 |
| 54 | 2y | 37 | MIA | C8-N7 | 2.40 | 1.36 | 1.31 |
| 54 | 1w | 54 | 5MU | C4-N3 | -2.39 | 1.34 | 1.38 |
| 54 | 1y | 54 | 5MU | C4-C5 | 2.38 | 1.48 | 1.44 |
| 32 | 2a | 516 | PSU | C4-N3 | -2.38 | 1.34 | 1.38 |
| 55 | 1x | 54 | 5MU | C4-C5 | 2.38 | 1.48 | 1.44 |
| 54 | 1y | 54 | 5MU | C2-N1 | 2.37 | 1.42 | 1.38 |
| 1 | 2A | 2503 | 2MA | C5-N7 | -2.36 | 1.34 | 1.39 |
| 32 | 2a | 527 | 7MG | C6-N1 | -2.36 | 1.34 | 1.38 |
| 54 | 2y | 8 | 4SU | C2-N1 | 2.35 | 1.42 | 1.38 |
| 54 | 1w | 8 | 4SU | C2-N1 | 2.35 | 1.42 | 1.38 |
| 32 | 2a | 966 | M2G | C6-N1 | -2.35 | 1.34 | 1.38 |
| 32 | 1a | 967 | 5MC | C6-N1 | -2.35 | 1.34 | 1.38 |
| 1 | 1A | 2251 | OMG | C6-N1 | -2.34 | 1.34 | 1.38 |
| 1 | 2A | 1939 | 5MU | C4-C5 | 2.34 | 1.48 | 1.44 |
| 54 | 2y | 32 | PSU | C4-N3 | -2.34 | 1.34 | 1.38 |
| 55 | 2x | 8 | 4SU | C2-N1 | 2.34 | 1.42 | 1.38 |
| 1 | 1A | 2503 | 2MA | C8-N7 | 2.33 | 1.36 | 1.31 |
| 54 | 2w | 37 | MIA | C8-N7 | 2.33 | 1.36 | 1.31 |
| 54 | 1w | 37 | MIA | C8-N7 | 2.33 | 1.36 | 1.31 |
| 32 | 2a | 1207 | 2MG | C6-N1 | -2.32 | 1.34 | 1.38 |
| 1 | 2A | 1939 | 5MU | C6-N1 | -2.32 | 1.34 | 1.38 |
| 54 | 2y | 54 | 5MU | C2-N3 | -2.31 | 1.33 | 1.38 |
| 1 | 1A | 1942 | 5MC | C6-N1 | -2.30 | 1.34 | 1.38 |
| 54 | 2w | 54 | 5MU | C4-C5 | 2.30 | 1.48 | 1.44 |
| 1 | 2A | 1915 | 5MU | C2-N1 | 2.30 | 1.42 | 1.38 |
| 55 | 1x | 8 | 4SU | O2-C2 | 2.29 | 1.27 | 1.23 |
| 1 | 1A | 1915 | 5MU | C4-C5 | 2.29 | 1.48 | 1.44 |
| 55 | 1x | 54 | 5MU | C2-N1 | 2.28 | 1.42 | 1.38 |
| 54 | 2y | 54 | 5MU | C4-C5 | 2.28 | 1.48 | 1.44 |
| 54 | 1y | 46 | 7MG | C6-N1 | -2.28 | 1.34 | 1.38 |
| 1 | 2A | 1962 | 5MC | C6-N1 | -2.28 | 1.34 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 54 | 1w | 8 | 4SU | C2-N3 | -2.28 | 1.34 | 1.38 |
| 1 | 2A | 2503 | 2MA | C8-N7 | 2.27 | 1.36 | 1.31 |
| 54 | 2y | 8 | 4SU | C2-N3 | -2.26 | 1.34 | 1.38 |
| 32 | 1a | 1519 | MA6 | C8-N7 | 2.26 | 1.36 | 1.31 |
| 32 | 1a | 1519 | MA6 | C5-N7 | -2.26 | 1.35 | 1.39 |
| 32 | 1a | 1518 | MA6 | C8-N7 | 2.25 | 1.36 | 1.31 |
| 1 | 1A | 1939 | 5MU | C6-N1 | -2.25 | 1.34 | 1.38 |
| 1 | 1A | 1962 | 5MC | C6-N1 | -2.24 | 1.34 | 1.38 |
| 54 | 2w | 46 | 7MG | C6-N1 | -2.24 | 1.34 | 1.38 |
| 54 | 2w | 37 | MIA | C5-N7 | -2.23 | 1.35 | 1.39 |
| 32 | 1a | 527 | 7MG | C6-N1 | -2.23 | 1.34 | 1.38 |
| 1 | 1A | 1939 | 5MU | C2-N3 | -2.21 | 1.34 | 1.38 |
| 32 | 2a | 1519 | MA6 | C8-N7 | 2.19 | 1.35 | 1.31 |
| 54 | 1w | 54 | 5MU | C2-N1 | 2.19 | 1.41 | 1.38 |
| 54 | 1w | 37 | MIA | C5-N7 | -2.19 | 1.35 | 1.39 |
| 32 | 1a | 1498 | UR3 | C2-N1 | 2.19 | 1.41 | 1.38 |
| 55 | 1x | 32 | 5MC | C6-N1 | -2.19 | 1.34 | 1.38 |
| 1 | 2A | 2251 | OMG | C5-N7 | -2.18 | 1.34 | 1.39 |
| 54 | 1y | 54 | 5MU | C6-N1 | -2.18 | 1.34 | 1.38 |
| 1 | 2A | 1939 | 5MU | C2-N3 | -2.18 | 1.34 | 1.38 |
| 54 | 1w | 54 | 5MU | C6-N1 | -2.18 | 1.34 | 1.38 |
| 32 | 2a | 1518 | MA6 | C8-N7 | 2.18 | 1.35 | 1.31 |
| 1 | 2A | 1915 | 5MU | C6-N1 | -2.17 | 1.34 | 1.38 |
| 1 | 1A | 2503 | 2MA | C5-N7 | -2.17 | 1.35 | 1.39 |
| 32 | 2a | 1498 | UR3 | C2-N1 | 2.16 | 1.41 | 1.38 |
| 54 | 2y | 37 | MIA | C5-N7 | -2.16 | 1.35 | 1.39 |
| 32 | 1a | 1400 | 5MC | C6-N1 | -2.16 | 1.34 | 1.38 |
| 32 | 2a | 1498 | UR3 | C6-C5 | 2.15 | 1.40 | 1.35 |
| 55 | 2x | 54 | 5MU | C2-N1 | 2.15 | 1.41 | 1.38 |
| 1 | 1A | 1939 | 5MU | C4-C5 | 2.14 | 1.48 | 1.44 |
| 32 | 2a | 1404 | 5MC | C6-N1 | -2.14 | 1.34 | 1.38 |
| 1 | 2A | 1942 | 5MC | C6-N1 | -2.14 | 1.34 | 1.38 |
| 1 | 1A | 2251 | OMG | C5-N7 | -2.13 | 1.34 | 1.39 |
| 32 | 2a | 1407 | 5MC | C6-N1 | -2.13 | 1.34 | 1.38 |
| 32 | 2a | 1400 | 5MC | C6-N1 | -2.13 | 1.34 | 1.38 |
| 55 | 2x | 54 | 5MU | C2-N3 | -2.12 | 1.34 | 1.38 |
| 54 | 1y | 37 | MIA | C5-N7 | -2.11 | 1.35 | 1.39 |
| 55 | 1x | 8 | 4SU | C2-N1 | 2.11 | 1.41 | 1.38 |
| 55 | 1x | 54 | 5MU | C6-N1 | -2.11 | 1.34 | 1.38 |
| 1 | 2A | 2605 | PSU | C2-N3 | -2.11 | 1.34 | 1.37 |
| 32 | 2a | 1518 | MA6 | C4-N9 | -2.11 | 1.33 | 1.37 |
| 32 | 2a | 1519 | MA6 | C5-N7 | -2.10 | 1.35 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | 1A | 1939 | 5MU | C2-N1 | 2.10 | 1.41 | 1.38 |
| 54 | 1w | 46 | 7MG | C8-N9 | 2.10 | 1.47 | 1.45 |
| 32 | 1a | 1207 | 2MG | C2-N3 | 2.10 | 1.36 | 1.32 |
| 54 | 1y | 46 | 7MG | C8-N9 | 2.09 | 1.47 | 1.45 |
| 32 | 1a | 1404 | 5MC | C6-N1 | -2.09 | 1.34 | 1.38 |
| 1 | 2A | 2552 | 2MU | C2-N3 | -2.08 | 1.34 | 1.38 |
| 55 | 2x | 32 | 5MC | C6-N1 | -2.07 | 1.34 | 1.38 |
| 54 | 2w | 54 | 5MU | C2-N3 | -2.07 | 1.34 | 1.38 |
| 1 | 1A | 2552 | 2MU | C5-C4 | 2.06 | 1.48 | 1.43 |
| 54 | 2y | 54 | 5MU | C6-N1 | -2.06 | 1.34 | 1.38 |
| 32 | 2a | 1518 | MA6 | C5-N7 | -2.06 | 1.35 | 1.39 |
| 1 | 1A | 2503 | 2MA | C4-N9 | -2.06 | 1.33 | 1.37 |
| 32 | 1a | 1407 | 5MC | C6-N1 | -2.05 | 1.34 | 1.38 |
| 32 | 1a | 527 | 7MG | C8-N9 | 2.05 | 1.47 | 1.45 |
| 32 | 1a | 1207 | 2MG | C5-N7 | -2.04 | 1.35 | 1.39 |
| 1 | 1A | 1915 | 5MU | C6-N1 | -2.04 | 1.34 | 1.38 |
| 54 | 2w | 54 | 5MU | C2-N1 | 2.04 | 1.41 | 1.38 |
| 1 | 2A | 1939 | 5MU | C2-N1 | 2.04 | 1.41 | 1.38 |
| 32 | 2a | 966 | M2G | C5-N7 | -2.04 | 1.35 | 1.39 |
| 32 | 1a | 1518 | MA6 | C5-N7 | -2.03 | 1.35 | 1.39 |
| 55 | 2x | 54 | 5MU | C6-N1 | -2.03 | 1.34 | 1.38 |
| 54 | 2w | 46 | 7MG | C8-N9 | 2.03 | 1.47 | 1.45 |
| 54 | 1w | 54 | 5MU | C2-N3 | -2.01 | 1.34 | 1.38 |
| 32 | 2a | 1207 | 2MG | C2-N3 | 2.01 | 1.35 | 1.32 |
| 54 | 2y | 46 | 7MG | C8-N9 | 2.01 | 1.47 | 1.45 |
| 54 | 1y | 8 | 4SU | C2-N3 | -2.01 | 1.34 | 1.38 |
| 32 | 2a | 967 | 5MC | C6-N1 | -2.00 | 1.34 | 1.38 |

All (415) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 43 | 1l | 92 | 0TD | CSB-SB-CB | -11.01 | 82.57 | 102.36 |
| 54 | 2y | 46 | 7MG | N9-C4-N3 | 9.82 | 139.84 | 125.46 |
| 54 | 1y | 46 | 7MG | N9-C4-N3 | 9.20 | 138.94 | 125.46 |
| 32 | 2a | 527 | 7MG | N9-C4-N3 | 9.09 | 138.78 | 125.46 |
| 54 | 1w | 37 | MIA | C12-C13-C14 | -9.05 | 110.76 | 127.01 |
| 32 | 1a | 527 | 7MG | N9-C4-N3 | 8.89 | 138.49 | 125.46 |
| 54 | 1w | 46 | 7MG | N9-C4-N3 | 8.78 | 138.33 | 125.46 |
| 54 | 2w | 46 | 7MG | N9-C4-N3 | 8.54 | 137.97 | 125.46 |
| 54 | 2w | 37 | MIA | C5-C4-N3 | -8.33 | 118.41 | 127.18 |
| 1 | 2A | 2503 | 2MA | C5-C4-N3 | -8.13 | 118.61 | 127.18 |
| 54 | 2w | 8 | 4SU | C4-N3-C2 | -8.09 | 119.56 | 127.31 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 54 | 1w | 37 | MIA | C5-C4-N3 | -7.78 | 118.99 | 127.18 |
| 1 | 1A | 2503 | 2MA | C5-C4-N3 | -7.73 | 119.03 | 127.18 |
| 32 | 2a | 1498 | UR3 | C4-N3-C2 | -7.16 | 118.82 | 124.58 |
| 43 | 2l | 92 | 0TD | CSB-SB-CB | -7.11 | 89.59 | 102.36 |
| 32 | 2a | 1207 | 2MG | C2-N3-C4 | 7.06 | 120.84 | 112.00 |
| 32 | 1a | 1207 | 2MG | C2-N3-C4 | 6.95 | 120.70 | 112.00 |
| 32 | 1a | 1498 | UR3 | C4-N3-C2 | -6.82 | 119.09 | 124.58 |
| 54 | 2w | 37 | MIA | N3-C4-N9 | 6.74 | 135.54 | 126.99 |
| 55 | 2x | 55 | PSU | N1-C2-N3 | 6.42 | 121.94 | 115.17 |
| 1 | 2A | 2503 | 2MA | N3-C4-N9 | 6.41 | 135.13 | 126.99 |
| 54 | 1w | 55 | PSU | N1-C2-N3 | 6.41 | 121.93 | 115.17 |
| 1 | 1A | 1911 | PSU | N1-C2-N3 | 6.39 | 121.91 | 115.17 |
| 1 | 2A | 1917 | PSU | N1-C2-N3 | 6.39 | 121.91 | 115.17 |
| 54 | 1y | 39 | PSU | N1-C2-N3 | 6.37 | 121.88 | 115.17 |
| 54 | 2y | 55 | PSU | N1-C2-N3 | 6.33 | 121.85 | 115.17 |
| 54 | 1w | 39 | PSU | N1-C2-N3 | 6.33 | 121.84 | 115.17 |
| 1 | 2A | 2605 | PSU | N1-C2-N3 | 6.32 | 121.84 | 115.17 |
| 54 | 2y | 32 | PSU | N1-C2-N3 | 6.30 | 121.81 | 115.17 |
| 55 | 1x | 55 | PSU | N1-C2-N3 | 6.26 | 121.78 | 115.17 |
| 54 | 2w | 32 | PSU | N1-C2-N3 | 6.26 | 121.77 | 115.17 |
| 1 | 2A | 1911 | PSU | N1-C2-N3 | 6.26 | 121.77 | 115.17 |
| 54 | 1y | 55 | PSU | N1-C2-N3 | 6.25 | 121.77 | 115.17 |
| 1 | 2A | 2251 | OMG | C5-C4-N3 | -6.24 | 118.45 | 128.39 |
| 54 | 2y | 39 | PSU | N1-C2-N3 | 6.24 | 121.75 | 115.17 |
| 1 | 1A | 1917 | PSU | N1-C2-N3 | 6.24 | 121.75 | 115.17 |
| 54 | 2w | 55 | PSU | N1-C2-N3 | 6.20 | 121.71 | 115.17 |
| 54 | 1y | 32 | PSU | N1-C2-N3 | 6.20 | 121.70 | 115.17 |
| 54 | 2w | 8 | 4SU | C5-C4-N3 | 6.15 | 120.47 | 114.75 |
| 1 | 1A | 2503 | 2MA | N3-C4-N9 | 6.13 | 134.78 | 126.99 |
| 54 | 1w | 32 | PSU | N1-C2-N3 | 6.12 | 121.62 | 115.17 |
| 32 | 2a | 966 | M2G | C5-C4-N3 | -6.10 | 118.68 | 128.39 |
| 54 | 1w | 37 | MIA | N3-C4-N9 | 6.05 | 134.67 | 126.99 |
| 32 | 1a | 516 | PSU | N1-C2-N3 | 6.05 | 121.55 | 115.17 |
| 1 | 1A | 2605 | PSU | N1-C2-N3 | 6.02 | 121.52 | 115.17 |
| 32 | 2a | 516 | PSU | N1-C2-N3 | 6.02 | 121.52 | 115.17 |
| 1 | 1A | 2251 | OMG | C5-C4-N3 | -5.99 | 118.86 | 128.39 |
| 54 | 1y | 8 | 4SU | C4-N3-C2 | -5.95 | 121.61 | 127.31 |
| 54 | 2y | 46 | 7MG | C5-C4-N3 | -5.94 | 116.99 | 128.13 |
| 32 | 1a | 1207 | 2MG | C5-C4-N3 | -5.93 | 118.96 | 128.39 |
| 32 | 1a | 966 | M2G | C5-C4-N3 | -5.90 | 119.00 | 128.39 |
| 54 | 2y | 37 | MIA | C5-C4-N3 | -5.85 | 118.66 | 126.72 |
| 32 | 2a | 1207 | 2MG | C5-C4-N3 | -5.79 | 119.18 | 128.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 54 | 2w | 39 | PSU | N1-C2-N3 | 5.73 | 121.22 | 115.17 |
| 54 | 2y | 8 | 4SU | C4-N3-C2 | -5.73 | 121.82 | 127.31 |
| 32 | 1a | 1519 | MA6 | C5-C4-N3 | -5.69 | 118.88 | 126.72 |
| 32 | 2a | 1519 | MA6 | C5-C4-N3 | -5.66 | 118.93 | 126.72 |
| 32 | 2a | 527 | 7MG | C5-C4-N3 | -5.59 | 117.64 | 128.13 |
| 1 | 2A | 1939 | 5MU | C4-N3-C2 | -5.59 | 120.02 | 127.34 |
| 54 | 1y | 37 | MIA | C5-C4-N3 | -5.56 | 119.06 | 126.72 |
| 54 | 2y | 8 | 4SU | C5-C4-N3 | 5.55 | 119.92 | 114.75 |
| 54 | 1y | 46 | 7MG | C5-C4-N3 | -5.53 | 117.74 | 128.13 |
| 32 | 1a | 1518 | MA6 | C5-C4-N3 | -5.44 | 119.23 | 126.72 |
| 1 | 2A | 1939 | 5MU | N3-C2-N1 | 5.44 | 121.97 | 114.89 |
| 54 | 2w | 46 | 7MG | N9-C8-N7 | -5.38 | 95.75 | 103.37 |
| 1 | 1A | 1939 | 5MU | C4-N3-C2 | -5.31 | 120.38 | 127.34 |
| 54 | 1w | 54 | 5MU | C4-N3-C2 | -5.29 | 120.41 | 127.34 |
| 32 | 1a | 527 | 7MG | C5-C4-N3 | -5.29 | 118.20 | 128.13 |
| 54 | 1w | 46 | 7MG | N9-C8-N7 | -5.28 | 95.89 | 103.37 |
| 54 | 2w | 8 | 4SU | C5-C4-S4 | -5.26 | 118.30 | 124.31 |
| 32 | 1a | 527 | 7MG | N9-C8-N7 | -5.25 | 95.94 | 103.37 |
| 1 | 1A | 1915 | 5MU | N3-C2-N1 | 5.24 | 121.71 | 114.89 |
| 54 | 1y | 54 | 5MU | C4-N3-C2 | -5.22 | 120.49 | 127.34 |
| 54 | 1y | 8 | 4SU | C5-C4-N3 | 5.21 | 119.59 | 114.75 |
| 54 | 1w | 54 | 5MU | N3-C2-N1 | 5.16 | 121.61 | 114.89 |
| 54 | 1y | 54 | 5MU | N3-C2-N1 | 5.16 | 121.61 | 114.89 |
| 1 | 2A | 2552 | 2MU | N3-C2-N1 | 5.16 | 121.60 | 114.89 |
| 54 | 1w | 8 | 4SU | C5-C4-N3 | 5.15 | 119.54 | 114.75 |
| 1 | 1A | 2552 | 2MU | N3-C2-N1 | 5.13 | 121.56 | 114.89 |
| 1 | 2A | 1915 | 5MU | N3-C2-N1 | 5.13 | 121.56 | 114.89 |
| 54 | 1w | 8 | 4SU | C4-N3-C2 | -5.11 | 122.42 | 127.31 |
| 32 | 2a | 527 | 7MG | N9-C8-N7 | -5.11 | 96.14 | 103.37 |
| 1 | 1A | 2251 | OMG | C2-N3-C4 | 5.09 | 121.06 | 112.30 |
| 32 | 2a | 1518 | MA6 | C5-C4-N3 | -5.08 | 119.72 | 126.72 |
| 1 | 2A | 1915 | 5MU | C4-N3-C2 | -5.01 | 120.77 | 127.34 |
| 32 | 2a | 1518 | MA6 | C9-N6-C6 | -5.00 | 107.80 | 120.52 |
| 1 | 1A | 1915 | 5MU | C4-N3-C2 | -5.00 | 120.78 | 127.34 |
| 54 | 2w | 46 | 7MG | C5-C4-N3 | -4.97 | 118.80 | 128.13 |
| 55 | 1x | 54 | 5MU | N3-C2-N1 | 4.97 | 121.36 | 114.89 |
| 55 | 2x | 54 | 5MU | N3-C2-N1 | 4.96 | 121.34 | 114.89 |
| 54 | 1y | 46 | 7MG | N9-C8-N7 | -4.96 | 96.36 | 103.37 |
| 1 | 1A | 1939 | 5MU | N3-C2-N1 | 4.93 | 121.31 | 114.89 |
| 1 | 2A | 2251 | OMG | C2-N3-C4 | 4.92 | 120.78 | 112.30 |
| 54 | 2y | 46 | 7MG | N9-C8-N7 | -4.91 | 96.42 | 103.37 |
| 1 | 1A | 2552 | 2MU | C4-N3-C2 | -4.88 | 120.55 | 126.61 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 55 | 2x | 54 | 5MU | C4-N3-C2 | -4.88 | 120.94 | 127.34 |
| 1 | 1A | 1939 | 5MU | C5-C4-N3 | 4.87 | 119.56 | 115.32 |
| 1 | 2A | 2251 | OMG | N9-C4-N3 | 4.86 | 135.66 | 125.95 |
| 55 | 2x | 8 | 4SU | C5-C4-N3 | 4.78 | 119.20 | 114.75 |
| 54 | 1w | 46 | 7MG | C5-C4-N3 | -4.77 | 119.17 | 128.13 |
| 1 | 2A | 2552 | 2MU | C4-N3-C2 | -4.77 | 120.69 | 126.61 |
| 54 | 2y | 37 | MIA | N3-C4-N9 | 4.73 | 135.21 | 127.17 |
| 55 | 1x | 54 | 5MU | C4-N3-C2 | -4.71 | 121.16 | 127.34 |
| 1 | 2A | 1939 | 5MU | C5-C4-N3 | 4.67 | 119.38 | 115.32 |
| 54 | 2y | 46 | 7MG | C2-N3-C4 | 4.63 | 120.28 | 112.30 |
| 54 | 2w | 8 | 4SU | N3-C2-N1 | 4.60 | 120.88 | 114.89 |
| 32 | 2a | 1518 | MA6 | C2-N1-C6 | 4.56 | 122.97 | 111.83 |
| 32 | 2a | 966 | M2G | N9-C4-N3 | 4.54 | 135.04 | 125.95 |
| 32 | 2a | 966 | M2G | C2-N3-C4 | 4.51 | 120.85 | 112.51 |
| 1 | 1A | 2251 | OMG | N9-C4-N3 | 4.48 | 134.92 | 125.95 |
| 54 | 1w | 54 | 5MU | C5-C4-N3 | 4.48 | 119.22 | 115.32 |
| 32 | 1a | 966 | M2G | C2-N3-C4 | 4.48 | 120.79 | 112.51 |
| 54 | 2w | 54 | 5MU | N3-C2-N1 | 4.46 | 120.69 | 114.89 |
| 54 | 1y | 46 | 7MG | C2-N3-C4 | 4.45 | 119.97 | 112.30 |
| 32 | 1a | 1518 | MA6 | C9-N6-C6 | -4.45 | 109.21 | 120.52 |
| 32 | 2a | 1518 | MA6 | C4-C5-N7 | -4.40 | 105.55 | 110.58 |
| 54 | 1y | 54 | 5MU | C5-C4-N3 | 4.40 | 119.15 | 115.32 |
| 54 | 1y | 37 | MIA | N3-C4-N9 | 4.40 | 134.65 | 127.17 |
| 32 | 2a | 527 | 7MG | C2-N3-C4 | 4.40 | 119.88 | 112.30 |
| 32 | 2a | 1519 | MA6 | C2-N1-C6 | 4.37 | 122.50 | 111.83 |
| 32 | 1a | 1518 | MA6 | C2-N1-C6 | 4.36 | 122.48 | 111.83 |
| 1 | 1A | 1939 | 5MU | O4-C4-C5 | -4.36 | 119.93 | 124.92 |
| 32 | 1a | 1519 | MA6 | C9-N6-C6 | -4.34 | 109.47 | 120.52 |
| 32 | 1a | 966 | M2G | N9-C4-N3 | 4.34 | 134.63 | 125.95 |
| 32 | 2a | 1519 | MA6 | N3-C4-N9 | 4.32 | 134.52 | 127.17 |
| 32 | 1a | 527 | 7MG | C2-N3-C4 | 4.32 | 119.74 | 112.30 |
| 55 | 2x | 54 | 5MU | C5-C4-N3 | 4.28 | 119.04 | 115.32 |
| 1 | 1A | 1915 | 5MU | C5-C4-N3 | 4.27 | 119.03 | 115.32 |
| 32 | 1a | 1207 | 2MG | N9-C4-N3 | 4.26 | 134.47 | 125.95 |
| 54 | 2w | 46 | 7MG | C2-N3-C4 | 4.26 | 119.63 | 112.30 |
| 54 | 1y | 39 | PSU | C4-N3-C2 | -4.26 | 120.51 | 126.37 |
| 54 | 2w | 54 | 5MU | C4-N3-C2 | -4.26 | 121.76 | 127.34 |
| 32 | 2a | 1519 | MA6 | C9-N6-C6 | -4.24 | 109.73 | 120.52 |
| 32 | 1a | 1519 | MA6 | N3-C4-N9 | 4.23 | 134.37 | 127.17 |
| 32 | 1a | 1519 | MA6 | C4-C5-N7 | -4.20 | 105.78 | 110.58 |
| 55 | 1x | 8 | 4SU | C5-C4-N3 | 4.19 | 118.65 | 114.75 |
| 1 | 2A | 2605 | PSU | C4-N3-C2 | -4.19 | 120.60 | 126.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 32 | 1a | 1519 | MA6 | C2-N1-C6 | 4.15 | 121.97 | 111.83 |
| 1 | 2A | 1917 | PSU | C4-N3-C2 | -4.13 | 120.67 | 126.37 |
| 54 | 2y | 55 | PSU | C4-N3-C2 | -4.13 | 120.68 | 126.37 |
| 32 | 2a | 1519 | MA6 | C4-C5-N7 | -4.13 | 105.86 | 110.58 |
| 1 | 1A | 1911 | PSU | C4-N3-C2 | -4.13 | 120.69 | 126.37 |
| 1 | 2A | 1915 | 5MU | C5-C4-N3 | 4.12 | 118.91 | 115.32 |
| 54 | 2y | 54 | 5MU | C5-C4-N3 | 4.12 | 118.90 | 115.32 |
| 54 | 1w | 54 | 5MU | O4-C4-C5 | -4.12 | 120.21 | 124.92 |
| 54 | 1y | 54 | 5MU | O4-C4-C5 | -4.11 | 120.21 | 124.92 |
| 55 | 2x | 8 | 4SU | C1'-N1-C2 | 4.11 | 124.97 | 117.59 |
| 54 | 1w | 46 | 7MG | C2-N3-C4 | 4.10 | 119.37 | 112.30 |
| 1 | 1A | 1917 | PSU | C4-N3-C2 | -4.09 | 120.74 | 126.37 |
| 32 | 1a | 1518 | MA6 | C4-C5-N7 | -4.07 | 105.92 | 110.58 |
| 54 | 2y | 39 | PSU | C4-N3-C2 | -4.07 | 120.77 | 126.37 |
| 54 | 1y | 55 | PSU | C4-N3-C2 | -4.06 | 120.78 | 126.37 |
| 1 | 1A | 1915 | 5MU | O4-C4-C5 | -4.06 | 120.28 | 124.92 |
| 55 | 1x | 55 | PSU | C4-N3-C2 | -4.04 | 120.81 | 126.37 |
| 1 | 2A | 1939 | 5MU | C5-C6-N1 | -4.04 | 118.93 | 123.31 |
| 1 | 2A | 1939 | 5MU | O4-C4-C5 | -4.03 | 120.30 | 124.92 |
| 1 | 2A | 1911 | PSU | C4-N3-C2 | -4.03 | 120.81 | 126.37 |
| 32 | 1a | 1518 | MA6 | N3-C4-N9 | 4.03 | 134.02 | 127.17 |
| 54 | 1w | 55 | PSU | O2-C2-N1 | -4.01 | 118.65 | 122.79 |
| 55 | 2x | 55 | PSU | C4-N3-C2 | -4.00 | 120.85 | 126.37 |
| 54 | 1w | 39 | PSU | C4-N3-C2 | -3.99 | 120.87 | 126.37 |
| 54 | 2y | 54 | 5MU | C4-N3-C2 | -3.99 | 122.11 | 127.34 |
| 1 | 1A | 1911 | PSU | O2-C2-N1 | -3.99 | 118.68 | 122.79 |
| 54 | 2y | 32 | PSU | C4-N3-C2 | -3.96 | 120.91 | 126.37 |
| 54 | 1w | 37 | MIA | C15-C14-C13 | -3.95 | 110.79 | 122.66 |
| 54 | 1y | 32 | PSU | C4-N3-C2 | -3.94 | 120.94 | 126.37 |
| 54 | 1w | 55 | PSU | C4-N3-C2 | -3.93 | 120.96 | 126.37 |
| 54 | 2w | 54 | 5MU | C5-C4-N3 | 3.93 | 118.74 | 115.32 |
| 54 | 2w | 32 | PSU | C4-N3-C2 | -3.91 | 120.99 | 126.37 |
| 1 | 1A | 1939 | 5MU | C5-C6-N1 | -3.90 | 119.08 | 123.31 |
| 54 | 2y | 54 | 5MU | O4-C4-C5 | -3.90 | 120.46 | 124.92 |
| 54 | 2y | 54 | 5MU | N3-C2-N1 | 3.88 | 119.94 | 114.89 |
| 32 | 2a | 1207 | 2MG | N9-C4-N3 | 3.87 | 133.70 | 125.95 |
| 55 | 1x | 54 | 5MU | C5-C4-N3 | 3.87 | 118.69 | 115.32 |
| 54 | 2w | 55 | PSU | C4-N3-C2 | -3.87 | 121.04 | 126.37 |
| 1 | 1A | 2605 | PSU | C4-N3-C2 | -3.85 | 121.06 | 126.37 |
| 32 | 1a | 516 | PSU | C4-N3-C2 | -3.83 | 121.10 | 126.37 |
| 55 | 2x | 54 | 5MU | O4-C4-C5 | -3.81 | 120.56 | 124.92 |
| 54 | 1y | 39 | PSU | O2-C2-N1 | -3.78 | 118.89 | 122.79 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 54 | 1y | 55 | PSU | O2-C2-N1 | -3.76 | 118.91 | 122.79 |
| 55 | 1x | 32 | 5MC | C5-C6-N1 | -3.76 | 119.23 | 123.31 |
| 54 | 1w | 32 | PSU | C4-N3-C2 | -3.75 | 121.20 | 126.37 |
| 54 | 1w | 37 | MIA | C16-C14-C13 | -3.75 | 111.40 | 122.66 |
| 1 | 2A | 1915 | 5MU | O4-C4-C5 | -3.74 | 120.64 | 124.92 |
| 32 | 2a | 1207 | 2MG | C6-C5-N7 | 3.73 | 137.07 | 130.29 |
| 54 | 2w | 55 | PSU | O2-C2-N1 | -3.71 | 118.97 | 122.79 |
| 32 | 1a | 516 | PSU | O2-C2-N1 | -3.70 | 118.97 | 122.79 |
| 54 | 2y | 37 | MIA | C2-N3-C4 | 3.70 | 120.86 | 111.83 |
| 1 | 2A | 1962 | 5MC | C5-C6-N1 | -3.69 | 119.30 | 123.31 |
| 32 | 1a | 1518 | MA6 | C2-N3-C4 | 3.69 | 120.84 | 111.83 |
| 32 | 2a | 1518 | MA6 | N3-C4-N9 | 3.68 | 133.43 | 127.17 |
| 54 | 1y | 8 | 4SU | N3-C2-N1 | 3.68 | 119.69 | 114.89 |
| 55 | 1x | 54 | 5MU | O4-C4-C5 | -3.68 | 120.70 | 124.92 |
| 32 | 2a | 516 | PSU | C4-N3-C2 | -3.67 | 121.31 | 126.37 |
| 32 | 2a | 1519 | MA6 | C2-N3-C4 | 3.66 | 120.76 | 111.83 |
| 54 | 1y | 37 | MIA | C2-N3-C4 | 3.65 | 120.75 | 111.83 |
| 54 | 2w | 39 | PSU | C4-N3-C2 | -3.65 | 121.34 | 126.37 |
| 55 | 2x | 55 | PSU | O2-C2-N1 | -3.63 | 119.04 | 122.79 |
| 54 | 1y | 8 | 4SU | C5-C4-S4 | -3.63 | 120.16 | 124.31 |
| 32 | 1a | 1519 | MA6 | C2-N3-C4 | 3.63 | 120.69 | 111.83 |
| 1 | 2A | 1917 | PSU | O2-C2-N1 | -3.62 | 119.05 | 122.79 |
| 54 | 2w | 32 | PSU | O2-C2-N1 | -3.62 | 119.05 | 122.79 |
| 1 | 1A | 1917 | PSU | O2-C2-N1 | -3.61 | 119.07 | 122.79 |
| 54 | 2y | 32 | PSU | O2-C2-N1 | -3.60 | 119.08 | 122.79 |
| 54 | 1y | 37 | MIA | N3-C2-N1 | -3.60 | 123.14 | 128.58 |
| 1 | 1A | 1942 | 5MC | C5-C6-N1 | -3.59 | 119.42 | 123.31 |
| 54 | 1w | 32 | PSU | O2-C2-N1 | -3.58 | 119.10 | 122.79 |
| 55 | 1x | 55 | PSU | O2-C2-N1 | -3.57 | 119.11 | 122.79 |
| 54 | 1w | 39 | PSU | O2-C2-N1 | -3.56 | 119.12 | 122.79 |
| 54 | 2y | 8 | 4SU | C5-C4-S4 | -3.52 | 120.28 | 124.31 |
| 32 | 2a | 1518 | MA6 | C2-N3-C4 | 3.52 | 120.43 | 111.83 |
| 54 | 1y | 37 | MIA | C4-C5-N7 | -3.51 | 106.57 | 110.58 |
| 54 | 2w | 54 | 5MU | O4-C4-C5 | -3.51 | 120.90 | 124.92 |
| 54 | 2w | 37 | MIA | C2-N3-C4 | 3.51 | 121.48 | 112.29 |
| 54 | 2y | 8 | 4SU | N3-C2-N1 | 3.51 | 119.46 | 114.89 |
| 54 | 2y | 37 | MIA | N3-C2-N1 | -3.50 | 123.28 | 128.58 |
| 1 | 2A | 1911 | PSU | O2-C2-N1 | -3.50 | 119.18 | 122.79 |
| 54 | 2y | 37 | MIA | C4-C5-N7 | -3.49 | 106.59 | 110.58 |
| 54 | 1y | 32 | PSU | O2-C2-N1 | -3.49 | 119.19 | 122.79 |
| 32 | 2a | 516 | PSU | O2-C2-N1 | -3.49 | 119.19 | 122.79 |
| 54 | 2y | 39 | PSU | O2-C2-N1 | -3.48 | 119.20 | 122.79 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 32 | 1a | 1518 | MA6 | N1-C2-N3 | -3.48 | 123.32 | 128.58 |
| 54 | 1y | 54 | 5MU | C5-C6-N1 | -3.47 | 119.54 | 123.31 |
| 43 | 2l | 92 | 0TD | OD2-CG-CB | 3.47 | 120.65 | 113.15 |
| 32 | 1a | 1404 | 5MC | C5-C6-N1 | -3.46 | 119.55 | 123.31 |
| 32 | 2a | 1404 | 5MC | C5-C6-N1 | -3.43 | 119.59 | 123.31 |
| 1 | 2A | 1915 | 5MU | C5-C6-N1 | -3.43 | 119.59 | 123.31 |
| 54 | 1w | 37 | MIA | C2-N3-C4 | 3.42 | 121.26 | 112.29 |
| 32 | 2a | 1518 | MA6 | N1-C2-N3 | -3.42 | 123.41 | 128.58 |
| 54 | 1w | 8 | 4SU | N3-C2-N1 | 3.42 | 119.34 | 114.89 |
| 32 | 1a | 1207 | 2MG | C6-C5-N7 | 3.40 | 136.47 | 130.29 |
| 55 | 1x | 8 | 4SU | C6-C5-C4 | -3.39 | 117.02 | 119.95 |
| 54 | 1w | 37 | MIA | C6-C5-N7 | 3.38 | 136.12 | 132.43 |
| 55 | 2x | 54 | 5MU | C5-C6-N1 | -3.38 | 119.64 | 123.31 |
| 1 | 1A | 2503 | 2MA | C4-C5-N7 | -3.37 | 106.72 | 110.58 |
| 1 | 2A | 2503 | 2MA | C4-C5-N7 | -3.34 | 106.76 | 110.58 |
| 54 | 1w | 37 | MIA | C4-C5-N7 | -3.33 | 106.77 | 110.58 |
| 54 | 1w | 8 | 4SU | C5-C4-S4 | -3.33 | 120.50 | 124.31 |
| 1 | 1A | 2552 | 2MU | O2-C2-N1 | -3.32 | 118.47 | 122.80 |
| 1 | 2A | 1942 | 5MC | C5-C6-N1 | -3.31 | 119.72 | 123.31 |
| 32 | 2a | 967 | 5MC | C5-C6-N1 | -3.29 | 119.73 | 123.31 |
| 54 | 2w | 37 | MIA | C4-C5-N7 | -3.28 | 106.83 | 110.58 |
| 32 | 1a | 966 | M2G | C6-C5-N7 | 3.28 | 136.25 | 130.29 |
| 32 | 1a | 1498 | UR3 | C5-C4-N3 | 3.26 | 119.33 | 115.04 |
| 32 | 2a | 1519 | MA6 | N1-C2-N3 | -3.26 | 123.65 | 128.58 |
| 54 | 2y | 55 | PSU | O2-C2-N1 | -3.25 | 119.44 | 122.79 |
| 1 | 1A | 2251 | OMG | C6-C5-N7 | 3.23 | 136.16 | 130.29 |
| 32 | 1a | 967 | 5MC | C5-C6-N1 | -3.22 | 119.81 | 123.31 |
| 1 | 1A | 1962 | 5MC | C5-C6-N1 | -3.18 | 119.86 | 123.31 |
| 54 | 1w | 54 | 5MU | C5-C6-N1 | -3.18 | 119.86 | 123.31 |
| 1 | 2A | 2605 | PSU | O2-C2-N1 | -3.17 | 119.52 | 122.79 |
| 1 | 1A | 2552 | 2MU | O4-C4-C5 | -3.17 | 119.69 | 125.16 |
| 32 | 2a | 966 | M2G | C6-C5-N7 | 3.16 | 136.05 | 130.29 |
| 32 | 1a | 1400 | 5MC | C5-C6-N1 | -3.14 | 119.91 | 123.31 |
| 55 | 1x | 54 | 5MU | C5-C6-N1 | -3.12 | 119.92 | 123.31 |
| 1 | 1A | 1915 | 5MU | C5-C6-N1 | -3.12 | 119.92 | 123.31 |
| 1 | 1A | 2552 | 2MU | C5-C4-N3 | 3.11 | 119.16 | 114.80 |
| 1 | 1A | 2552 | 2MU | C2'-C1'-N1 | -3.11 | 108.35 | 114.24 |
| 32 | 2a | 1498 | UR3 | C5-C4-N3 | 3.09 | 119.11 | 115.04 |
| 32 | 2a | 1400 | 5MC | C5-C6-N1 | -3.08 | 119.96 | 123.31 |
| 1 | 2A | 2552 | 2MU | C5-C4-N3 | 3.08 | 119.11 | 114.80 |
| 43 | 1l | 92 | 0TD | OD2-CG-CB | 3.07 | 119.78 | 113.15 |
| 32 | 1a | 1519 | MA6 | N1-C2-N3 | -3.07 | 123.94 | 128.58 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 55 | 1x | 32 | 5MC | C5-C4-N3 | -3.05 | 118.63 | 121.75 |
| 55 | 1x | 8 | 4SU | O2-C2-N1 | 3.04 | 126.75 | 122.80 |
| 32 | 2a | 1407 | 5MC | C5-C4-N3 | -3.03 | 118.65 | 121.75 |
| 55 | 2x | 32 | 5MC | C5-C6-N1 | -3.03 | 120.03 | 123.31 |
| 32 | 1a | 1407 | 5MC | C5-C6-N1 | -3.01 | 120.04 | 123.31 |
| 54 | 2y | 54 | 5MU | C5-C6-N1 | -3.01 | 120.05 | 123.31 |
| 54 | 1w | 46 | 7MG | C5-C4-N9 | -3.00 | 102.50 | 106.33 |
| 54 | 2w | 8 | 4SU | C1'-N1-C2 | 2.99 | 122.97 | 117.59 |
| 32 | 2a | 1518 | MA6 | C5-N7-C8 | 2.99 | 108.14 | 103.45 |
| 32 | 1a | 1518 | MA6 | C10-N6-C6 | -2.98 | 112.93 | 120.52 |
| 55 | 1x | 8 | 4SU | C1'-N1-C2 | 2.98 | 122.95 | 117.59 |
| 32 | 2a | 1207 | 2MG | C4-C5-N7 | -2.98 | 105.95 | 110.67 |
| 32 | 2a | 1404 | 5MC | C5-C4-N3 | -2.97 | 118.71 | 121.75 |
| 1 | 1A | 2503 | 2MA | C4-N9-C8 | 2.97 | 108.86 | 105.74 |
| 1 | 2A | 2503 | 2MA | N6-C6-N1 | 2.95 | 121.01 | 117.03 |
| 1 | 1A | 2503 | 2MA | N6-C6-N1 | 2.94 | 120.99 | 117.03 |
| 1 | 2A | 1939 | 5MU | O2-C2-N1 | -2.93 | 118.98 | 122.80 |
| 32 | 1a | 1519 | MA6 | C5-N7-C8 | 2.93 | 108.05 | 103.45 |
| 32 | 2a | 1519 | MA6 | C5-N7-C8 | 2.88 | 107.98 | 103.45 |
| 55 | 2x | 32 | 5MC | C5-C4-N3 | -2.88 | 118.81 | 121.75 |
| 1 | 2A | 2251 | OMG | C6-C5-N7 | 2.86 | 135.49 | 130.29 |
| 1 | 2A | 1942 | 5MC | C5-C4-N3 | -2.84 | 118.85 | 121.75 |
| 32 | 1a | 1518 | MA6 | C5-N7-C8 | 2.84 | 107.91 | 103.45 |
| 32 | 1a | 1407 | 5MC | C5-C4-N3 | -2.84 | 118.85 | 121.75 |
| 54 | 2w | 37 | MIA | C6-C5-N7 | 2.82 | 135.51 | 132.43 |
| 1 | 2A | 2552 | 2MU | O2-C2-N1 | -2.82 | 119.13 | 122.80 |
| 32 | 1a | 527 | 7MG | C5-C6-N1 | 2.80 | 115.87 | 110.94 |
| 1 | 1A | 2605 | PSU | O2-C2-N1 | -2.79 | 119.91 | 122.79 |
| 1 | 1A | 1962 | 5MC | C5-C4-N3 | -2.79 | 118.90 | 121.75 |
| 32 | 2a | 1407 | 5MC | C5-C6-N1 | -2.77 | 120.30 | 123.31 |
| 32 | 1a | 1400 | 5MC | C5-C4-N3 | -2.77 | 118.91 | 121.75 |
| 1 | 1A | 2503 | 2MA | C2-N1-C6 | 2.77 | 122.36 | 118.10 |
| 32 | 2a | 1400 | 5MC | C5-C4-N3 | -2.76 | 118.92 | 121.75 |
| 54 | 2w | 54 | 5MU | C5-C6-N1 | -2.76 | 120.31 | 123.31 |
| 32 | 2a | 1518 | MA6 | C4-N9-C8 | 2.74 | 108.61 | 105.74 |
| 55 | 2x | 8 | 4SU | C4-N3-C2 | -2.74 | 124.69 | 127.31 |
| 32 | 2a | 1518 | MA6 | C6-C5-N7 | 2.73 | 137.79 | 133.43 |
| 32 | 1a | 1207 | 2MG | C4-C5-N7 | -2.73 | 106.35 | 110.67 |
| 32 | 2a | 1207 | 2MG | N1-C2-N2 | 2.73 | 119.34 | 116.56 |
| 32 | 2a | 967 | 5MC | C5-C4-N3 | -2.72 | 118.97 | 121.75 |
| 32 | 1a | 1404 | 5MC | C5-C4-N3 | -2.71 | 118.97 | 121.75 |
| 54 | 1y | 54 | 5MU | O2-C2-N1 | -2.71 | 119.27 | 122.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 54 | 2y | 37 | MIA | C4-N9-C8 | 2.70 | 108.58 | 105.74 |
| 32 | 2a | 527 | 7MG | C5-C6-N1 | 2.70 | 115.70 | 110.94 |
| 54 | 2w | 37 | MIA | C12-N6-C6 | -2.70 | 120.35 | 122.85 |
| 1 | 1A | 1942 | 5MC | C5-C4-N3 | -2.67 | 119.02 | 121.75 |
| 1 | 2A | 2503 | 2MA | C4-N9-C8 | 2.66 | 108.53 | 105.74 |
| 54 | 1w | 54 | 5MU | O2-C2-N1 | -2.66 | 119.33 | 122.80 |
| 32 | 1a | 1518 | MA6 | C4-N9-C8 | 2.65 | 108.52 | 105.74 |
| 54 | 2w | 39 | PSU | O2-C2-N1 | -2.64 | 120.07 | 122.79 |
| 32 | 1a | 1519 | MA6 | C4-N9-C8 | 2.64 | 108.50 | 105.74 |
| 54 | 2y | 37 | MIA | C5-N7-C8 | 2.63 | 107.58 | 103.45 |
| 32 | 2a | 966 | M2G | C4-C5-N7 | -2.61 | 106.53 | 110.67 |
| 1 | 1A | 1939 | 5MU | O2-C2-N1 | -2.61 | 119.39 | 122.80 |
| 54 | 2y | 46 | 7MG | C5-C6-N1 | 2.61 | 115.54 | 110.94 |
| 54 | 2w | 8 | 4SU | O2-C2-N1 | -2.61 | 119.40 | 122.80 |
| 54 | 1y | 37 | MIA | C4-N9-C8 | 2.60 | 108.47 | 105.74 |
| 54 | 1y | 37 | MIA | C5-N7-C8 | 2.58 | 107.51 | 103.45 |
| 32 | 2a | 1519 | MA6 | C4-N9-C8 | 2.57 | 108.43 | 105.74 |
| 43 | 2l | 92 | 0TD | OD1-CG-CB | -2.55 | 117.09 | 122.44 |
| 1 | 2A | 2503 | 2MA | C2-N1-C6 | 2.54 | 122.00 | 118.10 |
| 32 | 1a | 967 | 5MC | C5-C4-N3 | -2.54 | 119.15 | 121.75 |
| 54 | 1w | 37 | MIA | C2-N1-C6 | 2.53 | 122.34 | 117.54 |
| 54 | 1w | 37 | MIA | N3-C2-N1 | -2.52 | 122.39 | 127.00 |
| 1 | 2A | 1962 | 5MC | C5-C4-N3 | -2.52 | 119.17 | 121.75 |
| 54 | 1y | 46 | 7MG | C5-C6-N1 | 2.52 | 115.37 | 110.94 |
| 54 | 1w | 54 | 5MU | C5M-C5-C4 | 2.51 | 121.46 | 118.78 |
| 54 | 2w | 46 | 7MG | C5-C6-N1 | 2.50 | 115.34 | 110.94 |
| 32 | 1a | 1519 | MA6 | C10-N6-C6 | -2.50 | 114.17 | 120.52 |
| 54 | 2y | 46 | 7MG | C5-C4-N9 | -2.48 | 103.15 | 106.33 |
| 1 | 1A | 2503 | 2MA | C5-N7-C8 | 2.48 | 107.35 | 103.45 |
| 54 | 2w | 37 | MIA | N3-C2-N1 | -2.48 | 122.48 | 127.00 |
| 1 | 1A | 2251 | OMG | C4-C5-N7 | -2.48 | 106.75 | 110.67 |
| 55 | 2x | 54 | 5MU | O2-C2-N1 | -2.47 | 119.58 | 122.80 |
| 54 | 2w | 37 | MIA | C5-N7-C8 | 2.46 | 107.32 | 103.45 |
| 1 | 2A | 2503 | 2MA | C5-N7-C8 | 2.44 | 107.29 | 103.45 |
| 54 | 2w | 37 | MIA | C4-N9-C8 | 2.44 | 108.30 | 105.74 |
| 54 | 2w | 46 | 7MG | C5-C4-N9 | -2.43 | 103.22 | 106.33 |
| 32 | 1a | 966 | M2G | C4-C5-N7 | -2.41 | 106.86 | 110.67 |
| 32 | 1a | 1518 | MA6 | C6-C5-N7 | 2.40 | 137.27 | 133.43 |
| 54 | 2w | 37 | MIA | C2-N1-C6 | 2.40 | 122.09 | 117.54 |
| 32 | 1a | 527 | 7MG | C5-C4-N9 | -2.38 | 103.28 | 106.33 |
| 32 | 2a | 1519 | MA6 | C10-N6-C6 | -2.38 | 114.47 | 120.52 |
| 1 | 1A | 2251 | OMG | O6-C6-C5 | -2.38 | 120.26 | 126.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 32 | 1a | 1518 | MA6 | C10-N6-C9 | -2.37 | 108.58 | 116.18 |
| 54 | 1y | 46 | 7MG | C5-C4-N9 | -2.36 | 103.31 | 106.33 |
| 32 | 2a | 1404 | 5MC | O2-C2-N3 | -2.35 | 118.62 | 122.33 |
| 1 | 2A | 2552 | 2MU | C2'-C1'-N1 | -2.35 | 109.78 | 114.24 |
| 1 | 2A | 1915 | 5MU | O2-C2-N1 | -2.35 | 119.74 | 122.80 |
| 1 | 2A | 2251 | OMG | C4-C5-N7 | -2.34 | 106.96 | 110.67 |
| 55 | 2x | 32 | 5MC | O2-C2-N3 | -2.34 | 118.65 | 122.33 |
| 54 | 1w | 37 | MIA | C4-N9-C8 | 2.33 | 108.19 | 105.74 |
| 32 | 2a | 1518 | MA6 | C10-N6-C9 | -2.33 | 108.71 | 116.18 |
| 32 | 2a | 1498 | UR3 | C3U-N3-C4 | 2.32 | 121.09 | 117.87 |
| 55 | 2x | 8 | 4SU | C6-C5-C4 | -2.31 | 117.95 | 119.95 |
| 55 | 2x | 8 | 4SU | C1'-N1-C6 | -2.30 | 115.87 | 120.78 |
| 54 | 1w | 37 | MIA | C5-N7-C8 | 2.29 | 107.05 | 103.45 |
| 32 | 1a | 1498 | UR3 | C3U-N3-C4 | 2.29 | 121.05 | 117.87 |
| 55 | 1x | 54 | 5MU | O2-C2-N1 | -2.29 | 119.82 | 122.80 |
| 1 | 1A | 1920 | 4OC | O2-C2-N3 | -2.29 | 118.73 | 122.33 |
| 54 | 2w | 54 | 5MU | C5M-C5-C4 | 2.28 | 121.22 | 118.78 |
| 54 | 2y | 55 | PSU | C5-C6-N1 | -2.28 | 118.97 | 122.14 |
| 55 | 1x | 8 | 4SU | O2-C2-N3 | -2.28 | 117.29 | 121.49 |
| 1 | 1A | 2503 | 2MA | C6-C5-N7 | 2.27 | 136.47 | 132.09 |
| 54 | 1w | 37 | MIA | C11-S10-C2 | -2.26 | 100.55 | 102.25 |
| 1 | 2A | 2552 | 2MU | O4-C4-C5 | -2.26 | 121.26 | 125.16 |
| 32 | 1a | 527 | 7MG | O6-C6-C5 | -2.25 | 122.10 | 127.62 |
| 55 | 2x | 8 | 4SU | O2-C2-N3 | -2.23 | 117.37 | 121.49 |
| 54 | 2y | 39 | PSU | C5-C6-N1 | -2.21 | 119.07 | 122.14 |
| 32 | 1a | 1402 | 4OC | C6-C5-C4 | 2.21 | 119.66 | 117.00 |
| 1 | 2A | 1920 | 4OC | O2-C2-N3 | -2.20 | 118.86 | 122.33 |
| 32 | 1a | 1400 | 5MC | O2-C2-N3 | -2.20 | 118.86 | 122.33 |
| 1 | 2A | 2251 | OMG | O6-C6-C5 | -2.19 | 120.75 | 126.53 |
| 1 | 2A | 2605 | PSU | C5-C6-N1 | -2.19 | 119.10 | 122.14 |
| 43 | 1l | 92 | 0TD | OD1-CG-CB | -2.19 | 117.86 | 122.44 |
| 54 | 1w | 8 | 4SU | C1'-N1-C2 | 2.19 | 121.52 | 117.59 |
| 32 | 1a | 1404 | 5MC | O2-C2-N3 | -2.18 | 118.89 | 122.33 |
| 32 | 1a | 1519 | MA6 | C6-C5-N7 | 2.18 | 136.91 | 133.43 |
| 32 | 2a | 1518 | MA6 | N9-C8-N7 | -2.18 | 110.85 | 113.94 |
| 54 | 1w | 46 | 7MG | C5-C6-N1 | 2.17 | 114.77 | 110.94 |
| 32 | 2a | 967 | 5MC | O2-C2-N3 | -2.17 | 118.91 | 122.33 |
| 54 | 2y | 54 | 5MU | C5M-C5-C4 | 2.17 | 121.10 | 118.78 |
| 32 | 2a | 1519 | MA6 | C6-C5-N7 | 2.17 | 136.89 | 133.43 |
| 32 | 2a | 527 | 7MG | C5-C4-N9 | -2.16 | 103.57 | 106.33 |
| 1 | 1A | 1911 | PSU | C5-C6-N1 | -2.16 | 119.15 | 122.14 |
| 1 | 1A | 2503 | 2MA | N9-C8-N7 | -2.15 | 110.88 | 113.94 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 32 | 1a | 1518 | MA6 | N9-C8-N7 | -2.14 | 110.89 | 113.94 |
| 32 | 1a | 1519 | MA6 | N9-C8-N7 | -2.14 | 110.90 | 113.94 |
| 54 | 2w | 54 | 5MU | O2-C2-N1 | -2.13 | 120.02 | 122.80 |
| 54 | 2y | 8 | 4SU | C1'-N1-C2 | 2.13 | 121.42 | 117.59 |
| 55 | 1x | 55 | PSU | C5-C6-N1 | -2.13 | 119.18 | 122.14 |
| 55 | 2x | 8 | 4SU | C5-C4-S4 | -2.12 | 121.88 | 124.31 |
| 32 | 1a | 1207 | 2MG | N1-C2-N2 | 2.12 | 118.72 | 116.56 |
| 54 | 1y | 37 | MIA | C6-C5-N7 | 2.12 | 136.17 | 132.09 |
| 32 | 2a | 1402 | 4OC | C6-C5-C4 | 2.10 | 119.53 | 117.00 |
| 54 | 1w | 39 | PSU | C5-C6-N1 | -2.09 | 119.24 | 122.14 |
| 32 | 1a | 1519 | MA6 | N1-C6-N6 | 2.09 | 119.40 | 116.86 |
| 32 | 2a | 966 | M2G | O6-C6-C5 | -2.07 | 121.08 | 126.53 |
| 1 | 2A | 1917 | PSU | C5-C6-N1 | -2.06 | 119.28 | 122.14 |
| 54 | 1y | 39 | PSU | C5-C6-N1 | -2.06 | 119.28 | 122.14 |
| 54 | 2w | 46 | 7MG | O6-C6-C5 | -2.06 | 122.57 | 127.62 |
| 32 | 2a | 527 | 7MG | O6-C6-C5 | -2.05 | 122.59 | 127.62 |
| 32 | 2a | 1207 | 2MG | N2-C2-N3 | -2.05 | 117.90 | 120.51 |
| 1 | 1A | 1917 | PSU | C5-C6-N1 | -2.04 | 119.31 | 122.14 |
| 1 | 1A | 1915 | 5MU | O2-C2-N1 | -2.04 | 120.15 | 122.80 |
| 55 | 2x | 55 | PSU | C5-C6-N1 | -2.03 | 119.32 | 122.14 |
| 54 | 1w | 46 | 7MG | C4-C5-N7 | 2.03 | 107.77 | 105.38 |
| 54 | 2y | 32 | PSU | O4'-C1'-C2' | 2.02 | 107.94 | 105.15 |
| 32 | 2a | 1407 | 5MC | O2-C2-N3 | -2.02 | 119.15 | 122.33 |
| 54 | 1y | 46 | 7MG | O6-C6-C5 | -2.01 | 122.67 | 127.62 |
| 54 | 1w | 46 | 7MG | O6-C6-C5 | -2.00 | 122.70 | 127.62 |
| 54 | 2y | 54 | 5MU | C1'-N1-C6 | -2.00 | 117.85 | 121.15 |

There are no chirality outliers.

All (54) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 32 | 1a | 1519 | MA6 | O4'-C4'-C5'-O5' |
| 32 | 2a | 1402 | 4OC | O4'-C4'-C5'-O5' |
| 32 | 2a | 1518 | MA6 | C5-C6-N6-C9 |
| 32 | 2a | 1519 | MA6 | O4'-C4'-C5'-O5' |
| 43 | 2l | 92 | 0TD | O-C-CA-CB |
| 54 | 2y | 8 | 4SU | O4'-C4'-C5'-O5' |
| 54 | 1w | 37 | MIA | C12-C13-C14-C16 |
| 54 | 1y | 46 | 7MG | C4'-C5'-O5'-P |
| 54 | 2y | 46 | 7MG | C4'-C5'-O5'-P |
| 32 | 1a | 1402 | 4OC | O4'-C4'-C5'-O5' |
| 1 | 1A | 1915 | 5MU | C3'-C4'-C5'-O5' |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 1 | 1A | 1915 | 5MU | O4'-C4'-C5'-O5' |
| 54 | 2y | 8 | 4SU | C3'-C4'-C5'-O5' |
| 54 | 1y | 8 | 4SU | C3'-C4'-C5'-O5' |
| 54 | 1y | 8 | 4SU | O4'-C4'-C5'-O5' |
| 32 | 2a | 1518 | MA6 | N1-C6-N6-C9 |
| 32 | 1a | 1519 | MA6 | C3'-C4'-C5'-O5' |
| 32 | 2a | 1402 | 4OC | C3'-C4'-C5'-O5' |
| 32 | 2a | 1519 | MA6 | C3'-C4'-C5'-O5' |
| 32 | 1a | 527 | 7MG | C3'-C4'-C5'-O5' |
| 32 | 2a | 1519 | MA6 | N1-C6-N6-C9 |
| 32 | 1a | 1402 | 4OC | C3'-C4'-C5'-O5' |
| 32 | 1a | 1518 | MA6 | C5-C6-N6-C10 |
| 32 | 1a | 1519 | MA6 | C5-C6-N6-C10 |
| 32 | 2a | 1519 | MA6 | C5-C6-N6-C9 |
| 32 | 1a | 1400 | 5MC | O4'-C4'-C5'-O5' |
| 54 | 2w | 46 | 7MG | C2'-C1'-N9-C8 |
| 54 | 2y | 46 | 7MG | C2'-C1'-N9-C8 |
| 54 | 1w | 46 | 7MG | C2'-C1'-N9-C8 |
| 54 | 1y | 46 | 7MG | C2'-C1'-N9-C8 |
| 43 | 2l | 92 | 0TD | CG-CB-SB-CSB |
| 32 | 1a | 527 | 7MG | O4'-C4'-C5'-O5' |
| 54 | 2w | 39 | PSU | O4'-C1'-C5-C4 |
| 32 | 1a | 1400 | 5MC | C3'-C4'-C5'-O5' |
| 32 | 1a | 1518 | MA6 | C5-C6-N6-C9 |
| 32 | 2a | 1519 | MA6 | C5-C6-N6-C10 |
| 32 | 2a | 1519 | MA6 | C4'-C5'-O5'-P |
| 1 | 1A | 2503 | 2MA | C4'-C5'-O5'-P |
| 54 | 1y | 54 | 5MU | O4'-C4'-C5'-O5' |
| 32 | 2a | 527 | 7MG | C4'-C5'-O5'-P |
| 54 | 1w | 46 | 7MG | O4'-C1'-N9-C8 |
| 54 | 2w | 39 | PSU | O4'-C1'-C5-C6 |
| 32 | 1a | 967 | 5MC | O4'-C4'-C5'-O5' |
| 54 | 1y | 46 | 7MG | O4'-C1'-N9-C8 |
| 54 | 2w | 46 | 7MG | O4'-C1'-N9-C8 |
| 54 | 2y | 46 | 7MG | O4'-C1'-N9-C8 |
| 43 | 1l | 92 | 0TD | CG-CB-SB-CSB |
| 32 | 2a | 1400 | 5MC | O4'-C4'-C5'-O5' |
| 32 | 1a | 527 | 7MG | C4'-C5'-O5'-P |
| 32 | 1a | 1519 | MA6 | C4'-C5'-O5'-P |
| 1 | 2A | 2251 | OMG | C4'-C5'-O5'-P |
| 54 | 1y | 8 | 4SU | C4'-C5'-O5'-P |
| 1 | 1A | 1920 | 4OC | C2'-C1'-N1-C2 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 55 | 2x | 8 | 4SU | C2'-C1'-N1-C2 |

There are no ring outliers.

46 monomers are involved in 63 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 54 | 2y | 55 | PSU | 2 | 0 |
| 1 | 2A | 1917 | PSU | 1 | 0 |
| 54 | 1w | 46 | 7MG | 1 | 0 |
| 1 | 1A | 1920 | 4OC | 1 | 0 |
| 1 | 2A | 2552 | 2MU | 1 | 0 |
| 1 | 2A | 2251 | OMG | 2 | 0 |
| 54 | 2y | 39 | PSU | 1 | 0 |
| 54 | 1y | 46 | 7MG | 1 | 0 |
| 54 | 2w | 39 | PSU | 1 | 0 |
| 1 | 2A | 2503 | 2MA | 1 | 0 |
| 54 | 1w | 54 | 5MU | 1 | 0 |
| 32 | 1a | 1518 | MA6 | 3 | 0 |
| 55 | 2x | 8 | 4SU | 2 | 0 |
| 32 | 2a | 1404 | 5MC | 1 | 0 |
| 32 | 2a | 1518 | MA6 | 3 | 0 |
| 54 | 2w | 32 | PSU | 1 | 0 |
| 54 | 2y | 37 | MIA | 1 | 0 |
| 1 | 2A | 1920 | 4OC | 2 | 0 |
| 54 | 2y | 46 | 7MG | 2 | 0 |
| 32 | 2a | 1407 | 5MC | 1 | 0 |
| 1 | 1A | 2552 | 2MU | 1 | 0 |
| 54 | 2y | 54 | 5MU | 1 | 0 |
| 32 | 2a | 967 | 5MC | 2 | 0 |
| 32 | 2a | 966 | M2G | 2 | 0 |
| 1 | 2A | 1939 | 5MU | 1 | 0 |
| 32 | 2a | 516 | PSU | 1 | 0 |
| 54 | 2w | 8 | 4SU | 5 | 0 |
| 55 | 1x | 32 | 5MC | 1 | 0 |
| 54 | 1y | 8 | 4SU | 1 | 0 |
| 54 | 1w | 55 | PSU | 1 | 0 |
| 54 | 2w | 37 | MIA | 1 | 0 |
| 55 | 2x | 32 | 5MC | 1 | 0 |
| 32 | 1a | 1519 | MA6 | 3 | 0 |
| 32 | 2a | 1519 | MA6 | 2 | 0 |
| 32 | 2a | 1498 | UR3 | 2 | 0 |
| 54 | 2w | 54 | 5MU | 1 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 54 | 1y | 39 | PSU | 1 | 0 |
| 1 | 1A | 1939 | 5MU | 2 | 0 |
| 54 | 1w | 39 | PSU | 1 | 0 |
| 54 | 1y | 37 | MIA | 1 | 0 |
| 32 | 1a | 1402 | 4OC | 2 | 0 |
| 43 | 2l | 92 | 0TD | 1 | 0 |
| 54 | 1w | 37 | MIA | 1 | 0 |
| 1 | 2A | 1915 | 5MU | 1 | 0 |
| 55 | 1x | 8 | 4SU | 2 | 0 |
| 32 | 2a | 1402 | 4OC | 2 | 0 |

## 5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry (i)

Of 2840 ligands modelled in this entry, 2836 are monoatomic - leaving 4 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 57 | CLM | 2A | 3888 | - | 20,20,20 | 0.93 | 2 (10%) | 23,27,27 | 1.00 | 1 (4%) |
| 60 | SF4 | 2d | 302 | 35 | 0,12,12 | - | - | - | | |
| 57 | CLM | 1A | 4102 | - | 20,20,20 | 0.91 | 2 (10%) | 23,27,27 | 0.74 | 0 |
| 60 | SF4 | 1d | 302 | 35 | 0,12,12 | - | - | - | | |

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 |
|---|---|---|---|---|---|---|---|
| 57 | CLM | 2A | 3888 | - | - | 6/20/22/22 | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 60 | SF4 | 2d | 302 | 35 | - | - | 0/6/5/5 |
| 57 | CLM | 1A | 4102 | - | - | 7/20/22/22 | 0/1/1/1 |
| 60 | SF4 | 1d | 302 | 35 | - | - | 0/6/5/5 |

All (4) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 57 | 2A | 3888 | CLM | C6-C5 | -2.44 | 1.48 | 1.51 |
| 57 | 2A | 3888 | CLM | C9-N9 | -2.15 | 1.40 | 1.45 |
| 57 | 1A | 4102 | CLM | C6-C5 | -2.12 | 1.48 | 1.51 |
| 57 | 1A | 4102 | CLM | C9-N9 | -2.02 | 1.40 | 1.45 |

All (1) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | 2A | 3888 | CLM | C6-C5-C3 | -2.82 | 106.66 | 111.72 |

There are no chirality outliers.

All (13) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 57 | 2A | 3888 | CLM | C1-C2-N2-C3 |
| 57 | 2A | 3888 | CLM | O2-C2-N2-C3 |
| 57 | 2A | 3888 | CLM | C4-C3-N2-C2 |
| 57 | 2A | 3888 | CLM | N2-C3-C4-O4 |
| 57 | 2A | 3888 | CLM | C5-C3-C4-O4 |
| 57 | 1A | 4102 | CLM | O2-C2-N2-C3 |
| 57 | 1A | 4102 | CLM | C1-C2-N2-C3 |
| 57 | 1A | 4102 | CLM | C5-C3-C4-O4 |
| 57 | 1A | 4102 | CLM | N2-C3-C4-O4 |
| 57 | 1A | 4102 | CLM | C5-C3-N2-C2 |
| 57 | 1A | 4102 | CLM | C4-C3-N2-C2 |
| 57 | 1A | 4102 | CLM | C4-C3-C5-O5 |
| 57 | 2A | 3888 | CLM | C4-C3-C5-O5 |

There are no ring outliers.

3 monomers are involved in 15 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 57 | 2A | 3888 | CLM | 1 | 0 |

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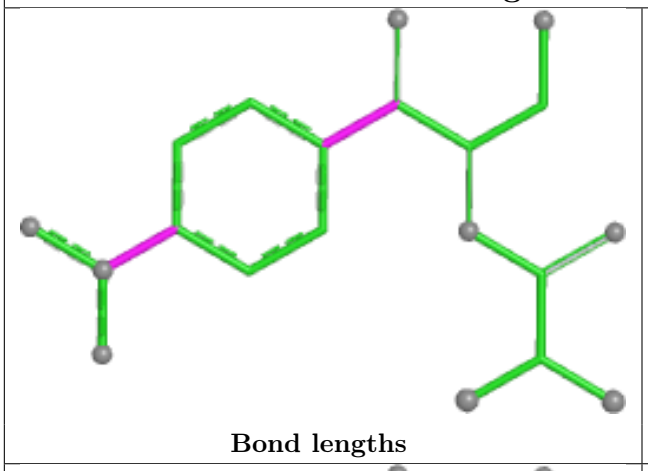
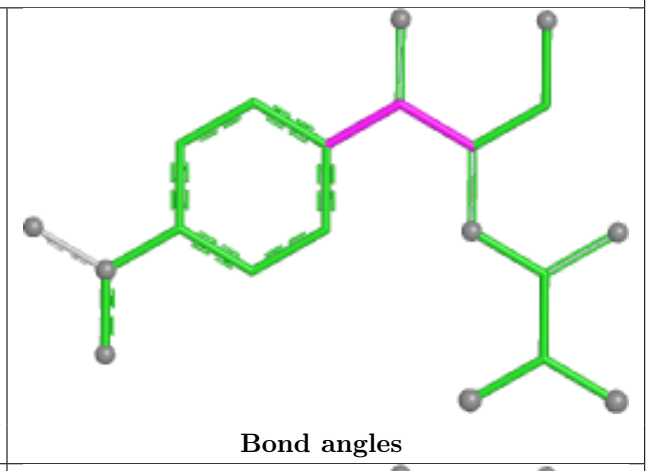
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 60 | 2d | 302 | SF4 | 3 | 0 |
| 60 | 1d | 302 | SF4 | 11 | 0 |

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

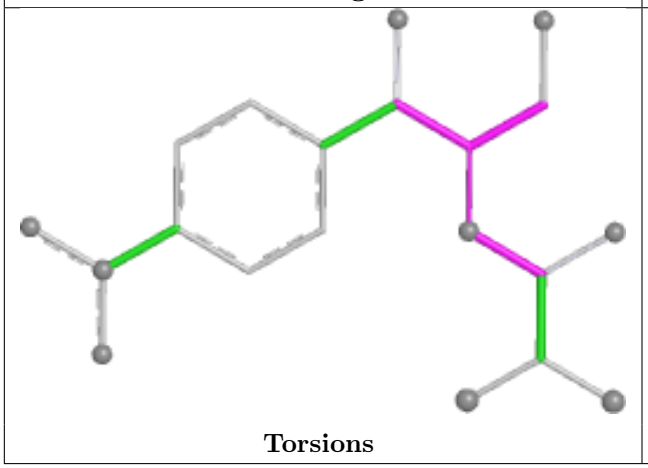
**Ligand CLM 2A 3888**



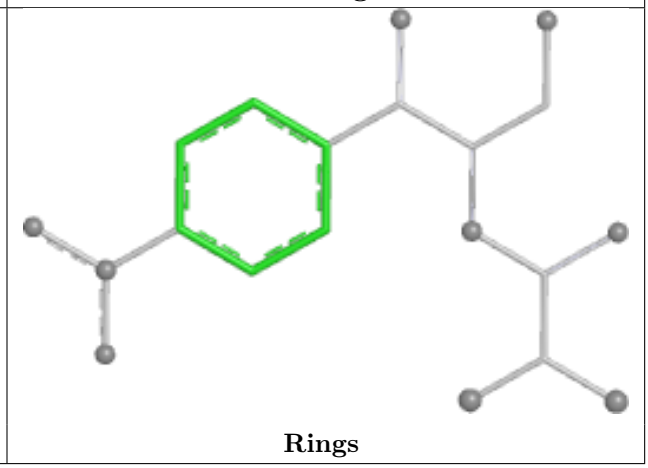
**Bond lengths**



**Bond angles**

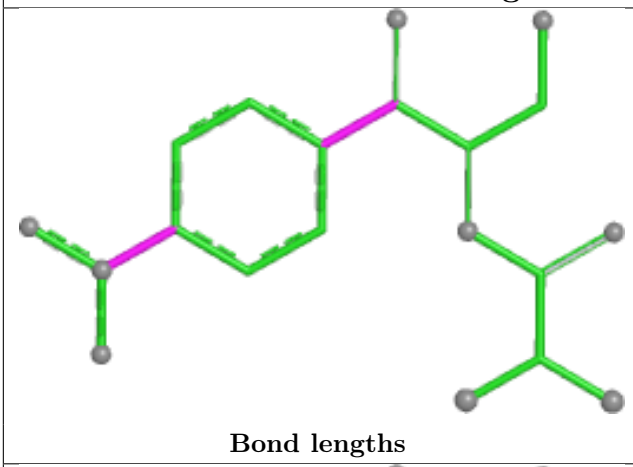


**Torsions**

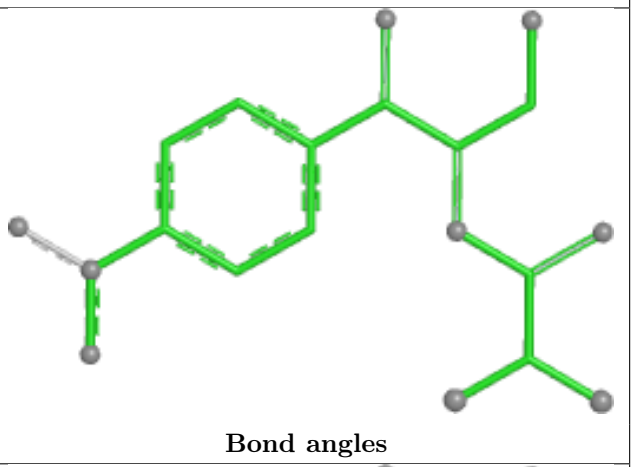


**Rings**

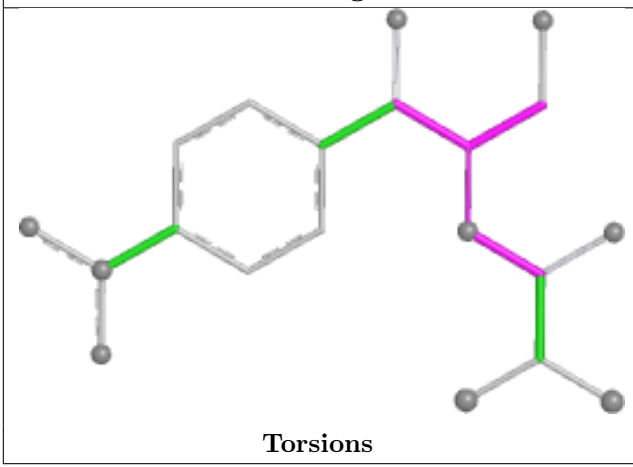
**Ligand CLM 1A 4102**



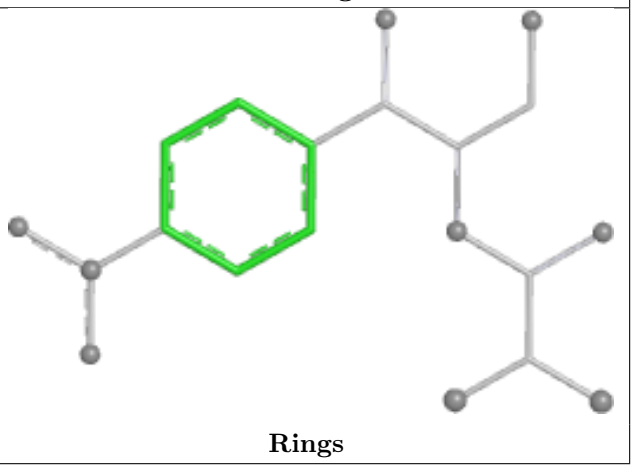
Bond lengths



Bond angles



Torsions



Rings

## 5.7 Other polymers (i)

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

# 6 Fit of model and data

## 6.1 Protein, DNA and RNA chains

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

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|
| 1 | 1A | 2860/2915 (98%) | -0.41 | 102 (3%) 46 40 | 17, 34, 87, 101 | 0 |
| 1 | 2A | 2789/2915 (95%) | 0.13 | 94 (3%) 48 42 | 34, 57, 87, 102 | 0 |
| 2 | 1B | 120/121 (99%) | -0.29 | 0 100 100 | 27, 48, 58, 79 | 0 |
| 2 | 2B | 120/121 (99%) | 1.04 | 9 (7%) 20 16 | 58, 78, 85, 87 | 0 |
| 3 | 1D | 275/276 (99%) | -0.01 | 4 (1%) 72 68 | 20, 35, 50, 73 | 0 |
| 3 | 2D | 275/276 (99%) | 0.44 | 2 (0%) 84 82 | 33, 51, 62, 73 | 0 |
| 4 | 1E | 204/206 (99%) | -0.04 | 1 (0%) 87 85 | 18, 40, 57, 73 | 0 |
| 4 | 2E | 204/206 (99%) | 0.55 | 9 (4%) 39 33 | 35, 58, 69, 79 | 0 |
| 5 | 1F | 203/210 (96%) | -0.01 | 2 (0%) 79 76 | 16, 41, 63, 80 | 0 |
| 5 | 2F | 203/210 (96%) | 0.64 | 6 (2%) 52 47 | 37, 64, 77, 83 | 0 |
| 6 | 1G | 181/182 (99%) | 0.55 | 8 (4%) 39 33 | 39, 56, 69, 78 | 0 |
| 6 | 2G | 181/182 (99%) | 1.21 | 23 (12%) 8 6 | 68, 77, 85, 93 | 0 |
| 7 | 1H | 174/180 (96%) | 0.30 | 3 (1%) 69 64 | 37, 50, 62, 71 | 0 |
| 7 | 2H | 174/180 (96%) | 1.38 | 39 (22%) 2 2 | 67, 78, 84, 91 | 0 |
| 8 | 1I | 146/148 (98%) | 0.89 | 4 (2%) 56 50 | 45, 70, 77, 81 | 0 |
| 8 | 2I | 146/148 (98%) | 1.13 | 16 (10%) 10 8 | 53, 70, 80, 85 | 0 |
| 9 | 1N | 140/140 (100%) | 0.01 | 1 (0%) 84 82 | 26, 38, 54, 72 | 0 |
| 9 | 2N | 140/140 (100%) | 0.64 | 4 (2%) 53 48 | 46, 64, 75, 80 | 0 |
| 10 | 1O | 122/122 (100%) | -0.03 | 0 100 100 | 26, 40, 55, 61 | 0 |
| 10 | 2O | 122/122 (100%) | 0.58 | 1 (0%) 82 80 | 44, 57, 68, 73 | 0 |
| 11 | 1P | 149/150 (99%) | 0.10 | 0 100 100 | 17, 44, 64, 72 | 0 |
| 11 | 2P | 149/150 (99%) | 0.66 | 1 (0%) 84 82 | 38, 64, 77, 83 | 0 |
| 12 | 1Q | 141/141 (100%) | 0.10 | 1 (0%) 84 82 | 27, 41, 54, 74 | 0 |
| 12 | 2Q | 141/141 (100%) | 1.01 | 12 (8%) 16 13 | 52, 65, 74, 80 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|
| 13 | 1R | 118/118 (100%) | -0.23 | 0 100 100 | 22, 34, 47, 55 | 0 |
| 13 | 2R | 118/118 (100%) | 0.29 | 0 100 100 | 38, 51, 59, 67 | 0 |
| 14 | 1S | 110/112 (98%) | 0.25 | 0 100 100 | 37, 49, 61, 65 | 0 |
| 14 | 2S | 110/112 (98%) | 1.56 | 35 (31%) 1 1 | 63, 73, 80, 84 | 0 |
| 15 | 1T | 131/146 (89%) | 0.18 | 2 (1%) 72 68 | 33, 43, 64, 70 | 0 |
| 15 | 2T | 131/146 (89%) | 0.65 | 4 (3%) 51 45 | 49, 59, 74, 79 | 0 |
| 16 | 1U | 116/118 (98%) | -0.21 | 1 (0%) 81 78 | 20, 29, 47, 60 | 0 |
| 16 | 2U | 116/118 (98%) | 0.84 | 5 (4%) 40 34 | 47, 61, 74, 80 | 0 |
| 17 | 1V | 101/101 (100%) | -0.19 | 0 100 100 | 20, 39, 56, 69 | 0 |
| 17 | 2V | 101/101 (100%) | 0.75 | 1 (0%) 79 76 | 42, 68, 76, 82 | 0 |
| 18 | 1W | 112/113 (99%) | -0.23 | 2 (1%) 67 63 | 21, 30, 46, 75 | 0 |
| 18 | 2W | 112/113 (99%) | 0.55 | 1 (0%) 81 78 | 38, 50, 66, 88 | 0 |
| 19 | 1X | 95/96 (98%) | -0.04 | 2 (2%) 63 58 | 24, 36, 55, 72 | 0 |
| 19 | 2X | 95/96 (98%) | 0.80 | 4 (4%) 40 35 | 44, 58, 70, 81 | 0 |
| 20 | 1Y | 107/110 (97%) | 0.41 | 1 (0%) 81 78 | 33, 48, 66, 74 | 0 |
| 20 | 2Y | 107/110 (97%) | 0.92 | 5 (4%) 36 30 | 59, 68, 75, 84 | 0 |
| 21 | 1Z | 154/206 (74%) | 0.67 | 9 (5%) 29 23 | 41, 60, 77, 85 | 0 |
| 21 | 2Z | 160/206 (77%) | 1.71 | 51 (31%) 1 1 | 66, 78, 86, 88 | 0 |
| 22 | 10 | 83/85 (97%) | 0.40 | 7 (8%) 17 13 | 27, 37, 60, 72 | 0 |
| 22 | 20 | 83/85 (97%) | 1.32 | 12 (14%) 6 4 | 53, 64, 74, 83 | 0 |
| 23 | 11 | 97/98 (98%) | 0.22 | 2 (2%) 63 58 | 24, 43, 63, 68 | 0 |
| 23 | 21 | 97/98 (98%) | 0.71 | 5 (5%) 33 27 | 40, 56, 71, 73 | 0 |
| 24 | 12 | 70/72 (97%) | 0.19 | 2 (2%) 53 48 | 32, 46, 57, 65 | 0 |
| 24 | 22 | 70/72 (97%) | 0.97 | 5 (7%) 22 17 | 54, 68, 73, 76 | 0 |
| 25 | 13 | 59/60 (98%) | -0.04 | 1 (1%) 69 64 | 25, 36, 58, 78 | 0 |
| 25 | 23 | 59/60 (98%) | 0.64 | 1 (1%) 69 64 | 53, 64, 77, 79 | 0 |
| 26 | 14 | 69/71 (97%) | 1.04 | 11 (15%) 5 4 | 49, 71, 81, 85 | 0 |
| 26 | 24 | 69/71 (97%) | 1.50 | 18 (26%) 1 1 | 76, 82, 88, 91 | 0 |
| 27 | 15 | 59/60 (98%) | -0.32 | 1 (1%) 69 64 | 18, 29, 45, 63 | 0 |
| 27 | 25 | 59/60 (98%) | 0.32 | 2 (3%) 48 42 | 38, 50, 63, 67 | 0 |
| 28 | 16 | 53/54 (98%) | 0.07 | 0 100 100 | 30, 41, 55, 61 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|
| 28 | 26 | 53/54 (98%) | 1.17 | 6 (11%) 10 8 | 49, 61, 68, 75 | 0 |
| 29 | 17 | 48/49 (97%) | -0.12 | 0 100 100 | 18, 24, 52, 58 | 0 |
| 29 | 27 | 48/49 (97%) | 0.23 | 4 (8%) 17 13 | 32, 41, 60, 68 | 0 |
| 30 | 18 | 64/65 (98%) | -0.03 | 1 (1%) 70 66 | 26, 31, 38, 54 | 0 |
| 30 | 28 | 64/65 (98%) | 0.67 | 2 (3%) 51 45 | 45, 54, 60, 71 | 0 |
| 31 | 19 | 37/37 (100%) | -0.13 | 0 100 100 | 27, 38, 54, 57 | 0 |
| 31 | 29 | 37/37 (100%) | 1.15 | 3 (8%) 18 14 | 59, 66, 73, 76 | 0 |
| 32 | 1a | 1488/1521 (97%) | 0.39 | 45 (3%) 52 47 | 33, 65, 87, 100 | 0 |
| 32 | 2a | 1491/1521 (98%) | 0.90 | 157 (10%) 11 9 | 50, 75, 91, 99 | 0 |
| 33 | 1b | 231/256 (90%) | 1.35 | 44 (19%) 3 2 | 63, 74, 82, 87 | 0 |
| 33 | 2b | 231/256 (90%) | 1.53 | 60 (25%) 1 1 | 71, 83, 88, 92 | 0 |
| 34 | 1c | 206/239 (86%) | 0.91 | 15 (7%) 21 17 | 59, 70, 78, 83 | 0 |
| 34 | 2c | 206/239 (86%) | 2.08 | 102 (49%) 0 0 | 72, 82, 87, 91 | 0 |
| 35 | 1d | 208/209 (99%) | 1.10 | 24 (11%) 9 7 | 56, 69, 80, 84 | 0 |
| 35 | 2d | 208/209 (99%) | 0.97 | 13 (6%) 26 20 | 57, 67, 75, 82 | 0 |
| 36 | 1e | 148/162 (91%) | 0.66 | 4 (2%) 56 50 | 49, 63, 70, 76 | 0 |
| 36 | 2e | 148/162 (91%) | 1.30 | 23 (15%) 5 4 | 67, 76, 81, 88 | 0 |
| 37 | 1f | 100/101 (99%) | 0.64 | 2 (2%) 65 60 | 50, 64, 70, 73 | 0 |
| 37 | 2f | 100/101 (99%) | 1.19 | 13 (13%) 7 5 | 60, 70, 77, 81 | 0 |
| 38 | 1g | 155/156 (99%) | 1.01 | 17 (10%) 10 8 | 50, 67, 76, 87 | 0 |
| 38 | 2g | 155/156 (99%) | 1.31 | 27 (17%) 4 3 | 66, 75, 82, 88 | 0 |
| 39 | 1h | 137/138 (99%) | 0.50 | 2 (1%) 72 68 | 56, 64, 71, 75 | 0 |
| 39 | 2h | 137/138 (99%) | 1.20 | 17 (12%) 8 6 | 67, 75, 80, 86 | 0 |
| 40 | 1i | 127/128 (99%) | 1.32 | 26 (20%) 2 2 | 52, 72, 77, 79 | 0 |
| 40 | 2i | 127/128 (99%) | 2.05 | 67 (52%) 0 0 | 68, 80, 86, 89 | 0 |
| 41 | 1j | 97/105 (92%) | 1.29 | 22 (22%) 2 1 | 58, 76, 83, 89 | 0 |
| 41 | 2j | 96/105 (91%) | 2.67 | 74 (77%) 0 0 | 71, 82, 88, 96 | 0 |
| 42 | 1k | 114/129 (88%) | 0.69 | 4 (3%) 47 41 | 38, 61, 70, 74 | 0 |
| 42 | 2k | 114/129 (88%) | 1.17 | 19 (16%) 4 3 | 56, 72, 77, 82 | 0 |
| 43 | 1l | 121/132 (91%) | 0.70 | 10 (8%) 17 13 | 42, 56, 66, 69 | 0 |
| 43 | 2l | 121/132 (91%) | 1.44 | 24 (19%) 3 2 | 58, 69, 76, 80 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|
| 44 | 1m | 123/126 (97%) | 0.98 | 10 (8%) 18 14 | 55, 67, 75, 81 | 0 |
| 44 | 2m | 122/126 (96%) | 1.94 | 47 (38%) 1 0 | 71, 79, 85, 88 | 0 |
| 45 | 1n | 60/61 (98%) | 1.28 | 8 (13%) 7 5 | 60, 68, 73, 76 | 0 |
| 45 | 2n | 60/61 (98%) | 2.55 | 44 (73%) 0 0 | 74, 82, 86, 90 | 0 |
| 46 | 1o | 88/89 (98%) | 0.81 | 5 (5%) 29 24 | 48, 60, 70, 74 | 0 |
| 46 | 2o | 88/89 (98%) | 1.14 | 15 (17%) 4 3 | 60, 70, 78, 82 | 0 |
| 47 | 1p | 82/88 (93%) | 1.33 | 12 (14%) 6 4 | 56, 70, 76, 79 | 0 |
| 47 | 2p | 82/88 (93%) | 1.11 | 6 (7%) 21 17 | 58, 65, 74, 80 | 0 |
| 48 | 1q | 99/105 (94%) | 1.23 | 16 (16%) 4 3 | 50, 63, 71, 73 | 0 |
| 48 | 2q | 99/105 (94%) | 0.99 | 8 (8%) 18 14 | 62, 69, 77, 81 | 0 |
| 49 | 1r | 68/88 (77%) | 0.75 | 6 (8%) 15 12 | 55, 64, 73, 75 | 0 |
| 49 | 2r | 68/88 (77%) | 1.04 | 3 (4%) 39 33 | 62, 71, 78, 82 | 0 |
| 50 | 1s | 83/93 (89%) | 1.06 | 9 (10%) 11 8 | 60, 70, 77, 80 | 0 |
| 50 | 2s | 83/93 (89%) | 2.47 | 58 (69%) 0 0 | 75, 82, 87, 91 | 0 |
| 51 | 1t | 96/106 (90%) | 1.06 | 8 (8%) 17 13 | 58, 68, 76, 81 | 0 |
| 51 | 2t | 96/106 (90%) | 1.28 | 17 (17%) 4 3 | 57, 69, 76, 79 | 0 |
| 52 | 1u | 23/27 (85%) | 1.42 | 4 (17%) 4 3 | 59, 64, 69, 71 | 0 |
| 52 | 2u | 23/27 (85%) | 2.10 | 12 (52%) 0 0 | 74, 77, 81, 85 | 0 |
| 53 | 1v | 13/24 (54%) | 0.80 | 1 (7%) 19 15 | 47, 66, 80, 86 | 0 |
| 53 | 2v | 13/24 (54%) | 2.51 | 8 (61%) 0 0 | 69, 82, 92, 92 | 0 |
| 54 | 1w | 67/76 (88%) | 1.56 | 15 (22%) 2 2 | 59, 87, 94, 98 | 0 |
| 54 | 1y | 67/76 (88%) | 0.83 | 3 (4%) 38 32 | 38, 86, 93, 96 | 0 |
| 54 | 2w | 65/76 (85%) | 1.76 | 23 (35%) 1 1 | 74, 91, 96, 101 | 0 |
| 54 | 2y | 66/76 (86%) | 1.41 | 10 (15%) 5 4 | 57, 92, 96, 99 | 0 |
| 55 | 1x | 72/77 (93%) | 0.42 | 3 (4%) 40 35 | 37, 62, 77, 85 | 0 |
| 55 | 2x | 72/77 (93%) | 0.84 | 2 (2%) 55 49 | 55, 78, 86, 89 | 0 |
| All | All | 20875/21748 (95%) | 0.53 | 1712 (8%) 17 14 | 16, 62, 85, 102 | 0 |

All (1712) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 44 | 2m | 124 | PRO | 8.5 |
| 45 | 1n | 2 | ALA | 8.0 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 38 | 2g | 80 | VAL | 7.6 |
| 34 | 2c | 2 | GLY | 7.4 |
| 38 | 1g | 80 | VAL | 7.0 |
| 44 | 2m | 6 | GLY | 6.7 |
| 50 | 2s | 79 | THR | 6.1 |
| 44 | 2m | 5 | ALA | 6.0 |
| 32 | 2a | 1034 | G | 5.9 |
| 32 | 1a | 1036 | G | 5.5 |
| 44 | 2m | 102 | ARG | 5.5 |
| 23 | 21 | 2 | SER | 5.5 |
| 44 | 1m | 124 | PRO | 5.3 |
| 32 | 2a | 1033 | G | 5.3 |
| 1 | 1A | 2159 | G | 5.1 |
| 21 | 2Z | 174 | VAL | 5.1 |
| 50 | 2s | 9 | VAL | 5.1 |
| 45 | 2n | 7 | ILE | 5.0 |
| 44 | 1m | 2 | ALA | 5.0 |
| 47 | 1p | 82 | GLN | 5.0 |
| 44 | 2m | 121 | LYS | 4.8 |
| 41 | 2j | 49 | VAL | 4.8 |
| 36 | 2e | 22 | GLY | 4.8 |
| 34 | 2c | 187 | ALA | 4.7 |
| 53 | 2v | 24 | A | 4.7 |
| 44 | 2m | 123 | ALA | 4.7 |
| 54 | 1w | 73 | A | 4.7 |
| 33 | 2b | 187 | LEU | 4.6 |
| 41 | 2j | 40 | LEU | 4.6 |
| 41 | 2j | 65 | LEU | 4.6 |
| 43 | 2l | 13 | LYS | 4.6 |
| 1 | 1A | 2112 | G | 4.6 |
| 32 | 2a | 1030(B) | C | 4.5 |
| 15 | 1T | 130 | ALA | 4.5 |
| 41 | 2j | 27 | ALA | 4.5 |
| 38 | 2g | 84 | ASN | 4.5 |
| 38 | 2g | 81 | GLY | 4.5 |
| 21 | 2Z | 172 | ALA | 4.5 |
| 41 | 2j | 34 | VAL | 4.5 |
| 52 | 2u | 14 | TRP | 4.5 |
| 32 | 2a | 1036 | G | 4.5 |
| 45 | 2n | 3 | ARG | 4.5 |
| 22 | 10 | 7 | LEU | 4.4 |
| 33 | 2b | 237 | ALA | 4.4 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 38 | 1g | 85 | TYR | 4.4 |
| 45 | 2n | 44 | LEU | 4.4 |
| 1 | 2A | 1536 | C | 4.4 |
| 22 | 10 | 6 | GLY | 4.4 |
| 26 | 14 | 56 | VAL | 4.4 |
| 40 | 2i | 14 | VAL | 4.4 |
| 40 | 2i | 102 | LEU | 4.4 |
| 45 | 2n | 25 | VAL | 4.4 |
| 45 | 2n | 39 | LEU | 4.3 |
| 33 | 1b | 237 | ALA | 4.3 |
| 45 | 2n | 47 | LEU | 4.3 |
| 15 | 1T | 131 | ALA | 4.3 |
| 50 | 2s | 76 | PRO | 4.3 |
| 1 | 2A | 883 | G | 4.3 |
| 41 | 2j | 76 | ASN | 4.3 |
| 33 | 1b | 202 | PRO | 4.2 |
| 6 | 2G | 20 | ILE | 4.2 |
| 41 | 2j | 47 | PHE | 4.2 |
| 1 | 1A | 2115 | G | 4.2 |
| 12 | 2Q | 104 | PHE | 4.2 |
| 7 | 2H | 45 | VAL | 4.2 |
| 5 | 2F | 166 | ALA | 4.2 |
| 21 | 1Z | 146 | ILE | 4.2 |
| 41 | 2j | 50 | ILE | 4.2 |
| 40 | 2i | 41 | VAL | 4.2 |
| 41 | 2j | 85 | LEU | 4.2 |
| 1 | 1A | 2113 | U | 4.2 |
| 1 | 2A | 2146 | C | 4.2 |
| 34 | 2c | 77 | ILE | 4.2 |
| 22 | 10 | 3 | HIS | 4.2 |
| 1 | 1A | 1059 | G | 4.2 |
| 41 | 2j | 32 | ALA | 4.1 |
| 45 | 2n | 2 | ALA | 4.1 |
| 33 | 2b | 185 | ILE | 4.1 |
| 34 | 1c | 39 | ILE | 4.1 |
| 34 | 2c | 4 | LYS | 4.1 |
| 44 | 2m | 122 | LYS | 4.1 |
| 51 | 2t | 103 | GLY | 4.1 |
| 33 | 1b | 127 | ILE | 4.1 |
| 1 | 1A | 1078 | U | 4.1 |
| 32 | 1a | 1531 | A | 4.1 |
| 44 | 2m | 66 | LEU | 4.1 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 41 | 2j | 55 | LYS | 4.1 |
| 21 | 2Z | 171 | ILE | 4.1 |
| 40 | 2i | 126 | SER | 4.1 |
| 50 | 2s | 11 | VAL | 4.1 |
| 54 | 1w | 1 | G | 4.0 |
| 15 | 2T | 131 | ALA | 4.0 |
| 34 | 2c | 67 | THR | 4.0 |
| 1 | 2A | 2133 | G | 4.0 |
| 3 | 2D | 2 | ALA | 4.0 |
| 36 | 2e | 109 | ILE | 4.0 |
| 40 | 2i | 36 | TYR | 4.0 |
| 42 | 2k | 25 | TYR | 4.0 |
| 1 | 2A | 2155 | G | 4.0 |
| 50 | 2s | 53 | ASN | 4.0 |
| 43 | 1l | 14 | GLY | 4.0 |
| 45 | 2n | 6 | LEU | 4.0 |
| 22 | 10 | 5 | LYS | 4.0 |
| 32 | 2a | 1220 | G | 3.9 |
| 32 | 2a | 1310 | G | 3.9 |
| 34 | 2c | 5 | ILE | 3.9 |
| 34 | 2c | 3 | ASN | 3.9 |
| 32 | 1a | 1532 | U | 3.9 |
| 32 | 2a | 1224 | G | 3.9 |
| 34 | 2c | 52 | LEU | 3.9 |
| 19 | 1X | 95 | LEU | 3.9 |
| 43 | 2l | 56 | ALA | 3.9 |
| 50 | 2s | 15 | LEU | 3.9 |
| 32 | 2a | 1222 | G | 3.9 |
| 45 | 2n | 33 | VAL | 3.9 |
| 22 | 10 | 4 | LYS | 3.9 |
| 1 | 1A | 1064 | C | 3.9 |
| 33 | 1b | 230 | VAL | 3.9 |
| 40 | 2i | 105 | ASP | 3.9 |
| 32 | 2a | 1001(A) | G | 3.8 |
| 53 | 2v | 13 | A | 3.8 |
| 34 | 2c | 9 | GLY | 3.8 |
| 54 | 2w | 3 | C | 3.8 |
| 43 | 2l | 9 | GLN | 3.8 |
| 50 | 2s | 14 | HIS | 3.8 |
| 21 | 2Z | 21 | ALA | 3.8 |
| 34 | 2c | 129 | ALA | 3.8 |
| 26 | 24 | 65 | ASP | 3.8 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 52 | 2u | 5 | ASP | 3.8 |
| 34 | 2c | 167 | TRP | 3.8 |
| 34 | 2c | 149 | ALA | 3.8 |
| 21 | 2Z | 146 | ILE | 3.8 |
| 34 | 2c | 189 | ALA | 3.8 |
| 33 | 2b | 71 | VAL | 3.8 |
| 34 | 2c | 153 | VAL | 3.8 |
| 33 | 1b | 129 | GLU | 3.7 |
| 41 | 2j | 42 | THR | 3.7 |
| 33 | 1b | 229 | VAL | 3.7 |
| 53 | 2v | 12 | A | 3.7 |
| 5 | 2F | 131 | GLY | 3.7 |
| 1 | 2A | 2118 | U | 3.7 |
| 14 | 2S | 3 | ARG | 3.7 |
| 1 | 1A | 1058 | G | 3.7 |
| 54 | 1w | 71 | G | 3.7 |
| 38 | 1g | 154 | TYR | 3.7 |
| 40 | 2i | 125 | TYR | 3.7 |
| 31 | 29 | 37 | GLY | 3.7 |
| 34 | 2c | 53 | ALA | 3.7 |
| 40 | 2i | 82 | ALA | 3.7 |
| 45 | 2n | 38 | GLY | 3.7 |
| 1 | 1A | 1057 | A | 3.7 |
| 41 | 2j | 44 | VAL | 3.7 |
| 32 | 2a | 1030(A) | G | 3.7 |
| 50 | 2s | 13 | ASP | 3.7 |
| 26 | 24 | 63 | TYR | 3.7 |
| 33 | 2b | 165 | VAL | 3.7 |
| 32 | 2a | 1035 | A | 3.6 |
| 38 | 2g | 16 | LEU | 3.6 |
| 50 | 2s | 22 | LEU | 3.6 |
| 1 | 2A | 2112 | G | 3.6 |
| 32 | 2a | 1032 | G | 3.6 |
| 35 | 2d | 183 | GLY | 3.6 |
| 50 | 2s | 82 | GLY | 3.6 |
| 26 | 24 | 50 | VAL | 3.6 |
| 34 | 1c | 12 | LEU | 3.6 |
| 34 | 2c | 192 | THR | 3.6 |
| 45 | 1n | 7 | ILE | 3.6 |
| 32 | 2a | 1001 | A | 3.6 |
| 21 | 2Z | 173 | ALA | 3.6 |
| 7 | 2H | 21 | PRO | 3.6 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | 1A | 1094 | U | 3.6 |
| 32 | 2a | 1225 | A | 3.6 |
| 33 | 1b | 17 | PHE | 3.6 |
| 50 | 1s | 9 | VAL | 3.6 |
| 1 | 2A | 2145 | C | 3.6 |
| 1 | 1A | 2116 | G | 3.6 |
| 32 | 2a | 1002 | G | 3.6 |
| 32 | 2a | 1221 | G | 3.6 |
| 45 | 2n | 22 | THR | 3.6 |
| 34 | 2c | 168 | ALA | 3.6 |
| 41 | 2j | 91 | PRO | 3.6 |
| 35 | 1d | 150 | GLU | 3.6 |
| 43 | 2l | 16 | GLU | 3.6 |
| 51 | 1t | 14 | LYS | 3.6 |
| 34 | 2c | 134 | ILE | 3.5 |
| 50 | 2s | 63 | THR | 3.5 |
| 1 | 2A | 2174 | C | 3.5 |
| 32 | 1a | 1002 | G | 3.5 |
| 34 | 2c | 145 | GLY | 3.5 |
| 38 | 2g | 83 | ALA | 3.5 |
| 40 | 2i | 127 | LYS | 3.5 |
| 1 | 1A | 1081 | U | 3.5 |
| 35 | 1d | 135 | LEU | 3.5 |
| 40 | 2i | 64 | THR | 3.5 |
| 54 | 1w | 72 | C | 3.5 |
| 1 | 1A | 1087 | G | 3.5 |
| 1 | 2A | 2159 | G | 3.5 |
| 50 | 2s | 80 | TYR | 3.5 |
| 32 | 2a | 239 | U | 3.5 |
| 32 | 1a | 1035 | A | 3.5 |
| 32 | 2a | 1286 | A | 3.5 |
| 22 | 10 | 8 | GLY | 3.5 |
| 33 | 2b | 161 | ALA | 3.5 |
| 34 | 2c | 65 | ALA | 3.5 |
| 44 | 1m | 123 | ALA | 3.5 |
| 50 | 1s | 84 | GLY | 3.5 |
| 33 | 2b | 7 | VAL | 3.5 |
| 38 | 1g | 153 | HIS | 3.5 |
| 45 | 2n | 21 | TYR | 3.5 |
| 32 | 1a | 1257 | U | 3.5 |
| 44 | 1m | 122 | LYS | 3.5 |
| 6 | 1G | 51 | ARG | 3.5 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | 1A | 1097 | U | 3.4 |
| 1 | 2A | 2156 | G | 3.4 |
| 1 | 2A | 2319 | G | 3.4 |
| 8 | 2I | 20 | ASP | 3.4 |
| 1 | 1A | 2158 | A | 3.4 |
| 26 | 14 | 50 | VAL | 3.4 |
| 44 | 1m | 3 | ARG | 3.4 |
| 44 | 2m | 60 | VAL | 3.4 |
| 42 | 2k | 50 | TYR | 3.4 |
| 51 | 1t | 103 | GLY | 3.4 |
| 19 | 2X | 92 | LEU | 3.4 |
| 22 | 20 | 84 | LEU | 3.4 |
| 34 | 2c | 188 | LEU | 3.4 |
| 1 | 2A | 2144 | U | 3.4 |
| 33 | 1b | 28 | PHE | 3.4 |
| 40 | 2i | 10 | ARG | 3.4 |
| 32 | 2a | 1003 | G | 3.4 |
| 1 | 1A | 2117 | A | 3.4 |
| 7 | 2H | 2 | SER | 3.4 |
| 22 | 20 | 2 | ALA | 3.4 |
| 34 | 2c | 200 | ALA | 3.4 |
| 36 | 2e | 17 | ALA | 3.4 |
| 50 | 2s | 2 | PRO | 3.4 |
| 34 | 2c | 207 | VAL | 3.4 |
| 1 | 1A | 1060 | U | 3.4 |
| 54 | 1w | 70 | G | 3.4 |
| 41 | 2j | 87 | THR | 3.4 |
| 21 | 2Z | 164 | ALA | 3.4 |
| 44 | 2m | 90 | LEU | 3.4 |
| 34 | 1c | 207 | VAL | 3.4 |
| 1 | 1A | 1065 | U | 3.3 |
| 32 | 1a | 1037 | C | 3.3 |
| 32 | 2a | 1219 | U | 3.3 |
| 33 | 2b | 196 | LEU | 3.3 |
| 34 | 2c | 12 | LEU | 3.3 |
| 41 | 2j | 36 | GLY | 3.3 |
| 51 | 2t | 22 | ARG | 3.3 |
| 14 | 2S | 34 | HIS | 3.3 |
| 33 | 2b | 186 | ALA | 3.3 |
| 33 | 2b | 122 | PHE | 3.3 |
| 41 | 2j | 89 | ASP | 3.3 |
| 43 | 2l | 18 | VAL | 3.3 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | 1A | 1509 | C | 3.3 |
| 24 | 12 | 69 | ARG | 3.3 |
| 32 | 2a | 1321 | C | 3.3 |
| 54 | 1w | 2 | C | 3.3 |
| 44 | 2m | 100 | GLY | 3.3 |
| 46 | 1o | 89 | GLY | 3.3 |
| 6 | 2G | 160 | VAL | 3.3 |
| 9 | 1N | 140 | VAL | 3.3 |
| 34 | 2c | 68 | VAL | 3.3 |
| 34 | 2c | 70 | VAL | 3.3 |
| 34 | 2c | 76 | VAL | 3.3 |
| 32 | 2a | 1016 | A | 3.3 |
| 32 | 2a | 1236 | A | 3.3 |
| 1 | 1A | 2160 | G | 3.3 |
| 32 | 2a | 238 | G | 3.3 |
| 23 | 11 | 2 | SER | 3.3 |
| 42 | 2k | 126 | ARG | 3.3 |
| 41 | 2j | 13 | HIS | 3.3 |
| 41 | 2j | 93 | GLY | 3.3 |
| 1 | 1A | 2145 | C | 3.3 |
| 1 | 2A | 2166 | G | 3.3 |
| 21 | 2Z | 33 | LEU | 3.3 |
| 21 | 2Z | 149 | SER | 3.3 |
| 41 | 2j | 18 | ALA | 3.3 |
| 26 | 24 | 59 | PHE | 3.3 |
| 41 | 2j | 96 | ILE | 3.3 |
| 33 | 1b | 24 | TRP | 3.2 |
| 32 | 2a | 965 | A | 3.2 |
| 51 | 2t | 24 | LEU | 3.2 |
| 1 | 2A | 2125 | G | 3.2 |
| 26 | 24 | 56 | VAL | 3.2 |
| 34 | 2c | 55 | VAL | 3.2 |
| 41 | 2j | 66 | ARG | 3.2 |
| 14 | 2S | 58 | LEU | 3.2 |
| 41 | 1j | 77 | PRO | 3.2 |
| 41 | 2j | 41 | PRO | 3.2 |
| 41 | 2j | 83 | GLU | 3.2 |
| 50 | 2s | 71 | LEU | 3.2 |
| 7 | 1H | 2 | SER | 3.2 |
| 41 | 2j | 59 | SER | 3.2 |
| 52 | 2u | 16 | GLY | 3.2 |
| 1 | 2A | 2119 | A | 3.2 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | 2A | 2169 | A | 3.2 |
| 40 | 1i | 106 | ALA | 3.2 |
| 6 | 2G | 28 | VAL | 3.2 |
| 7 | 2H | 24 | VAL | 3.2 |
| 41 | 2j | 74 | ILE | 3.2 |
| 50 | 2s | 40 | ILE | 3.2 |
| 44 | 2m | 88 | ARG | 3.2 |
| 1 | 1A | 1026 | U | 3.2 |
| 26 | 14 | 57 | GLU | 3.2 |
| 50 | 1s | 5 | LEU | 3.2 |
| 7 | 2H | 55 | PRO | 3.2 |
| 27 | 25 | 29 | THR | 3.2 |
| 38 | 2g | 82 | GLY | 3.2 |
| 32 | 2a | 1038 | C | 3.2 |
| 32 | 2a | 1226 | C | 3.2 |
| 41 | 2j | 30 | SER | 3.2 |
| 40 | 2i | 114 | TYR | 3.2 |
| 41 | 1j | 65 | LEU | 3.2 |
| 32 | 2a | 1017 | G | 3.2 |
| 12 | 2Q | 61 | GLY | 3.2 |
| 39 | 2h | 90 | GLY | 3.2 |
| 34 | 2c | 160 | ALA | 3.2 |
| 41 | 2j | 23 | ILE | 3.2 |
| 7 | 2H | 44 | VAL | 3.2 |
| 40 | 2i | 28 | VAL | 3.2 |
| 1 | 2A | 2111 | C | 3.1 |
| 32 | 2a | 1030 | C | 3.1 |
| 50 | 1s | 13 | ASP | 3.1 |
| 50 | 2s | 70 | LYS | 3.1 |
| 6 | 1G | 139 | LEU | 3.1 |
| 40 | 2i | 19 | LEU | 3.1 |
| 53 | 1v | 12 | A | 3.1 |
| 26 | 14 | 52 | THR | 3.1 |
| 26 | 14 | 54 | GLY | 3.1 |
| 45 | 2n | 61 | TRP | 3.1 |
| 50 | 2s | 84 | GLY | 3.1 |
| 8 | 1I | 146 | ALA | 3.1 |
| 26 | 24 | 49 | PHE | 3.1 |
| 34 | 2c | 198 | VAL | 3.1 |
| 41 | 2j | 54 | PHE | 3.1 |
| 26 | 14 | 67 | TYR | 3.1 |
| 32 | 1a | 1034 | G | 3.1 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 32 | 2a | 1190 | G | 3.1 |
| 50 | 2s | 52 | TYR | 3.1 |
| 54 | 1w | 65 | G | 3.1 |
| 36 | 2e | 25 | ARG | 3.1 |
| 41 | 2j | 99 | LYS | 3.1 |
| 32 | 2a | 995 | C | 3.1 |
| 41 | 2j | 39 | PRO | 3.1 |
| 32 | 2a | 1183 | A | 3.1 |
| 33 | 1b | 7 | VAL | 3.1 |
| 41 | 2j | 35 | SER | 3.1 |
| 50 | 2s | 60 | VAL | 3.1 |
| 14 | 2S | 57 | LYS | 3.1 |
| 45 | 2n | 34 | TYR | 3.1 |
| 33 | 2b | 10 | LEU | 3.1 |
| 36 | 2e | 31 | LEU | 3.1 |
| 41 | 2j | 88 | LEU | 3.1 |
| 1 | 2A | 2318 | G | 3.1 |
| 40 | 2i | 124 | GLN | 3.1 |
| 34 | 2c | 8 | ILE | 3.1 |
| 49 | 2r | 60 | ALA | 3.1 |
| 21 | 2Z | 71 | VAL | 3.1 |
| 41 | 2j | 72 | VAL | 3.1 |
| 14 | 2S | 32 | LEU | 3.1 |
| 32 | 2a | 1196 | U | 3.1 |
| 32 | 2a | 1532 | U | 3.1 |
| 34 | 2c | 17 | ASP | 3.1 |
| 21 | 2Z | 106 | GLY | 3.1 |
| 41 | 2j | 75 | ILE | 3.1 |
| 43 | 2l | 15 | ARG | 3.1 |
| 1 | 1A | 886 | C | 3.1 |
| 1 | 1A | 1100 | C | 3.1 |
| 1 | 2A | 885 | C | 3.1 |
| 32 | 2a | 1059 | C | 3.1 |
| 40 | 1i | 59 | PHE | 3.1 |
| 54 | 2w | 13 | C | 3.1 |
| 36 | 2e | 133 | TYR | 3.0 |
| 38 | 2g | 85 | TYR | 3.0 |
| 41 | 2j | 71 | LEU | 3.0 |
| 33 | 1b | 167 | PRO | 3.0 |
| 41 | 2j | 37 | PRO | 3.0 |
| 41 | 1j | 48 | THR | 3.0 |
| 35 | 1d | 5 | ILE | 3.0 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 40 | 2i | 9 | ARG | 3.0 |
| 51 | 2t | 8 | ARG | 3.0 |
| 1 | 2A | 2157 | G | 3.0 |
| 1 | 1A | 34 | C | 3.0 |
| 32 | 2a | 824 | C | 3.0 |
| 32 | 2a | 1118 | C | 3.0 |
| 32 | 2a | 1119 | C | 3.0 |
| 34 | 2c | 69 | HIS | 3.0 |
| 40 | 1i | 2 | GLU | 3.0 |
| 43 | 2l | 8 | ASN | 3.0 |
| 51 | 2t | 9 | ASN | 3.0 |
| 1 | 2A | 2173 | A | 3.0 |
| 47 | 2p | 76 | GLN | 3.0 |
| 3 | 1D | 276 | LYS | 3.0 |
| 22 | 20 | 5 | LYS | 3.0 |
| 40 | 2i | 11 | LYS | 3.0 |
| 42 | 1k | 123 | LYS | 3.0 |
| 14 | 2S | 20 | ARG | 3.0 |
| 14 | 2S | 35 | ILE | 3.0 |
| 44 | 2m | 78 | ILE | 3.0 |
| 44 | 2m | 103 | THR | 3.0 |
| 49 | 2r | 65 | ILE | 3.0 |
| 35 | 1d | 195 | ALA | 3.0 |
| 40 | 2i | 13 | ALA | 3.0 |
| 5 | 2F | 6 | VAL | 3.0 |
| 33 | 1b | 163 | PHE | 3.0 |
| 33 | 2b | 112 | VAL | 3.0 |
| 4 | 2E | 195 | LEU | 3.0 |
| 6 | 2G | 19 | LEU | 3.0 |
| 14 | 2S | 92 | TYR | 3.0 |
| 40 | 2i | 123 | PRO | 3.0 |
| 1 | 1A | 1093 | G | 3.0 |
| 7 | 2H | 175 | LYS | 3.0 |
| 1 | 1A | 2138 | C | 3.0 |
| 32 | 2a | 1054 | C | 3.0 |
| 26 | 14 | 58 | ARG | 3.0 |
| 52 | 1u | 24 | ARG | 3.0 |
| 53 | 2v | 14 | A | 3.0 |
| 21 | 1Z | 147 | GLY | 3.0 |
| 40 | 2i | 81 | ILE | 3.0 |
| 50 | 2s | 49 | ILE | 3.0 |
| 45 | 2n | 10 | ALA | 3.0 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 32 | 2a | 1040 | U | 3.0 |
| 21 | 2Z | 141 | VAL | 3.0 |
| 45 | 1n | 56 | VAL | 3.0 |
| 21 | 2Z | 125 | LEU | 3.0 |
| 40 | 1i | 126 | SER | 3.0 |
| 50 | 2s | 4 | SER | 3.0 |
| 34 | 2c | 72 | LYS | 3.0 |
| 1 | 1A | 2190 | G | 3.0 |
| 1 | 2A | 2154 | G | 3.0 |
| 1 | 2A | 645 | C | 3.0 |
| 6 | 2G | 50 | ALA | 3.0 |
| 34 | 2c | 71 | ALA | 3.0 |
| 50 | 2s | 24 | ALA | 3.0 |
| 54 | 2w | 34 | G | 3.0 |
| 32 | 2a | 1322 | C | 3.0 |
| 33 | 2b | 163 | PHE | 3.0 |
| 33 | 1b | 11 | LEU | 2.9 |
| 48 | 2q | 98 | LEU | 2.9 |
| 1 | 1A | 271(K) | U | 2.9 |
| 33 | 1b | 19 | HIS | 2.9 |
| 50 | 2s | 66 | MET | 2.9 |
| 36 | 2e | 85 | GLY | 2.9 |
| 52 | 2u | 11 | GLY | 2.9 |
| 40 | 2i | 7 | THR | 2.9 |
| 8 | 2I | 146 | ALA | 2.9 |
| 40 | 1i | 43 | ALA | 2.9 |
| 7 | 2H | 19 | VAL | 2.9 |
| 40 | 2i | 99 | LEU | 2.9 |
| 1 | 1A | 1062 | G | 2.9 |
| 1 | 1A | 2141 | G | 2.9 |
| 32 | 2a | 972 | C | 2.9 |
| 32 | 2a | 979 | C | 2.9 |
| 32 | 2a | 1027 | C | 2.9 |
| 1 | 2A | 229 | A | 2.9 |
| 32 | 2a | 1061 | G | 2.9 |
| 32 | 2a | 1114 | C | 2.9 |
| 32 | 2a | 1216 | G | 2.9 |
| 33 | 1b | 134 | GLU | 2.9 |
| 32 | 2a | 1285 | A | 2.9 |
| 45 | 2n | 17 | LYS | 2.9 |
| 53 | 2v | 23 | A | 2.9 |
| 54 | 2w | 76 | A | 2.9 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 50 | 2s | 78 | ARG | 2.9 |
| 47 | 2p | 38 | TYR | 2.9 |
| 12 | 2Q | 33 | GLY | 2.9 |
| 51 | 1t | 69 | GLY | 2.9 |
| 50 | 2s | 33 | THR | 2.9 |
| 5 | 2F | 89 | VAL | 2.9 |
| 41 | 1j | 40 | LEU | 2.9 |
| 41 | 2j | 16 | LEU | 2.9 |
| 41 | 2j | 90 | LEU | 2.9 |
| 8 | 2I | 64 | GLU | 2.9 |
| 8 | 2I | 85 | GLU | 2.9 |
| 21 | 2Z | 166 | SER | 2.9 |
| 26 | 24 | 66 | SER | 2.9 |
| 34 | 2c | 144 | SER | 2.9 |
| 1 | 1A | 1080 | C | 2.9 |
| 28 | 26 | 37 | ARG | 2.9 |
| 34 | 2c | 190 | ARG | 2.9 |
| 54 | 2w | 4 | C | 2.9 |
| 1 | 1A | 1089 | G | 2.9 |
| 1 | 2A | 2131 | G | 2.9 |
| 1 | 2A | 2149 | G | 2.9 |
| 1 | 2A | 2893 | G | 2.9 |
| 32 | 1a | 1026 | G | 2.9 |
| 38 | 1g | 37 | ASN | 2.9 |
| 41 | 2j | 6 | ILE | 2.9 |
| 4 | 2E | 167 | VAL | 2.9 |
| 33 | 2b | 184 | VAL | 2.9 |
| 33 | 2b | 215 | LEU | 2.9 |
| 34 | 2c | 33 | LEU | 2.9 |
| 35 | 1d | 194 | LEU | 2.9 |
| 45 | 2n | 56 | VAL | 2.9 |
| 40 | 2i | 2 | GLU | 2.9 |
| 21 | 2Z | 57 | ILE | 2.9 |
| 1 | 1A | 1054 | A | 2.9 |
| 1 | 1A | 2129 | C | 2.9 |
| 1 | 1A | 2132 | U | 2.9 |
| 5 | 2F | 208 | GLY | 2.9 |
| 26 | 24 | 64 | GLY | 2.9 |
| 32 | 1a | 344 | A | 2.9 |
| 32 | 2a | 948 | C | 2.9 |
| 33 | 2b | 31 | TYR | 2.9 |
| 40 | 1i | 67 | GLY | 2.9 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | 1A | 1099 | G | 2.9 |
| 1 | 1A | 2165 | G | 2.9 |
| 1 | 2A | 2751 | G | 2.9 |
| 12 | 2Q | 121 | ALA | 2.9 |
| 15 | 2T | 130 | ALA | 2.9 |
| 33 | 1b | 133 | LYS | 2.9 |
| 33 | 2b | 11 | LEU | 2.9 |
| 34 | 2c | 47 | LEU | 2.9 |
| 34 | 2c | 138 | VAL | 2.9 |
| 39 | 2h | 112 | LEU | 2.9 |
| 51 | 1t | 74 | LYS | 2.9 |
| 40 | 2i | 117 | HIS | 2.9 |
| 45 | 2n | 49 | HIS | 2.9 |
| 51 | 2t | 80 | ARG | 2.8 |
| 35 | 1d | 173 | TRP | 2.8 |
| 50 | 2s | 38 | SER | 2.8 |
| 33 | 2b | 201 | ILE | 2.8 |
| 38 | 1g | 84 | ASN | 2.8 |
| 51 | 2t | 26 | ASN | 2.8 |
| 50 | 2s | 61 | TYR | 2.8 |
| 29 | 27 | 45 | ALA | 2.8 |
| 33 | 2b | 138 | LEU | 2.8 |
| 36 | 2e | 108 | ALA | 2.8 |
| 1 | 1A | 1066 | U | 2.8 |
| 16 | 2U | 90 | VAL | 2.8 |
| 34 | 2c | 75 | VAL | 2.8 |
| 34 | 2c | 106 | VAL | 2.8 |
| 34 | 2c | 195 | VAL | 2.8 |
| 32 | 2a | 1110 | A | 2.8 |
| 32 | 2a | 1019 | C | 2.8 |
| 32 | 2a | 1116 | C | 2.8 |
| 32 | 2a | 1214 | C | 2.8 |
| 32 | 2a | 1260 | C | 2.8 |
| 52 | 2u | 23 | PRO | 2.8 |
| 1 | 2A | 1533 | G | 2.8 |
| 32 | 1a | 1030(A) | G | 2.8 |
| 38 | 1g | 5 | ARG | 2.8 |
| 34 | 2c | 170 | GLN | 2.8 |
| 34 | 2c | 124 | ILE | 2.8 |
| 44 | 2m | 4 | ILE | 2.8 |
| 48 | 1q | 62 | SER | 2.8 |
| 50 | 2s | 54 | GLY | 2.8 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 52 | 1u | 2 | GLY | 2.8 |
| 33 | 1b | 236 | TYR | 2.8 |
| 41 | 2j | 8 | LEU | 2.8 |
| 38 | 2g | 152 | ALA | 2.8 |
| 40 | 2i | 4 | TYR | 2.8 |
| 40 | 2i | 56 | LEU | 2.8 |
| 50 | 2s | 5 | LEU | 2.8 |
| 50 | 2s | 16 | LEU | 2.8 |
| 44 | 2m | 105 | THR | 2.8 |
| 7 | 2H | 107 | VAL | 2.8 |
| 21 | 2Z | 96 | VAL | 2.8 |
| 43 | 2l | 32 | PHE | 2.8 |
| 33 | 1b | 12 | GLU | 2.8 |
| 38 | 1g | 79 | ARG | 2.8 |
| 40 | 2i | 49 | PRO | 2.8 |
| 1 | 1A | 1095 | A | 2.8 |
| 1 | 2A | 2170 | A | 2.8 |
| 16 | 1U | 117 | GLN | 2.8 |
| 32 | 1a | 1001 | A | 2.8 |
| 32 | 2a | 974 | A | 2.8 |
| 41 | 2j | 38 | ILE | 2.8 |
| 47 | 2p | 3 | LYS | 2.8 |
| 32 | 2a | 954 | G | 2.8 |
| 32 | 2a | 971 | G | 2.8 |
| 35 | 2d | 154 | ASN | 2.8 |
| 44 | 2m | 106 | ASN | 2.8 |
| 54 | 2w | 70 | G | 2.8 |
| 14 | 2S | 56 | LEU | 2.8 |
| 33 | 2b | 152 | PHE | 2.8 |
| 41 | 2j | 86 | MET | 2.8 |
| 44 | 2m | 99 | ARG | 2.8 |
| 50 | 2s | 36 | ARG | 2.8 |
| 38 | 2g | 86 | GLN | 2.8 |
| 1 | 1A | 2130 | U | 2.8 |
| 32 | 2a | 1235 | U | 2.8 |
| 1 | 1A | 1092 | C | 2.8 |
| 1 | 2A | 1043 | C | 2.8 |
| 32 | 2a | 1066 | C | 2.8 |
| 45 | 2n | 60 | SER | 2.8 |
| 48 | 2q | 99 | SER | 2.8 |
| 21 | 2Z | 150 | LEU | 2.8 |
| 36 | 2e | 23 | GLY | 2.8 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 38 | 1g | 82 | GLY | 2.8 |
| 41 | 2j | 52 | GLY | 2.8 |
| 51 | 2t | 73 | HIS | 2.8 |
| 21 | 1Z | 168 | GLU | 2.8 |
| 22 | 20 | 68 | GLU | 2.8 |
| 28 | 26 | 52 | VAL | 2.8 |
| 34 | 2c | 120 | VAL | 2.8 |
| 1 | 1A | 1176 | G | 2.8 |
| 33 | 2b | 199 | TYR | 2.8 |
| 4 | 1E | 56 | PRO | 2.7 |
| 33 | 1b | 131 | PRO | 2.7 |
| 8 | 2I | 17 | GLN | 2.7 |
| 6 | 2G | 157 | ILE | 2.7 |
| 33 | 2b | 127 | ILE | 2.7 |
| 33 | 2b | 214 | ILE | 2.7 |
| 44 | 2m | 96 | LEU | 2.7 |
| 1 | 2A | 2171 | A | 2.7 |
| 32 | 2a | 983 | A | 2.7 |
| 1 | 1A | 888 | C | 2.7 |
| 1 | 2A | 2128 | C | 2.7 |
| 1 | 2A | 2164 | C | 2.7 |
| 7 | 2H | 43 | VAL | 2.7 |
| 8 | 2I | 3 | VAL | 2.7 |
| 21 | 2Z | 152 | ALA | 2.7 |
| 33 | 2b | 123 | ALA | 2.7 |
| 26 | 14 | 59 | PHE | 2.7 |
| 32 | 2a | 984 | C | 2.7 |
| 40 | 2i | 128 | ARG | 2.7 |
| 41 | 2j | 43 | ARG | 2.7 |
| 50 | 2s | 67 | VAL | 2.7 |
| 23 | 21 | 68 | PRO | 2.7 |
| 44 | 2m | 21 | TYR | 2.7 |
| 1 | 1A | 2162 | G | 2.7 |
| 54 | 1y | 18 | G | 2.7 |
| 33 | 1b | 214 | ILE | 2.7 |
| 34 | 2c | 202 | ILE | 2.7 |
| 47 | 1p | 19 | ILE | 2.7 |
| 8 | 2I | 12 | LEU | 2.7 |
| 33 | 1b | 10 | LEU | 2.7 |
| 40 | 2i | 96 | LEU | 2.7 |
| 8 | 2I | 1 | MET | 2.7 |
| 20 | 2Y | 5 | MET | 2.7 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 34 | 2c | 6 | HIS | 2.7 |
| 40 | 2i | 39 | GLY | 2.7 |
| 44 | 2m | 64 | TRP | 2.7 |
| 44 | 2m | 95 | GLY | 2.7 |
| 1 | 1A | 2167 | U | 2.7 |
| 35 | 1d | 192 | GLU | 2.7 |
| 35 | 2d | 3 | ARG | 2.7 |
| 43 | 1l | 16 | GLU | 2.7 |
| 3 | 1D | 2 | ALA | 2.7 |
| 33 | 2b | 164 | VAL | 2.7 |
| 38 | 1g | 2 | ALA | 2.7 |
| 44 | 2m | 104 | ARG | 2.7 |
| 45 | 2n | 13 | THR | 2.7 |
| 48 | 1q | 68 | ARG | 2.7 |
| 49 | 1r | 24 | ALA | 2.7 |
| 1 | 1A | 1084 | A | 2.7 |
| 1 | 2A | 896 | A | 2.7 |
| 6 | 2G | 2 | PRO | 2.7 |
| 33 | 2b | 236 | TYR | 2.7 |
| 38 | 2g | 154 | TYR | 2.7 |
| 42 | 2k | 124 | LYS | 2.7 |
| 1 | 2A | 2175 | C | 2.7 |
| 32 | 2a | 1223 | C | 2.7 |
| 45 | 2n | 53 | LEU | 2.7 |
| 49 | 1r | 78 | LEU | 2.7 |
| 21 | 2Z | 26 | GLY | 2.7 |
| 21 | 2Z | 121 | HIS | 2.7 |
| 26 | 14 | 64 | GLY | 2.7 |
| 32 | 2a | 973 | G | 2.7 |
| 32 | 2a | 1026 | G | 2.7 |
| 54 | 2y | 18 | G | 2.7 |
| 55 | 2x | 70 | G | 2.7 |
| 41 | 1j | 78 | ASN | 2.7 |
| 22 | 20 | 69 | PHE | 2.7 |
| 36 | 1e | 67 | VAL | 2.7 |
| 37 | 2f | 6 | VAL | 2.7 |
| 40 | 2i | 18 | PHE | 2.7 |
| 40 | 2i | 43 | ALA | 2.7 |
| 41 | 2j | 94 | VAL | 2.7 |
| 1 | 1A | 1101 | U | 2.7 |
| 1 | 2A | 2113 | U | 2.7 |
| 52 | 1u | 23 | PRO | 2.7 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 54 | 1y | 20 | U | 2.7 |
| 1 | 1A | 2119 | A | 2.7 |
| 1 | 2A | 1847 | A | 2.7 |
| 34 | 2c | 182 | ILE | 2.7 |
| 41 | 1j | 74 | ILE | 2.7 |
| 1 | 1A | 885 | C | 2.7 |
| 32 | 2a | 1203 | C | 2.7 |
| 54 | 1w | 74 | C | 2.7 |
| 44 | 2m | 70 | LEU | 2.7 |
| 14 | 2S | 45 | GLY | 2.7 |
| 26 | 24 | 61 | ARG | 2.7 |
| 41 | 1j | 79 | ARG | 2.7 |
| 45 | 2n | 29 | ARG | 2.7 |
| 46 | 2o | 20 | GLY | 2.7 |
| 46 | 2o | 68 | ARG | 2.7 |
| 7 | 2H | 123 | PHE | 2.7 |
| 43 | 2l | 104 | VAL | 2.7 |
| 50 | 2s | 7 | LYS | 2.7 |
| 52 | 2u | 3 | LYS | 2.7 |
| 39 | 2h | 4 | ASP | 2.7 |
| 1 | 2A | 2160 | G | 2.6 |
| 32 | 1a | 1001(A) | G | 2.6 |
| 32 | 1a | 1003 | G | 2.6 |
| 32 | 2a | 951 | G | 2.6 |
| 40 | 2i | 73 | GLN | 2.6 |
| 26 | 24 | 67 | TYR | 2.6 |
| 32 | 2a | 1126 | U | 2.6 |
| 44 | 2m | 22 | ILE | 2.6 |
| 21 | 2Z | 144 | LEU | 2.6 |
| 32 | 2a | 1333 | A | 2.6 |
| 33 | 1b | 196 | LEU | 2.6 |
| 1 | 1A | 2161 | C | 2.6 |
| 3 | 1D | 38 | LYS | 2.6 |
| 32 | 1a | 345 | C | 2.6 |
| 54 | 1w | 4 | C | 2.6 |
| 54 | 2w | 74 | C | 2.6 |
| 55 | 1x | 69 | C | 2.6 |
| 22 | 20 | 12 | ASN | 2.6 |
| 41 | 2j | 78 | ASN | 2.6 |
| 21 | 1Z | 141 | VAL | 2.6 |
| 21 | 2Z | 88 | PHE | 2.6 |
| 21 | 2Z | 139 | VAL | 2.6 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 21 | 2Z | 167 | PRO | 2.6 |
| 26 | 24 | 42 | PHE | 2.6 |
| 51 | 2t | 98 | PRO | 2.6 |
| 6 | 2G | 146 | TYR | 2.6 |
| 1 | 1A | 1082 | U | 2.6 |
| 55 | 2x | 47 | U | 2.6 |
| 22 | 20 | 7 | LEU | 2.6 |
| 33 | 2b | 121 | LEU | 2.6 |
| 34 | 2c | 101 | LEU | 2.6 |
| 43 | 2l | 10 | LEU | 2.6 |
| 7 | 2H | 60 | ARG | 2.6 |
| 41 | 2j | 68 | HIS | 2.6 |
| 8 | 1I | 70 | GLU | 2.6 |
| 33 | 1b | 228 | GLY | 2.6 |
| 34 | 2c | 13 | GLY | 2.6 |
| 35 | 1d | 169 | LYS | 2.6 |
| 40 | 2i | 115 | GLY | 2.6 |
| 45 | 2n | 4 | LYS | 2.6 |
| 45 | 2n | 55 | GLY | 2.6 |
| 2 | 2B | 59 | A | 2.6 |
| 32 | 2a | 1306 | A | 2.6 |
| 8 | 2I | 19 | VAL | 2.6 |
| 33 | 1b | 25 | ASN | 2.6 |
| 14 | 2S | 12 | PHE | 2.6 |
| 37 | 1f | 90 | VAL | 2.6 |
| 38 | 2g | 7 | ALA | 2.6 |
| 40 | 1i | 15 | ALA | 2.6 |
| 50 | 2s | 41 | VAL | 2.6 |
| 33 | 2b | 97 | TRP | 2.6 |
| 1 | 1A | 2111 | C | 2.6 |
| 32 | 1a | 1027 | C | 2.6 |
| 32 | 2a | 1045 | C | 2.6 |
| 32 | 2a | 1249 | C | 2.6 |
| 47 | 1p | 1 | MET | 2.6 |
| 47 | 2p | 19 | ILE | 2.6 |
| 43 | 2l | 19 | ARG | 2.6 |
| 46 | 1o | 88 | ARG | 2.6 |
| 52 | 1u | 6 | ARG | 2.6 |
| 32 | 2a | 1308 | U | 2.6 |
| 41 | 2j | 22 | LYS | 2.6 |
| 51 | 2t | 74 | LYS | 2.6 |
| 44 | 2m | 67 | GLU | 2.6 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 7 | 2H | 174 | GLY | 2.6 |
| 18 | 1W | 112 | GLY | 2.6 |
| 34 | 2c | 41 | GLY | 2.6 |
| 45 | 1n | 51 | GLY | 2.6 |
| 50 | 1s | 8 | GLY | 2.6 |
| 32 | 1a | 1024 | G | 2.6 |
| 32 | 2a | 1047 | G | 2.6 |
| 32 | 2a | 1202 | G | 2.6 |
| 32 | 2a | 1331 | G | 2.6 |
| 54 | 2w | 15 | G | 2.6 |
| 34 | 2c | 137 | ALA | 2.6 |
| 42 | 2k | 89 | ALA | 2.6 |
| 46 | 2o | 19 | PRO | 2.6 |
| 34 | 2c | 107 | GLN | 2.6 |
| 1 | 1A | 548 | A | 2.6 |
| 32 | 1a | 1005 | A | 2.6 |
| 32 | 2a | 949 | A | 2.6 |
| 6 | 2G | 52 | ILE | 2.6 |
| 33 | 2b | 200 | ILE | 2.6 |
| 46 | 1o | 87 | ILE | 2.6 |
| 50 | 2s | 31 | ILE | 2.6 |
| 32 | 1a | 221 | C | 2.6 |
| 32 | 2a | 985 | C | 2.6 |
| 32 | 2a | 1384 | C | 2.6 |
| 40 | 2i | 47 | LEU | 2.6 |
| 54 | 2w | 2 | C | 2.6 |
| 12 | 2Q | 60 | ARG | 2.6 |
| 34 | 2c | 79 | ARG | 2.6 |
| 45 | 2n | 12 | ARG | 2.6 |
| 48 | 2q | 32 | TYR | 2.6 |
| 12 | 2Q | 22 | LYS | 2.6 |
| 21 | 2Z | 143 | GLY | 2.6 |
| 43 | 2l | 63 | GLY | 2.6 |
| 7 | 2H | 52 | VAL | 2.6 |
| 32 | 2a | 960 | U | 2.6 |
| 45 | 2n | 40 | CYS | 2.6 |
| 34 | 2c | 73 | PRO | 2.6 |
| 41 | 1j | 32 | ALA | 2.6 |
| 41 | 1j | 47 | PHE | 2.6 |
| 45 | 2n | 16 | PHE | 2.6 |
| 41 | 1j | 100 | THR | 2.5 |
| 41 | 2j | 100 | THR | 2.5 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | 2A | 2165 | G | 2.5 |
| 32 | 1a | 1023 | G | 2.5 |
| 32 | 2a | 1253 | G | 2.5 |
| 54 | 2y | 5 | G | 2.5 |
| 1 | 1A | 2135 | A | 2.5 |
| 32 | 1a | 1447 | A | 2.5 |
| 44 | 2m | 19 | LEU | 2.5 |
| 14 | 2S | 17 | ARG | 2.5 |
| 34 | 2c | 176 | HIS | 2.5 |
| 34 | 2c | 48 | TYR | 2.5 |
| 40 | 2i | 62 | TYR | 2.5 |
| 1 | 2A | 884 | C | 2.5 |
| 50 | 2s | 26 | GLY | 2.5 |
| 21 | 2Z | 165 | VAL | 2.5 |
| 41 | 2j | 77 | PRO | 2.5 |
| 42 | 1k | 14 | VAL | 2.5 |
| 50 | 2s | 42 | PRO | 2.5 |
| 24 | 12 | 70 | GLN | 2.5 |
| 40 | 1i | 13 | ALA | 2.5 |
| 42 | 1k | 97 | ALA | 2.5 |
| 43 | 1l | 6 | THR | 2.5 |
| 54 | 2y | 45 | U | 2.5 |
| 21 | 2Z | 157 | LEU | 2.5 |
| 34 | 2c | 172 | ARG | 2.5 |
| 45 | 1n | 3 | ARG | 2.5 |
| 48 | 2q | 100 | LYS | 2.5 |
| 1 | 1A | 1055 | G | 2.5 |
| 1 | 1A | 1068 | G | 2.5 |
| 32 | 2a | 1031 | G | 2.5 |
| 1 | 2A | 1913 | A | 2.5 |
| 26 | 24 | 57 | GLU | 2.5 |
| 32 | 2a | 1251 | A | 2.5 |
| 32 | 2a | 1447 | A | 2.5 |
| 33 | 1b | 31 | TYR | 2.5 |
| 33 | 1b | 33 | TYR | 2.5 |
| 45 | 2n | 28 | GLY | 2.5 |
| 46 | 1o | 19 | PRO | 2.5 |
| 34 | 2c | 128 | PHE | 2.5 |
| 38 | 1g | 7 | ALA | 2.5 |
| 40 | 2i | 106 | ALA | 2.5 |
| 41 | 2j | 63 | PHE | 2.5 |
| 45 | 2n | 59 | ALA | 2.5 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | 1A | 889 | C | 2.5 |
| 1 | 1A | 2164 | C | 2.5 |
| 1 | 2A | 886 | C | 2.5 |
| 2 | 2B | 6 | C | 2.5 |
| 32 | 1a | 1030(B) | C | 2.5 |
| 32 | 2a | 1149 | C | 2.5 |
| 46 | 2o | 4 | THR | 2.5 |
| 43 | 2l | 52 | LEU | 2.5 |
| 44 | 2m | 34 | LEU | 2.5 |
| 45 | 2n | 23 | ARG | 2.5 |
| 46 | 2o | 3 | ILE | 2.5 |
| 50 | 2s | 32 | LYS | 2.5 |
| 7 | 2H | 51 | ARG | 2.5 |
| 21 | 2Z | 102 | LEU | 2.5 |
| 37 | 2f | 45 | LEU | 2.5 |
| 26 | 14 | 63 | TYR | 2.5 |
| 38 | 2g | 133 | GLY | 2.5 |
| 33 | 2b | 125 | PRO | 2.5 |
| 1 | 1A | 1098 | A | 2.5 |
| 1 | 2A | 2062 | A | 2.5 |
| 1 | 2A | 2117 | A | 2.5 |
| 32 | 2a | 1064 | G | 2.5 |
| 32 | 2a | 1117 | G | 2.5 |
| 32 | 2a | 1357 | A | 2.5 |
| 32 | 2a | 1370 | G | 2.5 |
| 33 | 1b | 136 | VAL | 2.5 |
| 40 | 2i | 53 | VAL | 2.5 |
| 50 | 2s | 45 | VAL | 2.5 |
| 55 | 1x | 70 | G | 2.5 |
| 4 | 2E | 51 | PHE | 2.5 |
| 10 | 2O | 99 | PHE | 2.5 |
| 41 | 2j | 26 | ALA | 2.5 |
| 43 | 2l | 68 | ALA | 2.5 |
| 45 | 2n | 37 | PHE | 2.5 |
| 51 | 1t | 12 | ALA | 2.5 |
| 14 | 2S | 19 | LYS | 2.5 |
| 39 | 2h | 135 | CYS | 2.5 |
| 44 | 1m | 121 | LYS | 2.5 |
| 48 | 1q | 87 | LYS | 2.5 |
| 51 | 2t | 30 | LYS | 2.5 |
| 6 | 2G | 133 | LEU | 2.5 |
| 33 | 2b | 130 | ARG | 2.5 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 34 | 2c | 119 | ARG | 2.5 |
| 34 | 2c | 157 | ILE | 2.5 |
| 34 | 2c | 56 | ASP | 2.5 |
| 6 | 2G | 24 | GLY | 2.5 |
| 33 | 2b | 91 | PRO | 2.5 |
| 28 | 26 | 48 | VAL | 2.5 |
| 35 | 2d | 198 | VAL | 2.5 |
| 40 | 1i | 14 | VAL | 2.5 |
| 44 | 2m | 7 | VAL | 2.5 |
| 51 | 1t | 18 | GLN | 2.5 |
| 12 | 2Q | 58 | PHE | 2.5 |
| 50 | 2s | 10 | PHE | 2.5 |
| 50 | 2s | 6 | LYS | 2.4 |
| 40 | 1i | 7 | THR | 2.4 |
| 1 | 1A | 1069 | A | 2.4 |
| 32 | 2a | 1363(A) | A | 2.4 |
| 35 | 2d | 49 | ARG | 2.4 |
| 16 | 2U | 62 | ILE | 2.4 |
| 21 | 2Z | 91 | LEU | 2.4 |
| 33 | 2b | 208 | ILE | 2.4 |
| 34 | 2c | 57 | ILE | 2.4 |
| 1 | 1A | 2133 | G | 2.4 |
| 1 | 2A | 2110 | G | 2.4 |
| 32 | 2a | 953 | G | 2.4 |
| 32 | 2a | 1233 | G | 2.4 |
| 33 | 2b | 109 | SER | 2.4 |
| 54 | 1y | 19 | G | 2.4 |
| 54 | 2w | 10 | G | 2.4 |
| 54 | 2w | 71 | G | 2.4 |
| 54 | 2y | 6 | G | 2.4 |
| 47 | 2p | 48 | TRP | 2.4 |
| 1 | 1A | 2794 | C | 2.4 |
| 32 | 1a | 1006 | C | 2.4 |
| 1 | 2A | 2132 | U | 2.4 |
| 32 | 1a | 1025 | U | 2.4 |
| 32 | 2a | 950 | U | 2.4 |
| 32 | 2a | 1150 | U | 2.4 |
| 21 | 2Z | 95 | PRO | 2.4 |
| 34 | 2c | 171 | GLY | 2.4 |
| 36 | 2e | 114 | GLY | 2.4 |
| 39 | 2h | 106 | GLY | 2.4 |
| 40 | 1i | 8 | GLY | 2.4 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 21 | 1Z | 100 | VAL | 2.4 |
| 34 | 2c | 199 | LYS | 2.4 |
| 37 | 2f | 90 | VAL | 2.4 |
| 38 | 2g | 75 | VAL | 2.4 |
| 14 | 2S | 29 | PHE | 2.4 |
| 21 | 2Z | 136 | PHE | 2.4 |
| 44 | 2m | 31 | LYS | 2.4 |
| 42 | 2k | 60 | ALA | 2.4 |
| 35 | 1d | 3 | ARG | 2.4 |
| 35 | 1d | 153 | ARG | 2.4 |
| 36 | 2e | 18 | ARG | 2.4 |
| 38 | 1g | 41 | ARG | 2.4 |
| 41 | 2j | 15 | THR | 2.4 |
| 52 | 2u | 8 | THR | 2.4 |
| 7 | 2H | 72 | ILE | 2.4 |
| 33 | 1b | 200 | ILE | 2.4 |
| 34 | 1c | 188 | LEU | 2.4 |
| 34 | 2c | 91 | LEU | 2.4 |
| 34 | 2c | 152 | ILE | 2.4 |
| 35 | 1d | 21 | LEU | 2.4 |
| 39 | 2h | 83 | ILE | 2.4 |
| 41 | 1j | 76 | ASN | 2.4 |
| 43 | 2l | 7 | ILE | 2.4 |
| 44 | 2m | 48 | LEU | 2.4 |
| 49 | 2r | 66 | LEU | 2.4 |
| 41 | 2j | 56 | HIS | 2.4 |
| 48 | 1q | 66 | SER | 2.4 |
| 1 | 1A | 2114 | A | 2.4 |
| 1 | 1A | 614(B) | G | 2.4 |
| 2 | 2B | 118 | G | 2.4 |
| 32 | 2a | 947 | G | 2.4 |
| 32 | 2a | 1048 | G | 2.4 |
| 32 | 2a | 1057 | G | 2.4 |
| 32 | 2a | 1283 | G | 2.4 |
| 33 | 1b | 125 | PRO | 2.4 |
| 38 | 2g | 112 | PRO | 2.4 |
| 1 | 1A | 1076 | C | 2.4 |
| 1 | 1A | 2146 | C | 2.4 |
| 2 | 2B | 88 | C | 2.4 |
| 27 | 15 | 60 | VAL | 2.4 |
| 32 | 1a | 1028 | C | 2.4 |
| 32 | 2a | 980 | C | 2.4 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 32 | 2a | 1069 | C | 2.4 |
| 33 | 1b | 165 | VAL | 2.4 |
| 34 | 2c | 141 | VAL | 2.4 |
| 35 | 1d | 20 | TYR | 2.4 |
| 44 | 2m | 117 | VAL | 2.4 |
| 54 | 2y | 48 | C | 2.4 |
| 1 | 2A | 2167 | U | 2.4 |
| 53 | 2v | 17 | U | 2.4 |
| 21 | 2Z | 131 | ARG | 2.4 |
| 38 | 2g | 4 | ARG | 2.4 |
| 41 | 2j | 46 | ARG | 2.4 |
| 45 | 2n | 31 | ARG | 2.4 |
| 21 | 2Z | 137 | ILE | 2.4 |
| 34 | 2c | 191 | THR | 2.4 |
| 40 | 2i | 79 | LEU | 2.4 |
| 7 | 2H | 56 | SER | 2.4 |
| 21 | 2Z | 168 | GLU | 2.4 |
| 26 | 24 | 51 | ASP | 2.4 |
| 41 | 2j | 64 | GLU | 2.4 |
| 41 | 2j | 73 | ASP | 2.4 |
| 45 | 2n | 8 | GLU | 2.4 |
| 1 | 2A | 2114 | A | 2.4 |
| 32 | 1a | 1503 | A | 2.4 |
| 32 | 2a | 1280 | A | 2.4 |
| 33 | 2b | 234 | PRO | 2.4 |
| 34 | 2c | 148 | GLY | 2.4 |
| 43 | 1l | 63 | GLY | 2.4 |
| 50 | 2s | 8 | GLY | 2.4 |
| 6 | 2G | 15 | VAL | 2.4 |
| 46 | 2o | 60 | VAL | 2.4 |
| 1 | 1A | 1063 | G | 2.4 |
| 1 | 2A | 2127 | G | 2.4 |
| 6 | 1G | 80 | PHE | 2.4 |
| 14 | 2S | 7 | TYR | 2.4 |
| 14 | 2S | 66 | ALA | 2.4 |
| 32 | 2a | 1127 | G | 2.4 |
| 38 | 2g | 149 | ARG | 2.4 |
| 47 | 1p | 81 | ARG | 2.4 |
| 28 | 26 | 11 | LEU | 2.4 |
| 38 | 2g | 12 | LEU | 2.4 |
| 50 | 2s | 48 | THR | 2.4 |
| 1 | 2A | 277 | C | 2.4 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 6 | 1G | 48 | GLU | 2.4 |
| 14 | 2S | 8 | GLU | 2.4 |
| 23 | 11 | 75 | GLU | 2.4 |
| 33 | 2b | 231 | GLU | 2.4 |
| 36 | 2e | 81 | GLU | 2.4 |
| 42 | 1k | 92 | GLU | 2.4 |
| 44 | 2m | 73 | GLU | 2.4 |
| 34 | 1c | 45 | LYS | 2.4 |
| 44 | 2m | 120 | LYS | 2.4 |
| 50 | 2s | 28 | LYS | 2.4 |
| 46 | 2o | 89 | GLY | 2.4 |
| 3 | 2D | 217 | ARG | 2.4 |
| 7 | 2H | 76 | VAL | 2.4 |
| 16 | 2U | 105 | VAL | 2.4 |
| 19 | 2X | 68 | ARG | 2.4 |
| 24 | 22 | 7 | ARG | 2.4 |
| 40 | 1i | 66 | ARG | 2.4 |
| 41 | 1j | 43 | ARG | 2.4 |
| 1 | 1A | 878 | A | 2.4 |
| 32 | 2a | 969 | A | 2.4 |
| 32 | 2a | 1044 | A | 2.4 |
| 47 | 1p | 7 | ALA | 2.4 |
| 47 | 1p | 80 | PHE | 2.4 |
| 6 | 2G | 34 | LEU | 2.3 |
| 21 | 2Z | 9 | TYR | 2.3 |
| 27 | 25 | 58 | LEU | 2.3 |
| 40 | 2i | 92 | TYR | 2.3 |
| 44 | 1m | 87 | TYR | 2.3 |
| 51 | 1t | 13 | LEU | 2.3 |
| 33 | 2b | 39 | ILE | 2.3 |
| 42 | 2k | 32 | ILE | 2.3 |
| 50 | 2s | 62 | ILE | 2.3 |
| 1 | 2A | 882 | G | 2.3 |
| 1 | 2A | 2109 | U | 2.3 |
| 1 | 2A | 2802 | G | 2.3 |
| 32 | 2a | 1030(C) | G | 2.3 |
| 54 | 2w | 5 | G | 2.3 |
| 16 | 2U | 89 | GLU | 2.3 |
| 1 | 1A | 898 | C | 2.3 |
| 1 | 2A | 2143 | C | 2.3 |
| 1 | 2A | 2896 | C | 2.3 |
| 3 | 1D | 275 | LYS | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 17 | 2V | 85 | LYS | 2.3 |
| 52 | 2u | 20 | LYS | 2.3 |
| 28 | 26 | 42 | TRP | 2.3 |
| 38 | 2g | 156 | TRP | 2.3 |
| 40 | 1i | 90 | PRO | 2.3 |
| 50 | 2s | 59 | PRO | 2.3 |
| 4 | 2E | 6 | GLY | 2.3 |
| 40 | 2i | 72 | GLY | 2.3 |
| 40 | 2i | 66 | ARG | 2.3 |
| 45 | 2n | 26 | ARG | 2.3 |
| 52 | 2u | 24 | ARG | 2.3 |
| 43 | 1l | 18 | VAL | 2.3 |
| 48 | 1q | 23 | VAL | 2.3 |
| 49 | 1r | 86 | VAL | 2.3 |
| 21 | 1Z | 150 | LEU | 2.3 |
| 33 | 1b | 29 | ALA | 2.3 |
| 33 | 2b | 17 | PHE | 2.3 |
| 34 | 2c | 50 | ALA | 2.3 |
| 34 | 2c | 178 | LEU | 2.3 |
| 33 | 1b | 201 | ILE | 2.3 |
| 35 | 1d | 158 | ILE | 2.3 |
| 37 | 2f | 52 | ILE | 2.3 |
| 51 | 2t | 63 | ILE | 2.3 |
| 19 | 2X | 18 | TYR | 2.3 |
| 34 | 2c | 23 | TYR | 2.3 |
| 35 | 1d | 4 | TYR | 2.3 |
| 42 | 2k | 75 | TYR | 2.3 |
| 1 | 2A | 2126 | A | 2.3 |
| 14 | 2S | 5 | THR | 2.3 |
| 32 | 2a | 1531 | A | 2.3 |
| 40 | 2i | 103 | THR | 2.3 |
| 21 | 2Z | 28 | MET | 2.3 |
| 34 | 2c | 19 | GLU | 2.3 |
| 34 | 2c | 161 | GLU | 2.3 |
| 37 | 2f | 95 | GLU | 2.3 |
| 39 | 2h | 9 | MET | 2.3 |
| 7 | 2H | 62 | LYS | 2.3 |
| 32 | 2a | 1000 | U | 2.3 |
| 41 | 2j | 58 | ASP | 2.3 |
| 1 | 2A | 1537 | G | 2.3 |
| 1 | 2A | 2147 | G | 2.3 |
| 1 | 2A | 2148 | G | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | 2A | 2168 | G | 2.3 |
| 7 | 2H | 10 | PRO | 2.3 |
| 32 | 2a | 976 | G | 2.3 |
| 32 | 2a | 1309 | G | 2.3 |
| 39 | 2h | 67 | PRO | 2.3 |
| 1 | 1A | 2128 | C | 2.3 |
| 1 | 1A | 2143 | C | 2.3 |
| 1 | 2A | 2297 | C | 2.3 |
| 30 | 28 | 46 | ARG | 2.3 |
| 32 | 1a | 1038 | C | 2.3 |
| 41 | 2j | 84 | GLN | 2.3 |
| 44 | 2m | 29 | ARG | 2.3 |
| 44 | 2m | 91 | ARG | 2.3 |
| 14 | 2S | 65 | VAL | 2.3 |
| 40 | 2i | 65 | VAL | 2.3 |
| 43 | 2l | 39 | VAL | 2.3 |
| 4 | 2E | 28 | ALA | 2.3 |
| 6 | 1G | 50 | ALA | 2.3 |
| 7 | 2H | 33 | LEU | 2.3 |
| 23 | 21 | 46 | LEU | 2.3 |
| 40 | 2i | 59 | PHE | 2.3 |
| 42 | 2k | 19 | ALA | 2.3 |
| 50 | 1s | 71 | LEU | 2.3 |
| 34 | 1c | 84 | ILE | 2.3 |
| 41 | 1j | 75 | ILE | 2.3 |
| 6 | 1G | 146 | TYR | 2.3 |
| 21 | 2Z | 69 | THR | 2.3 |
| 22 | 20 | 26 | TYR | 2.3 |
| 34 | 2c | 193 | TYR | 2.3 |
| 39 | 2h | 24 | THR | 2.3 |
| 40 | 2i | 27 | THR | 2.3 |
| 50 | 2s | 77 | THR | 2.3 |
| 12 | 2Q | 103 | MET | 2.3 |
| 33 | 1b | 126 | GLU | 2.3 |
| 41 | 2j | 7 | LYS | 2.3 |
| 51 | 2t | 27 | LYS | 2.3 |
| 1 | 1A | 1096 | A | 2.3 |
| 32 | 2a | 120 | A | 2.3 |
| 32 | 2a | 1398 | A | 2.3 |
| 54 | 2w | 36 | A | 2.3 |
| 54 | 2y | 36 | A | 2.3 |
| 41 | 1j | 30 | SER | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 34 | 1c | 38 | ARG | 2.3 |
| 38 | 1g | 156 | TRP | 2.3 |
| 38 | 2g | 78 | ARG | 2.3 |
| 40 | 1i | 9 | ARG | 2.3 |
| 40 | 2i | 83 | ARG | 2.3 |
| 44 | 2m | 113 | PRO | 2.3 |
| 52 | 2u | 6 | ARG | 2.3 |
| 12 | 2Q | 24 | GLY | 2.3 |
| 34 | 2c | 37 | GLN | 2.3 |
| 34 | 2c | 78 | GLY | 2.3 |
| 41 | 1j | 31 | GLY | 2.3 |
| 44 | 2m | 68 | GLY | 2.3 |
| 50 | 2s | 72 | GLY | 2.3 |
| 1 | 1A | 895 | U | 2.3 |
| 1 | 1A | 2109 | U | 2.3 |
| 7 | 2H | 50 | VAL | 2.3 |
| 21 | 2Z | 90 | VAL | 2.3 |
| 34 | 2c | 116 | VAL | 2.3 |
| 35 | 1d | 170 | VAL | 2.3 |
| 6 | 2G | 102 | PHE | 2.3 |
| 39 | 1h | 2 | LEU | 2.3 |
| 39 | 2h | 2 | LEU | 2.3 |
| 40 | 2i | 101 | PHE | 2.3 |
| 1 | 1A | 1071 | G | 2.3 |
| 1 | 1A | 2100 | G | 2.3 |
| 1 | 2A | 2108 | C | 2.3 |
| 1 | 2A | 2115 | G | 2.3 |
| 1 | 2A | 2116 | G | 2.3 |
| 6 | 2G | 39 | ILE | 2.3 |
| 36 | 2e | 21 | ALA | 2.3 |
| 36 | 2e | 54 | ALA | 2.3 |
| 40 | 2i | 61 | ALA | 2.3 |
| 18 | 1W | 111 | HIS | 2.3 |
| 32 | 2a | 926 | G | 2.3 |
| 32 | 2a | 1115 | C | 2.3 |
| 54 | 2w | 24 | G | 2.3 |
| 54 | 2y | 25 | C | 2.3 |
| 29 | 27 | 48 | LYS | 2.3 |
| 35 | 2d | 184 | LYS | 2.3 |
| 6 | 2G | 11 | TYR | 2.3 |
| 8 | 2I | 48 | GLU | 2.3 |
| 51 | 1t | 75 | ASN | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 21 | 2Z | 31 | ARG | 2.3 |
| 34 | 2c | 131 | ARG | 2.3 |
| 40 | 2i | 42 | ARG | 2.3 |
| 41 | 2j | 5 | ARG | 2.3 |
| 41 | 2j | 19 | SER | 2.3 |
| 50 | 2s | 81 | ARG | 2.3 |
| 52 | 2u | 15 | ARG | 2.3 |
| 1 | 1A | 896 | A | 2.3 |
| 1 | 1A | 1847 | A | 2.3 |
| 5 | 1F | 208 | GLY | 2.3 |
| 22 | 20 | 13 | GLY | 2.3 |
| 32 | 1a | 134 | A | 2.3 |
| 34 | 2c | 155 | GLY | 2.3 |
| 35 | 2d | 130 | GLY | 2.3 |
| 7 | 2H | 17 | VAL | 2.3 |
| 8 | 2I | 123 | LEU | 2.3 |
| 11 | 2P | 105 | LEU | 2.3 |
| 21 | 2Z | 105 | VAL | 2.3 |
| 34 | 2c | 32 | LEU | 2.3 |
| 35 | 1d | 105 | VAL | 2.3 |
| 39 | 2h | 61 | VAL | 2.3 |
| 48 | 1q | 35 | VAL | 2.3 |
| 21 | 1Z | 136 | PHE | 2.3 |
| 1 | 2A | 362 | U | 2.2 |
| 1 | 2A | 614(A) | U | 2.2 |
| 1 | 2A | 1026 | U | 2.2 |
| 22 | 10 | 2 | ALA | 2.2 |
| 33 | 1b | 172 | ILE | 2.2 |
| 33 | 2b | 162 | ILE | 2.2 |
| 35 | 2d | 32 | ALA | 2.2 |
| 41 | 1j | 38 | ILE | 2.2 |
| 44 | 1m | 4 | ILE | 2.2 |
| 45 | 2n | 24 | CYS | 2.2 |
| 50 | 2s | 75 | ALA | 2.2 |
| 51 | 2t | 97 | ALA | 2.2 |
| 50 | 1s | 14 | HIS | 2.2 |
| 36 | 2e | 10 | MET | 2.2 |
| 45 | 2n | 58 | LYS | 2.2 |
| 38 | 2g | 24 | THR | 2.2 |
| 41 | 2j | 48 | THR | 2.2 |
| 12 | 1Q | 80 | GLU | 2.2 |
| 36 | 2e | 60 | TYR | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | 2A | 2137 | C | 2.2 |
| 32 | 2a | 970 | C | 2.2 |
| 32 | 2a | 1039 | C | 2.2 |
| 32 | 2a | 1336 | C | 2.2 |
| 1 | 1A | 2131 | G | 2.2 |
| 1 | 2A | 2100 | G | 2.2 |
| 2 | 2B | 23 | G | 2.2 |
| 32 | 2a | 587 | G | 2.2 |
| 32 | 2a | 823 | G | 2.2 |
| 32 | 2a | 987 | G | 2.2 |
| 32 | 2a | 1365 | G | 2.2 |
| 54 | 1w | 24 | G | 2.2 |
| 6 | 2G | 51 | ARG | 2.2 |
| 14 | 2S | 97 | ARG | 2.2 |
| 33 | 2b | 21 | ARG | 2.2 |
| 40 | 2i | 111 | ARG | 2.2 |
| 46 | 1o | 65 | ARG | 2.2 |
| 26 | 24 | 29 | PRO | 2.2 |
| 41 | 2j | 21 | GLN | 2.2 |
| 21 | 2Z | 147 | GLY | 2.2 |
| 33 | 2b | 18 | GLY | 2.2 |
| 50 | 2s | 46 | GLY | 2.2 |
| 31 | 29 | 25 | VAL | 2.2 |
| 33 | 1b | 215 | LEU | 2.2 |
| 33 | 2b | 158 | LEU | 2.2 |
| 35 | 2d | 148 | VAL | 2.2 |
| 1 | 1A | 1070 | A | 2.2 |
| 1 | 2A | 2158 | A | 2.2 |
| 14 | 2S | 93 | LYS | 2.2 |
| 32 | 2a | 946 | A | 2.2 |
| 34 | 2c | 163 | ALA | 2.2 |
| 40 | 2i | 119 | ALA | 2.2 |
| 44 | 2m | 28 | ALA | 2.2 |
| 53 | 2v | 15 | A | 2.2 |
| 54 | 2w | 73 | A | 2.2 |
| 42 | 2k | 119 | CYS | 2.2 |
| 21 | 1Z | 119 | GLU | 2.2 |
| 32 | 2a | 1281 | U | 2.2 |
| 9 | 2N | 115 | ARG | 2.2 |
| 37 | 2f | 46 | ARG | 2.2 |
| 40 | 2i | 120 | ARG | 2.2 |
| 46 | 2o | 88 | ARG | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 47 | 1p | 75 | ARG | 2.2 |
| 49 | 1r | 87 | ARG | 2.2 |
| 33 | 1b | 234 | PRO | 2.2 |
| 40 | 2i | 21 | PRO | 2.2 |
| 1 | 1A | 2174 | C | 2.2 |
| 1 | 2A | 2136 | C | 2.2 |
| 2 | 2B | 5 | C | 2.2 |
| 32 | 1a | 1008 | C | 2.2 |
| 32 | 2a | 877 | C | 2.2 |
| 32 | 2a | 1029 | C | 2.2 |
| 54 | 1w | 75 | C | 2.2 |
| 31 | 29 | 12 | ASP | 2.2 |
| 40 | 2i | 67 | GLY | 2.2 |
| 40 | 2i | 69 | GLY | 2.2 |
| 50 | 2s | 12 | ASP | 2.2 |
| 1 | 1A | 275 | G | 2.2 |
| 1 | 2A | 1171 | G | 2.2 |
| 8 | 2I | 68 | LEU | 2.2 |
| 20 | 2Y | 31 | LEU | 2.2 |
| 32 | 1a | 230 | G | 2.2 |
| 32 | 2a | 945 | G | 2.2 |
| 6 | 2G | 29 | TRP | 2.2 |
| 14 | 2S | 11 | LYS | 2.2 |
| 14 | 2S | 33 | LYS | 2.2 |
| 14 | 2S | 59 | LYS | 2.2 |
| 23 | 21 | 69 | LYS | 2.2 |
| 34 | 2c | 173 | VAL | 2.2 |
| 36 | 2e | 115 | VAL | 2.2 |
| 38 | 2g | 141 | VAL | 2.2 |
| 43 | 2l | 40 | VAL | 2.2 |
| 44 | 2m | 53 | VAL | 2.2 |
| 6 | 1G | 52 | ILE | 2.2 |
| 15 | 2T | 1 | MET | 2.2 |
| 34 | 1c | 14 | ILE | 2.2 |
| 43 | 2l | 100 | ILE | 2.2 |
| 34 | 2c | 121 | ALA | 2.2 |
| 36 | 2e | 86 | ALA | 2.2 |
| 38 | 1g | 83 | ALA | 2.2 |
| 40 | 2i | 45 | ALA | 2.2 |
| 40 | 2i | 122 | ALA | 2.2 |
| 41 | 2j | 20 | ALA | 2.2 |
| 1 | 1A | 1067 | A | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | 1A | 1077 | A | 2.2 |
| 2 | 2B | 25 | A | 2.2 |
| 8 | 2I | 86 | THR | 2.2 |
| 26 | 24 | 52 | THR | 2.2 |
| 32 | 1a | 101 | A | 2.2 |
| 32 | 1a | 160 | A | 2.2 |
| 32 | 2a | 975 | A | 2.2 |
| 32 | 2a | 1250 | A | 2.2 |
| 34 | 1c | 15 | THR | 2.2 |
| 41 | 2j | 97 | GLU | 2.2 |
| 54 | 2w | 23 | A | 2.2 |
| 54 | 2y | 23 | A | 2.2 |
| 6 | 2G | 33 | ARG | 2.2 |
| 14 | 2S | 13 | ARG | 2.2 |
| 32 | 2a | 952 | U | 2.2 |
| 32 | 2a | 957 | U | 2.2 |
| 32 | 2a | 961 | U | 2.2 |
| 32 | 2a | 1049 | U | 2.2 |
| 37 | 2f | 87 | ARG | 2.2 |
| 48 | 1q | 92 | ARG | 2.2 |
| 54 | 1w | 20 | U | 2.2 |
| 37 | 2f | 7 | ASN | 2.2 |
| 38 | 2g | 37 | ASN | 2.2 |
| 7 | 2H | 36 | PRO | 2.2 |
| 34 | 2c | 7 | PRO | 2.2 |
| 48 | 1q | 28 | PRO | 2.2 |
| 48 | 2q | 47 | PRO | 2.2 |
| 6 | 2G | 41 | GLN | 2.2 |
| 35 | 2d | 45 | GLN | 2.2 |
| 46 | 2o | 62 | GLN | 2.2 |
| 22 | 20 | 37 | LEU | 2.2 |
| 24 | 22 | 60 | LEU | 2.2 |
| 33 | 1b | 44 | LEU | 2.2 |
| 33 | 2b | 98 | LEU | 2.2 |
| 35 | 1d | 120 | LEU | 2.2 |
| 35 | 1d | 188 | LEU | 2.2 |
| 43 | 1l | 60 | LEU | 2.2 |
| 50 | 2s | 20 | LEU | 2.2 |
| 51 | 2t | 10 | LEU | 2.2 |
| 51 | 2t | 64 | ASP | 2.2 |
| 26 | 24 | 35 | VAL | 2.2 |
| 33 | 2b | 15 | VAL | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 34 | 2c | 151 | VAL | 2.2 |
| 40 | 2i | 86 | VAL | 2.2 |
| 1 | 2A | 2294 | C | 2.2 |
| 22 | 20 | 45 | PHE | 2.2 |
| 32 | 2a | 1018 | C | 2.2 |
| 32 | 2a | 1189 | C | 2.2 |
| 32 | 2a | 1209 | C | 2.2 |
| 43 | 1l | 7 | ILE | 2.2 |
| 45 | 2n | 36 | PHE | 2.2 |
| 20 | 2Y | 16 | ALA | 2.2 |
| 33 | 2b | 207 | ALA | 2.2 |
| 1 | 2A | 2123 | G | 2.2 |
| 1 | 2A | 2182 | G | 2.2 |
| 30 | 18 | 65 | GLU | 2.2 |
| 32 | 1a | 1033 | G | 2.2 |
| 7 | 2H | 106 | THR | 2.2 |
| 41 | 2j | 92 | THR | 2.2 |
| 24 | 22 | 51 | ARG | 2.2 |
| 39 | 2h | 92 | ARG | 2.2 |
| 40 | 1i | 10 | ARG | 2.2 |
| 1 | 1A | 1045 | A | 2.2 |
| 1 | 1A | 1073 | A | 2.2 |
| 1 | 1A | 1088 | A | 2.2 |
| 1 | 2A | 2176 | A | 2.2 |
| 2 | 2B | 26 | A | 2.2 |
| 21 | 2Z | 34 | ASN | 2.2 |
| 32 | 2a | 1229 | A | 2.2 |
| 38 | 2g | 88 | PRO | 2.2 |
| 39 | 2h | 15 | ASN | 2.2 |
| 39 | 2h | 72 | PRO | 2.2 |
| 44 | 2m | 23 | TYR | 2.2 |
| 54 | 2w | 14 | A | 2.2 |
| 54 | 2w | 35 | A | 2.2 |
| 1 | 2A | 2172 | U | 2.2 |
| 6 | 2G | 74 | LYS | 2.2 |
| 4 | 2E | 10 | GLY | 2.2 |
| 7 | 2H | 103 | LEU | 2.2 |
| 34 | 2c | 197 | GLY | 2.2 |
| 35 | 2d | 196 | LEU | 2.2 |
| 38 | 1g | 81 | GLY | 2.2 |
| 40 | 2i | 57 | GLY | 2.2 |
| 41 | 1j | 8 | LEU | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 48 | 1q | 33 | GLY | 2.2 |
| 48 | 1q | 74 | LEU | 2.2 |
| 50 | 1s | 20 | LEU | 2.2 |
| 37 | 2f | 89 | MET | 2.2 |
| 7 | 2H | 35 | VAL | 2.2 |
| 7 | 2H | 38 | SER | 2.2 |
| 8 | 2I | 109 | ILE | 2.2 |
| 33 | 2b | 81 | VAL | 2.2 |
| 35 | 1d | 83 | SER | 2.2 |
| 34 | 2c | 14 | ILE | 2.2 |
| 36 | 2e | 69 | VAL | 2.2 |
| 40 | 1i | 117 | HIS | 2.2 |
| 43 | 2l | 55 | VAL | 2.2 |
| 21 | 2Z | 89 | PHE | 2.2 |
| 34 | 2c | 10 | PHE | 2.2 |
| 7 | 2H | 102 | ALA | 2.1 |
| 44 | 2m | 76 | ALA | 2.1 |
| 1 | 1A | 1079 | C | 2.1 |
| 1 | 2A | 888 | C | 2.1 |
| 1 | 2A | 2139 | C | 2.1 |
| 7 | 2H | 101 | ARG | 2.1 |
| 20 | 1Y | 50 | ARG | 2.1 |
| 26 | 24 | 68 | ARG | 2.1 |
| 29 | 27 | 23 | ARG | 2.1 |
| 32 | 1a | 163 | C | 2.1 |
| 32 | 1a | 1029 | C | 2.1 |
| 32 | 1a | 1030 | C | 2.1 |
| 41 | 2j | 60 | ARG | 2.1 |
| 42 | 2k | 31 | THR | 2.1 |
| 1 | 1A | 1056 | G | 2.1 |
| 1 | 1A | 2168 | G | 2.1 |
| 1 | 2A | 2153 | G | 2.1 |
| 25 | 23 | 2 | PRO | 2.1 |
| 32 | 1a | 1032 | G | 2.1 |
| 32 | 2a | 630 | G | 2.1 |
| 54 | 1w | 15 | G | 2.1 |
| 54 | 2w | 65 | G | 2.1 |
| 16 | 2U | 84 | LYS | 2.1 |
| 34 | 2c | 135 | LYS | 2.1 |
| 34 | 2c | 201 | TYR | 2.1 |
| 40 | 1i | 78 | LYS | 2.1 |
| 7 | 2H | 88 | LEU | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 9 | 2N | 112 | LEU | 2.1 |
| 37 | 1f | 19 | LEU | 2.1 |
| 49 | 1r | 79 | LEU | 2.1 |
| 7 | 2H | 5 | GLY | 2.1 |
| 32 | 2a | 964 | A | 2.1 |
| 32 | 2a | 1004 | A | 2.1 |
| 34 | 2c | 205 | GLY | 2.1 |
| 40 | 1i | 39 | GLY | 2.1 |
| 54 | 1w | 7 | A | 2.1 |
| 1 | 1A | 2172 | U | 2.1 |
| 7 | 2H | 79 | VAL | 2.1 |
| 24 | 22 | 52 | ASP | 2.1 |
| 26 | 14 | 51 | ASP | 2.1 |
| 18 | 2W | 13 | SER | 2.1 |
| 33 | 2b | 42 | ILE | 2.1 |
| 33 | 2b | 136 | VAL | 2.1 |
| 33 | 2b | 172 | ILE | 2.1 |
| 34 | 1c | 66 | VAL | 2.1 |
| 45 | 2n | 32 | SER | 2.1 |
| 46 | 2o | 27 | VAL | 2.1 |
| 53 | 2v | 22 | U | 2.1 |
| 34 | 2c | 100 | ALA | 2.1 |
| 45 | 2n | 30 | ALA | 2.1 |
| 46 | 2o | 14 | GLU | 2.1 |
| 50 | 1s | 27 | GLU | 2.1 |
| 5 | 1F | 17 | ARG | 2.1 |
| 7 | 2H | 6 | ARG | 2.1 |
| 12 | 2Q | 6 | ARG | 2.1 |
| 35 | 2d | 122 | ARG | 2.1 |
| 43 | 1l | 19 | ARG | 2.1 |
| 44 | 1m | 102 | ARG | 2.1 |
| 45 | 1n | 29 | ARG | 2.1 |
| 46 | 2o | 54 | ARG | 2.1 |
| 8 | 2I | 134 | PRO | 2.1 |
| 33 | 1b | 132 | LYS | 2.1 |
| 33 | 2b | 167 | PRO | 2.1 |
| 39 | 2h | 89 | PRO | 2.1 |
| 43 | 2l | 47 | LYS | 2.1 |
| 1 | 1A | 1052 | C | 2.1 |
| 1 | 1A | 2136 | C | 2.1 |
| 1 | 1A | 2140 | C | 2.1 |
| 32 | 2a | 1109 | C | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 32 | 2a | 1277 | C | 2.1 |
| 32 | 2a | 1314 | C | 2.1 |
| 42 | 2k | 13 | GLN | 2.1 |
| 33 | 1b | 187 | LEU | 2.1 |
| 33 | 2b | 101 | MET | 2.1 |
| 33 | 2b | 154 | LEU | 2.1 |
| 35 | 1d | 19 | LEU | 2.1 |
| 40 | 2i | 50 | LEU | 2.1 |
| 42 | 2k | 117 | ASN | 2.1 |
| 48 | 1q | 51 | TYR | 2.1 |
| 48 | 1q | 98 | LEU | 2.1 |
| 43 | 2l | 103 | GLY | 2.1 |
| 52 | 2u | 4 | GLY | 2.1 |
| 41 | 2j | 62 | HIS | 2.1 |
| 1 | 2A | 859 | G | 2.1 |
| 14 | 2S | 14 | VAL | 2.1 |
| 32 | 1a | 112 | G | 2.1 |
| 32 | 2a | 1184 | G | 2.1 |
| 32 | 2a | 1491 | G | 2.1 |
| 36 | 2e | 90 | VAL | 2.1 |
| 40 | 1i | 75 | ASP | 2.1 |
| 40 | 1i | 91 | ASP | 2.1 |
| 48 | 1q | 9 | VAL | 2.1 |
| 37 | 2f | 93 | SER | 2.1 |
| 1 | 2A | 528 | A | 2.1 |
| 1 | 2A | 2122 | U | 2.1 |
| 32 | 1a | 374 | A | 2.1 |
| 32 | 1a | 608 | A | 2.1 |
| 32 | 2a | 414 | A | 2.1 |
| 7 | 2H | 34 | GLU | 2.1 |
| 32 | 2a | 982 | U | 2.1 |
| 36 | 1e | 134 | ALA | 2.1 |
| 40 | 2i | 84 | ALA | 2.1 |
| 43 | 2l | 51 | ALA | 2.1 |
| 46 | 2o | 80 | ALA | 2.1 |
| 54 | 2y | 35 | A | 2.1 |
| 50 | 2s | 73 | GLU | 2.1 |
| 35 | 1d | 118 | ARG | 2.1 |
| 38 | 2g | 79 | ARG | 2.1 |
| 51 | 2t | 25 | ARG | 2.1 |
| 21 | 1Z | 156 | LYS | 2.1 |
| 50 | 2s | 18 | LYS | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 7 | 2H | 173 | PRO | 2.1 |
| 21 | 2Z | 25 | PRO | 2.1 |
| 25 | 13 | 2 | PRO | 2.1 |
| 40 | 2i | 3 | GLN | 2.1 |
| 34 | 2c | 34 | LEU | 2.1 |
| 37 | 2f | 98 | LEU | 2.1 |
| 39 | 2h | 39 | LEU | 2.1 |
| 47 | 2p | 6 | LEU | 2.1 |
| 48 | 2q | 76 | LEU | 2.1 |
| 8 | 1I | 106 | GLY | 2.1 |
| 19 | 1X | 94 | GLY | 2.1 |
| 19 | 2X | 69 | TYR | 2.1 |
| 21 | 2Z | 99 | TYR | 2.1 |
| 33 | 1b | 16 | HIS | 2.1 |
| 34 | 1c | 185 | GLY | 2.1 |
| 40 | 2i | 88 | TYR | 2.1 |
| 41 | 1j | 36 | GLY | 2.1 |
| 42 | 2k | 86 | GLY | 2.1 |
| 1 | 1A | 897 | C | 2.1 |
| 1 | 1A | 1075 | C | 2.1 |
| 1 | 2A | 897 | C | 2.1 |
| 1 | 2A | 2138 | C | 2.1 |
| 7 | 1H | 92 | ILE | 2.1 |
| 32 | 2a | 931 | C | 2.1 |
| 34 | 1c | 55 | VAL | 2.1 |
| 40 | 2i | 109 | VAL | 2.1 |
| 41 | 2j | 24 | VAL | 2.1 |
| 48 | 2q | 90 | ILE | 2.1 |
| 54 | 2w | 11 | C | 2.1 |
| 38 | 1g | 26 | PHE | 2.1 |
| 40 | 1i | 105 | ASP | 2.1 |
| 14 | 2S | 55 | ALA | 2.1 |
| 21 | 2Z | 103 | ARG | 2.1 |
| 24 | 22 | 66 | GLU | 2.1 |
| 29 | 27 | 47 | ARG | 2.1 |
| 33 | 1b | 9 | GLU | 2.1 |
| 33 | 2b | 34 | ALA | 2.1 |
| 33 | 2b | 129 | GLU | 2.1 |
| 36 | 1e | 81 | GLU | 2.1 |
| 36 | 2e | 27 | ARG | 2.1 |
| 40 | 2i | 55 | ALA | 2.1 |
| 45 | 1n | 5 | ALA | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 2 | 2B | 75 | G | 2.1 |
| 32 | 1a | 111 | G | 2.1 |
| 32 | 2a | 1305 | G | 2.1 |
| 42 | 2k | 42 | TRP | 2.1 |
| 37 | 2f | 54 | LYS | 2.1 |
| 40 | 1i | 113 | LYS | 2.1 |
| 43 | 1l | 46 | LYS | 2.1 |
| 43 | 1l | 126 | LYS | 2.1 |
| 48 | 1q | 14 | LYS | 2.1 |
| 54 | 2w | 28 | G | 2.1 |
| 1 | 2A | 271(L) | U | 2.1 |
| 32 | 1a | 149 | A | 2.1 |
| 32 | 2a | 997 | U | 2.1 |
| 32 | 2a | 1015 | A | 2.1 |
| 32 | 2a | 1252 | A | 2.1 |
| 36 | 2e | 16 | THR | 2.1 |
| 54 | 2y | 47 | U | 2.1 |
| 33 | 2b | 83 | MET | 2.1 |
| 9 | 2N | 69 | GLN | 2.1 |
| 34 | 2c | 118 | GLN | 2.1 |
| 34 | 2c | 162 | GLN | 2.1 |
| 8 | 2I | 35 | LEU | 2.1 |
| 14 | 2S | 80 | LEU | 2.1 |
| 34 | 1c | 52 | LEU | 2.1 |
| 46 | 2o | 31 | LEU | 2.1 |
| 4 | 2E | 121 | ASN | 2.1 |
| 47 | 1p | 14 | ASN | 2.1 |
| 14 | 2S | 90 | GLY | 2.1 |
| 14 | 2S | 36 | TYR | 2.1 |
| 33 | 2b | 33 | TYR | 2.1 |
| 37 | 2f | 63 | TYR | 2.1 |
| 40 | 2i | 63 | ILE | 2.1 |
| 41 | 1j | 4 | ILE | 2.1 |
| 47 | 1p | 38 | TYR | 2.1 |
| 48 | 1q | 95 | TYR | 2.1 |
| 21 | 2Z | 56 | VAL | 2.1 |
| 34 | 1c | 99 | VAL | 2.1 |
| 45 | 2n | 18 | VAL | 2.1 |
| 6 | 2G | 23 | PHE | 2.1 |
| 6 | 1G | 59 | GLU | 2.0 |
| 7 | 1H | 3 | ARG | 2.0 |
| 38 | 2g | 5 | ARG | 2.0 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 40 | 1i | 42 | ARG | 2.0 |
| 42 | 2k | 36 | ASP | 2.0 |
| 44 | 2m | 94 | ARG | 2.0 |
| 50 | 2s | 29 | ARG | 2.0 |
| 21 | 2Z | 142 | SER | 2.0 |
| 34 | 2c | 92 | ALA | 2.0 |
| 38 | 2g | 2 | ALA | 2.0 |
| 45 | 2n | 20 | ALA | 2.0 |
| 1 | 1A | 2142 | C | 2.0 |
| 1 | 2A | 2803 | C | 2.0 |
| 32 | 2a | 1037 | C | 2.0 |
| 32 | 2a | 1362 | C | 2.0 |
| 33 | 2b | 22 | LYS | 2.0 |
| 45 | 2n | 11 | LYS | 2.0 |
| 54 | 2w | 67 | C | 2.0 |
| 47 | 1p | 69 | THR | 2.0 |
| 39 | 1h | 72 | PRO | 2.0 |
| 1 | 1A | 2189 | U | 2.0 |
| 6 | 2G | 53 | LEU | 2.0 |
| 14 | 2S | 101 | LEU | 2.0 |
| 21 | 2Z | 76 | LEU | 2.0 |
| 32 | 2a | 1313 | U | 2.0 |
| 32 | 2a | 1358 | U | 2.0 |
| 33 | 1b | 154 | LEU | 2.0 |
| 33 | 2b | 44 | LEU | 2.0 |
| 34 | 1c | 107 | GLN | 2.0 |
| 34 | 2c | 175 | LEU | 2.0 |
| 35 | 1d | 101 | LEU | 2.0 |
| 35 | 2d | 155 | LEU | 2.0 |
| 47 | 1p | 49 | LEU | 2.0 |
| 50 | 2s | 30 | LEU | 2.0 |
| 1 | 1A | 1177 | A | 2.0 |
| 1 | 2A | 614(B) | G | 2.0 |
| 1 | 2A | 1125 | G | 2.0 |
| 1 | 2A | 2320 | A | 2.0 |
| 1 | 2A | 2805 | G | 2.0 |
| 32 | 1a | 1166 | G | 2.0 |
| 32 | 2a | 994 | A | 2.0 |
| 32 | 2a | 1356 | G | 2.0 |
| 20 | 2Y | 92 | ASN | 2.0 |
| 44 | 2m | 92 | HIS | 2.0 |
| 14 | 2S | 96 | GLY | 2.0 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 34 | 2c | 80 | GLY | 2.0 |
| 41 | 1j | 52 | GLY | 2.0 |
| 41 | 2j | 31 | GLY | 2.0 |
| 44 | 1m | 39 | ILE | 2.0 |
| 46 | 2o | 87 | ILE | 2.0 |
| 21 | 2Z | 27 | VAL | 2.0 |
| 26 | 24 | 32 | TYR | 2.0 |
| 33 | 2b | 93 | VAL | 2.0 |
| 36 | 2e | 82 | VAL | 2.0 |
| 44 | 2m | 87 | TYR | 2.0 |
| 12 | 2Q | 16 | ARG | 2.0 |
| 34 | 2c | 59 | ARG | 2.0 |
| 39 | 2h | 30 | ARG | 2.0 |
| 42 | 2k | 54 | ARG | 2.0 |
| 44 | 2m | 3 | ARG | 2.0 |
| 48 | 2q | 27 | PHE | 2.0 |
| 33 | 1b | 207 | ALA | 2.0 |
| 38 | 2g | 40 | ALA | 2.0 |
| 40 | 1i | 70 | LYS | 2.0 |
| 45 | 1n | 59 | ALA | 2.0 |
| 45 | 2n | 5 | ALA | 2.0 |
| 49 | 1r | 73 | ALA | 2.0 |
| 22 | 20 | 9 | SER | 2.0 |
| 33 | 2b | 48 | MET | 2.0 |
| 4 | 2E | 56 | PRO | 2.0 |
| 7 | 2H | 8 | PRO | 2.0 |
| 8 | 1I | 108 | THR | 2.0 |
| 9 | 2N | 48 | MET | 2.0 |
| 36 | 1e | 120 | THR | 2.0 |
| 41 | 1j | 86 | MET | 2.0 |
| 20 | 2Y | 53 | PRO | 2.0 |
| 33 | 1b | 232 | PRO | 2.0 |
| 41 | 1j | 39 | PRO | 2.0 |
| 41 | 2j | 53 | PRO | 2.0 |
| 41 | 2j | 67 | THR | 2.0 |
| 45 | 2n | 14 | PRO | 2.0 |
| 47 | 1p | 41 | PRO | 2.0 |
| 14 | 2S | 73 | LEU | 2.0 |
| 21 | 2Z | 155 | LEU | 2.0 |
| 32 | 2a | 1218 | C | 2.0 |
| 38 | 1g | 38 | LEU | 2.0 |
| 43 | 2l | 84 | LEU | 2.0 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 54 | 2w | 72 | C | 2.0 |
| 14 | 2S | 95 | HIS | 2.0 |
| 32 | 1a | 204 | U | 2.0 |
| 32 | 1a | 841 | U | 2.0 |
| 32 | 2a | 1257 | U | 2.0 |
| 5 | 2F | 16 | GLY | 2.0 |
| 12 | 2Q | 23 | GLY | 2.0 |
| 15 | 2T | 104 | ASN | 2.0 |
| 54 | 1w | 47 | U | 2.0 |
| 23 | 21 | 28 | GLY | 2.0 |
| 30 | 28 | 16 | ILE | 2.0 |
| 35 | 1d | 16 | GLY | 2.0 |
| 40 | 1i | 69 | GLY | 2.0 |
| 40 | 1i | 72 | GLY | 2.0 |
| 42 | 2k | 48 | ILE | 2.0 |
| 42 | 2k | 49 | GLY | 2.0 |
| 44 | 2m | 112 | GLY | 2.0 |
| 50 | 2s | 68 | GLY | 2.0 |
| 1 | 1A | 229 | A | 2.0 |
| 1 | 1A | 2170 | A | 2.0 |
| 1 | 2A | 901 | A | 2.0 |
| 7 | 2H | 49 | VAL | 2.0 |
| 14 | 2S | 28 | VAL | 2.0 |
| 28 | 26 | 5 | VAL | 2.0 |
| 35 | 1d | 139 | ARG | 2.0 |
| 43 | 2l | 11 | VAL | 2.0 |
| 55 | 1x | 76 | A | 2.0 |
| 4 | 2E | 151 | TYR | 2.0 |
| 7 | 2H | 157 | TYR | 2.0 |
| 48 | 1q | 88 | TYR | 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, $95^{th}$ percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 54 | 7MG | 2w | 46 | 24/25 | 0.51 | 0.16 | 80,93,101,121 | 0 |
| 54 | 7MG | 1w | 46 | 24/25 | 0.58 | 0.16 | 77,89,99,107 | 0 |
| 54 | 4SU | 2w | 8 | 20/21 | 0.60 | 0.15 | 83,93,104,117 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 54 | 7MG | 2y | 46 | 24/25 | 0.60 | 0.17 | 86,95,102,123 | 0 |
| 54 | PSU | 2w | 55 | 20/21 | 0.67 | 0.13 | 81,91,96,98 | 0 |
| 54 | PSU | 2y | 55 | 20/21 | 0.67 | 0.18 | 90,96,107,107 | 0 |
| 54 | 4SU | 2y | 8 | 20/21 | 0.69 | 0.13 | 88,93,99,104 | 0 |
| 54 | 7MG | 1y | 46 | 24/25 | 0.69 | 0.14 | 79,90,98,101 | 0 |
| 54 | MIA | 2y | 37 | 22/30 | 0.72 | 0.14 | 75,87,99,109 | 0 |
| 54 | 5MU | 2y | 54 | 21/22 | 0.72 | 0.15 | 84,91,99,112 | 0 |
| 54 | 5MU | 1y | 54 | 21/22 | 0.73 | 0.13 | 79,85,91,97 | 0 |
| 54 | PSU | 2y | 32 | 20/21 | 0.75 | 0.14 | 79,85,93,102 | 0 |
| 54 | 4SU | 1w | 8 | 20/21 | 0.75 | 0.14 | 80,85,93,94 | 0 |
| 54 | 4SU | 1y | 8 | 20/21 | 0.79 | 0.12 | 81,89,98,99 | 0 |
| 54 | PSU | 1y | 55 | 20/21 | 0.79 | 0.12 | 80,89,98,103 | 0 |
| 32 | 2MG | 2a | 1207 | 24/25 | 0.80 | 0.14 | 63,83,92,95 | 0 |
| 1 | 5MU | 2A | 1915 | 21/22 | 0.80 | 0.16 | 74,78,84,94 | 0 |
| 54 | PSU | 2w | 39 | 20/21 | 0.81 | 0.14 | 81,86,88,92 | 0 |
| 54 | MIA | 2w | 37 | 25/30 | 0.81 | 0.17 | 75,82,88,103 | 0 |
| 54 | PSU | 1y | 32 | 20/21 | 0.81 | 0.12 | 78,82,87,88 | 0 |
| 54 | 5MU | 2w | 54 | 21/22 | 0.81 | 0.11 | 67,82,87,93 | 0 |
| 54 | PSU | 1w | 55 | 20/21 | 0.82 | 0.11 | 74,83,92,95 | 0 |
| 54 | PSU | 2y | 39 | 20/21 | 0.82 | 0.13 | 79,84,92,96 | 0 |
| 55 | 4SU | 2x | 8 | 20/21 | 0.83 | 0.14 | 73,79,87,90 | 0 |
| 55 | PSU | 2x | 55 | 20/21 | 0.83 | 0.11 | 72,80,82,85 | 0 |
| 55 | 5MU | 2x | 54 | 21/22 | 0.84 | 0.12 | 68,77,82,94 | 0 |
| 32 | PSU | 2a | 516 | 20/21 | 0.86 | 0.12 | 70,77,83,85 | 0 |
| 1 | PSU | 2A | 1917 | 20/21 | 0.86 | 0.12 | 62,71,81,87 | 0 |
| 54 | MIA | 1y | 37 | 22/30 | 0.86 | 0.11 | 74,78,84,85 | 0 |
| 32 | M2G | 2a | 966 | 25/26 | 0.87 | 0.20 | 60,69,84,86 | 0 |
| 54 | PSU | 1y | 39 | 20/21 | 0.87 | 0.09 | 74,76,80,80 | 0 |
| 43 | 0TD | 2l | 92 | 10/11 | 0.87 | 0.14 | 67,71,72,79 | 0 |
| 55 | 5MU | 1x | 54 | 21/22 | 0.88 | 0.11 | 51,64,70,76 | 0 |
| 54 | PSU | 2w | 32 | 20/21 | 0.89 | 0.13 | 78,85,93,97 | 0 |
| 54 | PSU | 1w | 32 | 20/21 | 0.89 | 0.13 | 65,76,82,84 | 0 |
| 54 | MIA | 1w | 37 | 29/30 | 0.89 | 0.16 | 56,65,72,74 | 0 |
| 1 | 4OC | 2A | 1920 | 21/23 | 0.90 | 0.13 | 61,65,67,71 | 0 |
| 43 | 0TD | 1l | 92 | 10/11 | 0.90 | 0.12 | 47,55,60,75 | 0 |
| 1 | PSU | 2A | 1911 | 20/21 | 0.90 | 0.11 | 60,66,73,75 | 0 |
| 32 | 5MC | 2a | 967 | 21/22 | 0.90 | 0.16 | 61,70,78,82 | 0 |
| 55 | 4SU | 1x | 8 | 20/21 | 0.92 | 0.11 | 51,59,65,71 | 0 |
| 54 | 5MU | 1w | 54 | 21/22 | 0.92 | 0.09 | 64,72,79,82 | 0 |
| 55 | 5MC | 2x | 32 | 21/22 | 0.92 | 0.13 | 60,73,78,82 | 0 |
| 32 | 5MC | 2a | 1400 | 21/22 | 0.92 | 0.16 | 60,69,76,83 | 0 |
| 54 | PSU | 1w | 39 | 20/21 | 0.92 | 0.11 | 67,74,85,85 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 55 | PSU | 1x | 55 | 20/21 | 0.92 | 0.10 | 49,63,70,73 | 0 |
| 32 | 5MC | 2a | 1404 | 21/22 | 0.92 | 0.13 | 56,60,65,68 | 0 |
| 1 | 5MU | 1A | 1915 | 21/22 | 0.93 | 0.10 | 56,61,68,71 | 0 |
| 55 | 5MC | 1x | 32 | 21/22 | 0.93 | 0.13 | 46,54,60,74 | 0 |
| 32 | 4OC | 2a | 1402 | 22/23 | 0.93 | 0.13 | 53,65,69,70 | 0 |
| 32 | PSU | 1a | 516 | 20/21 | 0.93 | 0.10 | 60,66,71,71 | 0 |
| 32 | UR3 | 2a | 1498 | 21/22 | 0.93 | 0.13 | 55,61,65,66 | 0 |
| 32 | MA6 | 2a | 1518 | 24/25 | 0.93 | 0.12 | 55,65,68,71 | 0 |
| 32 | 7MG | 2a | 527 | 24/25 | 0.93 | 0.12 | 63,66,72,76 | 0 |
| 32 | MA6 | 2a | 1519 | 24/25 | 0.94 | 0.12 | 52,63,67,69 | 0 |
| 32 | 2MG | 1a | 1207 | 24/25 | 0.94 | 0.10 | 59,67,73,75 | 0 |
| 32 | 5MC | 1a | 967 | 21/22 | 0.94 | 0.11 | 52,59,63,64 | 0 |
| 1 | PSU | 1A | 1917 | 20/21 | 0.94 | 0.10 | 48,57,62,63 | 0 |
| 1 | 5MC | 2A | 1962 | 21/22 | 0.95 | 0.10 | 40,52,59,68 | 0 |
| 1 | 2MA | 2A | 2503 | 23/24 | 0.95 | 0.11 | 32,36,43,45 | 0 |
| 32 | 5MC | 2a | 1407 | 21/22 | 0.95 | 0.13 | 53,59,63,64 | 0 |
| 1 | 5MU | 2A | 1939 | 21/22 | 0.95 | 0.11 | 36,44,49,51 | 0 |
| 1 | 5MC | 2A | 1942 | 21/22 | 0.95 | 0.10 | 54,60,66,68 | 0 |
| 32 | 5MC | 1a | 1404 | 21/22 | 0.96 | 0.08 | 35,41,44,44 | 0 |
| 32 | 5MC | 1a | 1407 | 21/22 | 0.96 | 0.09 | 36,41,43,45 | 0 |
| 32 | MA6 | 1a | 1519 | 24/25 | 0.96 | 0.10 | 38,42,47,50 | 0 |
| 1 | PSU | 1A | 1911 | 20/21 | 0.96 | 0.09 | 40,49,57,57 | 0 |
| 32 | 7MG | 1a | 527 | 24/25 | 0.96 | 0.09 | 42,49,57,58 | 0 |
| 1 | OMG | 2A | 2251 | 24/25 | 0.96 | 0.09 | 42,45,51,56 | 0 |
| 1 | 5MC | 1A | 1942 | 21/22 | 0.96 | 0.09 | 31,40,43,49 | 0 |
| 1 | 2MU | 2A | 2552 | 21/23 | 0.96 | 0.09 | 35,42,46,62 | 0 |
| 32 | M2G | 1a | 966 | 25/26 | 0.96 | 0.09 | 49,55,59,66 | 0 |
| 32 | 5MC | 1a | 1400 | 21/22 | 0.96 | 0.09 | 39,50,54,59 | 0 |
| 32 | 4OC | 1a | 1402 | 22/23 | 0.96 | 0.09 | 37,45,51,57 | 0 |
| 32 | MA6 | 1a | 1518 | 24/25 | 0.97 | 0.08 | 34,41,45,49 | 0 |
| 1 | 5MC | 1A | 1962 | 21/22 | 0.97 | 0.07 | 29,36,41,44 | 0 |
| 1 | 2MU | 1A | 2552 | 21/23 | 0.97 | 0.08 | 21,29,33,39 | 0 |
| 1 | PSU | 2A | 2605 | 20/21 | 0.97 | 0.07 | 34,42,47,47 | 0 |
| 1 | 4OC | 1A | 1920 | 21/23 | 0.97 | 0.07 | 37,44,48,53 | 0 |
| 1 | 2MA | 1A | 2503 | 23/24 | 0.98 | 0.06 | 14,21,24,31 | 0 |
| 32 | UR3 | 1a | 1498 | 21/22 | 0.98 | 0.07 | 39,43,46,48 | 0 |
| 1 | 5MU | 1A | 1939 | 21/22 | 0.98 | 0.06 | 23,29,33,40 | 0 |
| 1 | PSU | 1A | 2605 | 20/21 | 0.98 | 0.07 | 19,26,35,35 | 0 |
| 1 | OMG | 1A | 2251 | 24/25 | 0.98 | 0.06 | 19,25,28,29 | 0 |

## 6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

## 6.4 Ligands (i)

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 1A | 3982 | 1/1 | 0.54 | 0.32 | 77,77,77,77 | 0 |
| 56 | MG | 1P | 206 | 1/1 | 0.57 | 0.20 | 62,62,62,62 | 0 |
| 56 | MG | 2a | 3225 | 1/1 | 0.57 | 0.40 | 73,73,73,73 | 0 |
| 56 | MG | 2A | 3698 | 1/1 | 0.63 | 0.16 | 56,56,56,56 | 0 |
| 56 | MG | 2A | 3762 | 1/1 | 0.64 | 0.20 | 59,59,59,59 | 0 |
| 56 | MG | 2A | 3650 | 1/1 | 0.66 | 0.18 | 67,67,67,67 | 0 |
| 56 | MG | 2a | 3199 | 1/1 | 0.66 | 0.27 | 70,70,70,70 | 0 |
| 56 | MG | 1A | 3402 | 1/1 | 0.66 | 0.16 | 85,85,85,85 | 0 |
| 56 | MG | 1a | 1784 | 1/1 | 0.67 | 0.21 | 56,56,56,56 | 0 |
| 56 | MG | 2a | 3227 | 1/1 | 0.67 | 0.16 | 78,78,78,78 | 0 |
| 56 | MG | 2a | 3209 | 1/1 | 0.68 | 0.31 | 73,73,73,73 | 0 |
| 56 | MG | 2A | 3516 | 1/1 | 0.68 | 0.26 | 74,74,74,74 | 0 |
| 56 | MG | 2A | 3636 | 1/1 | 0.68 | 0.28 | 55,55,55,55 | 0 |
| 56 | MG | 1A | 3771 | 1/1 | 0.69 | 0.13 | 19,19,19,19 | 0 |
| 56 | MG | 1A | 4083 | 1/1 | 0.70 | 0.14 | 51,51,51,51 | 0 |
| 56 | MG | 1a | 1755 | 1/1 | 0.70 | 0.21 | 88,88,88,88 | 0 |
| 56 | MG | 2A | 3687 | 1/1 | 0.70 | 0.17 | 71,71,71,71 | 0 |
| 56 | MG | 2a | 3239 | 1/1 | 0.70 | 0.24 | 66,66,66,66 | 0 |
| 56 | MG | 2A | 3817 | 1/1 | 0.71 | 0.21 | 75,75,75,75 | 0 |
| 56 | MG | 2B | 216 | 1/1 | 0.71 | 0.17 | 65,65,65,65 | 0 |
| 56 | MG | 2a | 3193 | 1/1 | 0.71 | 0.40 | 82,82,82,82 | 0 |
| 56 | MG | 2A | 3405 | 1/1 | 0.71 | 0.28 | 64,64,64,64 | 0 |
| 56 | MG | 2A | 3048 | 1/1 | 0.72 | 0.16 | 65,65,65,65 | 0 |
| 56 | MG | 2A | 3809 | 1/1 | 0.72 | 0.21 | 60,60,60,60 | 0 |
| 56 | MG | 2A | 3674 | 1/1 | 0.72 | 0.20 | 63,63,63,63 | 0 |
| 56 | MG | 2A | 3620 | 1/1 | 0.72 | 0.15 | 64,64,64,64 | 0 |
| 56 | MG | 1a | 1790 | 1/1 | 0.72 | 0.14 | 74,74,74,74 | 0 |
| 56 | MG | 2A | 3678 | 1/1 | 0.73 | 0.28 | 76,76,76,76 | 0 |
| 56 | MG | 1a | 1772 | 1/1 | 0.73 | 0.31 | 60,60,60,60 | 0 |
| 56 | MG | 1A | 3800 | 1/1 | 0.73 | 0.12 | 60,60,60,60 | 0 |
| 56 | MG | 2A | 3731 | 1/1 | 0.73 | 0.25 | 60,60,60,60 | 0 |
| 56 | MG | 2a | 3031 | 1/1 | 0.73 | 0.23 | 69,69,69,69 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 2a | 3107 | 1/1 | 0.73 | 0.39 | 74,74,74,74 | 0 |
| 56 | MG | 2v | 101 | 1/1 | 0.73 | 0.25 | 78,78,78,78 | 0 |
| 56 | MG | 2A | 3688 | 1/1 | 0.74 | 0.23 | 57,57,57,57 | 0 |
| 56 | MG | 1x | 111 | 1/1 | 0.74 | 0.27 | 71,71,71,71 | 0 |
| 56 | MG | 2a | 3003 | 1/1 | 0.74 | 0.21 | 63,63,63,63 | 0 |
| 56 | MG | 1A | 3341 | 1/1 | 0.74 | 0.18 | 50,50,50,50 | 0 |
| 56 | MG | 2A | 3285 | 1/1 | 0.74 | 0.14 | 62,62,62,62 | 0 |
| 56 | MG | 2A | 3334 | 1/1 | 0.74 | 0.19 | 74,74,74,74 | 0 |
| 56 | MG | 2A | 3773 | 1/1 | 0.75 | 0.13 | 73,73,73,73 | 0 |
| 56 | MG | 2A | 3396 | 1/1 | 0.75 | 0.20 | 63,63,63,63 | 0 |
| 56 | MG | 2A | 3709 | 1/1 | 0.75 | 0.17 | 48,48,48,48 | 0 |
| 56 | MG | 2A | 3712 | 1/1 | 0.75 | 0.20 | 70,70,70,70 | 0 |
| 56 | MG | 2A | 3713 | 1/1 | 0.75 | 0.17 | 48,48,48,48 | 0 |
| 56 | MG | 2A | 3040 | 1/1 | 0.75 | 0.26 | 88,88,88,88 | 0 |
| 56 | MG | 2j | 201 | 1/1 | 0.75 | 0.20 | 76,76,76,76 | 0 |
| 56 | MG | 2A | 3623 | 1/1 | 0.75 | 0.19 | 60,60,60,60 | 0 |
| 56 | MG | 2A | 3069 | 1/1 | 0.76 | 0.15 | 54,54,54,54 | 0 |
| 56 | MG | 1A | 4006 | 1/1 | 0.76 | 0.15 | 29,29,29,29 | 0 |
| 56 | MG | 2A | 3665 | 1/1 | 0.76 | 0.12 | 61,61,61,61 | 0 |
| 56 | MG | 1a | 1655 | 1/1 | 0.76 | 0.23 | 76,76,76,76 | 0 |
| 56 | MG | 2a | 3070 | 1/1 | 0.76 | 0.21 | 68,68,68,68 | 0 |
| 56 | MG | 2A | 3796 | 1/1 | 0.76 | 0.16 | 77,77,77,77 | 0 |
| 56 | MG | 1w | 104 | 1/1 | 0.76 | 0.23 | 72,72,72,72 | 0 |
| 56 | MG | 2A | 3602 | 1/1 | 0.77 | 0.20 | 55,55,55,55 | 0 |
| 56 | MG | 1A | 3667 | 1/1 | 0.77 | 0.14 | 28,28,28,28 | 0 |
| 56 | MG | 2A | 3333 | 1/1 | 0.77 | 0.15 | 65,65,65,65 | 0 |
| 56 | MG | 1A | 3852 | 1/1 | 0.77 | 0.21 | 39,39,39,39 | 0 |
| 56 | MG | 2A | 3828 | 1/1 | 0.77 | 0.14 | 59,59,59,59 | 0 |
| 56 | MG | 1A | 3930 | 1/1 | 0.77 | 0.13 | 30,30,30,30 | 0 |
| 56 | MG | 1A | 3425 | 1/1 | 0.77 | 0.20 | 60,60,60,60 | 0 |
| 56 | MG | 1s | 101 | 1/1 | 0.77 | 0.17 | 71,71,71,71 | 0 |
| 56 | MG | 2A | 3585 | 1/1 | 0.77 | 0.18 | 77,77,77,77 | 0 |
| 56 | MG | 1A | 3968 | 1/1 | 0.78 | 0.26 | 43,43,43,43 | 0 |
| 56 | MG | 1A | 3979 | 1/1 | 0.78 | 0.15 | 69,69,69,69 | 0 |
| 56 | MG | 2a | 3053 | 1/1 | 0.78 | 0.31 | 70,70,70,70 | 0 |
| 56 | MG | 2a | 3057 | 1/1 | 0.78 | 0.19 | 65,65,65,65 | 0 |
| 56 | MG | 18 | 105 | 1/1 | 0.78 | 0.23 | 45,45,45,45 | 0 |
| 56 | MG | 2A | 3715 | 1/1 | 0.78 | 0.21 | 68,68,68,68 | 0 |
| 56 | MG | 1A | 3801 | 1/1 | 0.78 | 0.11 | 53,53,53,53 | 0 |
| 56 | MG | 2a | 3196 | 1/1 | 0.78 | 0.20 | 76,76,76,76 | 0 |
| 56 | MG | 2A | 3350 | 1/1 | 0.78 | 0.31 | 68,68,68,68 | 0 |
| 56 | MG | 1a | 1700 | 1/1 | 0.78 | 0.23 | 68,68,68,68 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 1x | 117 | 1/1 | 0.78 | 0.12 | 71,71,71,71 | 0 |
| 56 | MG | 2A | 3452 | 1/1 | 0.78 | 0.37 | 70,70,70,70 | 0 |
| 56 | MG | 1A | 3948 | 1/1 | 0.78 | 0.14 | 36,36,36,36 | 0 |
| 56 | MG | 2A | 3532 | 1/1 | 0.78 | 0.27 | 61,61,61,61 | 0 |
| 56 | MG | 1A | 4043 | 1/1 | 0.78 | 0.20 | 66,66,66,66 | 0 |
| 56 | MG | 2A | 3171 | 1/1 | 0.79 | 0.32 | 74,74,74,74 | 0 |
| 56 | MG | 2a | 3036 | 1/1 | 0.79 | 0.24 | 72,72,72,72 | 0 |
| 56 | MG | 2A | 3661 | 1/1 | 0.79 | 0.15 | 59,59,59,59 | 0 |
| 56 | MG | 1A | 3626 | 1/1 | 0.79 | 0.15 | 47,47,47,47 | 0 |
| 56 | MG | 2A | 3750 | 1/1 | 0.79 | 0.16 | 55,55,55,55 | 0 |
| 56 | MG | 2A | 3671 | 1/1 | 0.79 | 0.13 | 59,59,59,59 | 0 |
| 56 | MG | 2a | 3170 | 1/1 | 0.79 | 0.14 | 73,73,73,73 | 0 |
| 56 | MG | 1a | 1693 | 1/1 | 0.79 | 0.28 | 69,69,69,69 | 0 |
| 56 | MG | 2A | 3543 | 1/1 | 0.79 | 0.13 | 45,45,45,45 | 0 |
| 56 | MG | 1A | 3791 | 1/1 | 0.79 | 0.20 | 63,63,63,63 | 0 |
| 56 | MG | 1a | 1739 | 1/1 | 0.79 | 0.14 | 77,77,77,77 | 0 |
| 56 | MG | 2A | 3823 | 1/1 | 0.79 | 0.11 | 50,50,50,50 | 0 |
| 56 | MG | 1A | 4060 | 1/1 | 0.79 | 0.27 | 52,52,52,52 | 0 |
| 56 | MG | 2A | 3402 | 1/1 | 0.79 | 0.15 | 65,65,65,65 | 0 |
| 56 | MG | 2G | 201 | 1/1 | 0.79 | 0.19 | 65,65,65,65 | 0 |
| 56 | MG | 2A | 3088 | 1/1 | 0.79 | 0.30 | 78,78,78,78 | 0 |
| 56 | MG | 2B | 220 | 1/1 | 0.80 | 0.20 | 65,65,65,65 | 0 |
| 56 | MG | 1a | 1767 | 1/1 | 0.80 | 0.20 | 67,67,67,67 | 0 |
| 56 | MG | 14 | 101 | 1/1 | 0.80 | 0.16 | 69,69,69,69 | 0 |
| 56 | MG | 1A | 3661 | 1/1 | 0.80 | 0.12 | 29,29,29,29 | 0 |
| 56 | MG | 2A | 3736 | 1/1 | 0.80 | 0.11 | 57,57,57,57 | 0 |
| 56 | MG | 2a | 3049 | 1/1 | 0.80 | 0.29 | 64,64,64,64 | 0 |
| 56 | MG | 1a | 1642 | 1/1 | 0.80 | 0.13 | 57,57,57,57 | 0 |
| 56 | MG | 2A | 3754 | 1/1 | 0.80 | 0.21 | 67,67,67,67 | 0 |
| 56 | MG | 2a | 3064 | 1/1 | 0.80 | 0.15 | 64,64,64,64 | 0 |
| 56 | MG | 2a | 3068 | 1/1 | 0.80 | 0.14 | 74,74,74,74 | 0 |
| 56 | MG | 1A | 4032 | 1/1 | 0.80 | 0.20 | 57,57,57,57 | 0 |
| 56 | MG | 1A | 4058 | 1/1 | 0.81 | 0.14 | 28,28,28,28 | 0 |
| 56 | MG | 2A | 3595 | 1/1 | 0.81 | 0.22 | 65,65,65,65 | 0 |
| 56 | MG | 2A | 3152 | 1/1 | 0.81 | 0.20 | 71,71,71,71 | 0 |
| 56 | MG | 1A | 3699 | 1/1 | 0.81 | 0.13 | 37,37,37,37 | 0 |
| 56 | MG | 2A | 3734 | 1/1 | 0.81 | 0.09 | 52,52,52,52 | 0 |
| 56 | MG | 2A | 3261 | 1/1 | 0.81 | 0.14 | 59,59,59,59 | 0 |
| 56 | MG | 2a | 3060 | 1/1 | 0.81 | 0.10 | 71,71,71,71 | 0 |
| 56 | MG | 1A | 4067 | 1/1 | 0.81 | 0.14 | 55,55,55,55 | 0 |
| 56 | MG | 1A | 3767 | 1/1 | 0.81 | 0.12 | 30,30,30,30 | 0 |
| 56 | MG | 1A | 3061 | 1/1 | 0.81 | 0.20 | 67,67,67,67 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 1A | 3103 | 1/1 | 0.81 | 0.17 | 60,60,60,60 | 0 |
| 56 | MG | 1A | 3317 | 1/1 | 0.81 | 0.28 | 65,65,65,65 | 0 |
| 56 | MG | 2A | 3804 | 1/1 | 0.81 | 0.14 | 53,53,53,53 | 0 |
| 56 | MG | 1A | 4000 | 1/1 | 0.81 | 0.18 | 62,62,62,62 | 0 |
| 56 | MG | 2A | 3676 | 1/1 | 0.81 | 0.13 | 61,61,61,61 | 0 |
| 56 | MG | 2A | 3819 | 1/1 | 0.81 | 0.19 | 69,69,69,69 | 0 |
| 56 | MG | 1A | 3693 | 1/1 | 0.81 | 0.20 | 42,42,42,42 | 0 |
| 56 | MG | 1A | 3808 | 1/1 | 0.81 | 0.25 | 65,65,65,65 | 0 |
| 56 | MG | 1A | 3697 | 1/1 | 0.81 | 0.15 | 38,38,38,38 | 0 |
| 56 | MG | 1a | 1721 | 1/1 | 0.81 | 0.34 | 54,54,54,54 | 0 |
| 56 | MG | 1a | 1731 | 1/1 | 0.81 | 0.40 | 69,69,69,69 | 0 |
| 56 | MG | 1A | 3263 | 1/1 | 0.82 | 0.22 | 64,64,64,64 | 0 |
| 56 | MG | 2D | 309 | 1/1 | 0.82 | 0.15 | 35,35,35,35 | 0 |
| 56 | MG | 1a | 1606 | 1/1 | 0.82 | 0.24 | 71,71,71,71 | 0 |
| 56 | MG | 2Q | 204 | 1/1 | 0.82 | 0.18 | 62,62,62,62 | 0 |
| 56 | MG | 2A | 3094 | 1/1 | 0.82 | 0.12 | 62,62,62,62 | 0 |
| 56 | MG | 2a | 3027 | 1/1 | 0.82 | 0.21 | 70,70,70,70 | 0 |
| 56 | MG | 1A | 3991 | 1/1 | 0.82 | 0.10 | 22,22,22,22 | 0 |
| 56 | MG | 1A | 3498 | 1/1 | 0.82 | 0.29 | 59,59,59,59 | 0 |
| 56 | MG | 2A | 3198 | 1/1 | 0.82 | 0.34 | 68,68,68,68 | 0 |
| 56 | MG | 2A | 3228 | 1/1 | 0.82 | 0.16 | 72,72,72,72 | 0 |
| 56 | MG | 2A | 3247 | 1/1 | 0.82 | 0.23 | 70,70,70,70 | 0 |
| 56 | MG | 2A | 3748 | 1/1 | 0.82 | 0.19 | 68,68,68,68 | 0 |
| 56 | MG | 1a | 1659 | 1/1 | 0.82 | 0.18 | 55,55,55,55 | 0 |
| 56 | MG | 2A | 3637 | 1/1 | 0.82 | 0.16 | 47,47,47,47 | 0 |
| 56 | MG | 2A | 3759 | 1/1 | 0.82 | 0.16 | 62,62,62,62 | 0 |
| 56 | MG | 2a | 3100 | 1/1 | 0.82 | 0.20 | 77,77,77,77 | 0 |
| 56 | MG | 2A | 3640 | 1/1 | 0.82 | 0.11 | 64,64,64,64 | 0 |
| 56 | MG | 1b | 302 | 1/1 | 0.82 | 0.20 | 71,71,71,71 | 0 |
| 56 | MG | 2A | 3315 | 1/1 | 0.82 | 0.16 | 62,62,62,62 | 0 |
| 56 | MG | 1A | 3551 | 1/1 | 0.82 | 0.18 | 50,50,50,50 | 0 |
| 56 | MG | 2A | 3805 | 1/1 | 0.82 | 0.10 | 67,67,67,67 | 0 |
| 56 | MG | 1w | 102 | 1/1 | 0.82 | 0.09 | 75,75,75,75 | 0 |
| 56 | MG | 1A | 4100 | 1/1 | 0.82 | 0.19 | 85,85,85,85 | 0 |
| 56 | MG | 1B | 237 | 1/1 | 0.82 | 0.16 | 68,68,68,68 | 0 |
| 56 | MG | 2a | 3233 | 1/1 | 0.82 | 0.21 | 67,67,67,67 | 0 |
| 56 | MG | 1A | 3605 | 1/1 | 0.82 | 0.12 | 37,37,37,37 | 0 |
| 56 | MG | 2a | 3240 | 1/1 | 0.82 | 0.17 | 67,67,67,67 | 0 |
| 56 | MG | 1A | 3845 | 1/1 | 0.82 | 0.23 | 57,57,57,57 | 0 |
| 56 | MG | 1a | 1753 | 1/1 | 0.82 | 0.17 | 53,53,53,53 | 0 |
| 56 | MG | 2w | 102 | 1/1 | 0.82 | 0.20 | 72,72,72,72 | 0 |
| 56 | MG | 1A | 3686 | 1/1 | 0.83 | 0.12 | 54,54,54,54 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 1a | 1779 | 1/1 | 0.83 | 0.12 | 88,88,88,88 | 0 |
| 56 | MG | 2A | 3493 | 1/1 | 0.83 | 0.11 | 61,61,61,61 | 0 |
| 56 | MG | 1A | 3532 | 1/1 | 0.83 | 0.20 | 52,52,52,52 | 0 |
| 56 | MG | 1a | 1666 | 1/1 | 0.83 | 0.22 | 63,63,63,63 | 0 |
| 56 | MG | 2a | 3017 | 1/1 | 0.83 | 0.21 | 71,71,71,71 | 0 |
| 56 | MG | 2a | 3021 | 1/1 | 0.83 | 0.23 | 69,69,69,69 | 0 |
| 56 | MG | 2a | 3023 | 1/1 | 0.83 | 0.24 | 76,76,76,76 | 0 |
| 56 | MG | 2A | 3173 | 1/1 | 0.83 | 0.21 | 72,72,72,72 | 0 |
| 56 | MG | 2A | 3729 | 1/1 | 0.83 | 0.20 | 68,68,68,68 | 0 |
| 56 | MG | 1a | 1800 | 1/1 | 0.83 | 0.11 | 50,50,50,50 | 0 |
| 56 | MG | 2a | 3041 | 1/1 | 0.83 | 0.28 | 66,66,66,66 | 0 |
| 56 | MG | 2a | 3046 | 1/1 | 0.83 | 0.24 | 66,66,66,66 | 0 |
| 56 | MG | 2A | 3214 | 1/1 | 0.83 | 0.13 | 62,62,62,62 | 0 |
| 56 | MG | 2A | 3599 | 1/1 | 0.83 | 0.23 | 68,68,68,68 | 0 |
| 56 | MG | 2a | 3054 | 1/1 | 0.83 | 0.19 | 71,71,71,71 | 0 |
| 56 | MG | 2A | 3739 | 1/1 | 0.83 | 0.20 | 59,59,59,59 | 0 |
| 56 | MG | 1a | 1692 | 1/1 | 0.83 | 0.23 | 70,70,70,70 | 0 |
| 56 | MG | 2A | 3609 | 1/1 | 0.83 | 0.12 | 29,29,29,29 | 0 |
| 56 | MG | 1E | 313 | 1/1 | 0.83 | 0.15 | 54,54,54,54 | 0 |
| 56 | MG | 1A | 3838 | 1/1 | 0.83 | 0.22 | 60,60,60,60 | 0 |
| 56 | MG | 2a | 3077 | 1/1 | 0.83 | 0.22 | 59,59,59,59 | 0 |
| 56 | MG | 1S | 201 | 1/1 | 0.83 | 0.26 | 40,40,40,40 | 0 |
| 56 | MG | 2a | 3101 | 1/1 | 0.83 | 0.27 | 68,68,68,68 | 0 |
| 56 | MG | 2A | 3302 | 1/1 | 0.83 | 0.19 | 61,61,61,61 | 0 |
| 56 | MG | 2A | 3310 | 1/1 | 0.83 | 0.28 | 65,65,65,65 | 0 |
| 56 | MG | 2a | 3173 | 1/1 | 0.83 | 0.17 | 70,70,70,70 | 0 |
| 56 | MG | 2a | 3174 | 1/1 | 0.83 | 0.14 | 75,75,75,75 | 0 |
| 56 | MG | 1x | 110 | 1/1 | 0.83 | 0.28 | 61,61,61,61 | 0 |
| 56 | MG | 1A | 3459 | 1/1 | 0.83 | 0.13 | 49,49,49,49 | 0 |
| 56 | MG | 2a | 3197 | 1/1 | 0.83 | 0.14 | 73,73,73,73 | 0 |
| 56 | MG | 1A | 3306 | 1/1 | 0.83 | 0.17 | 41,41,41,41 | 0 |
| 56 | MG | 2A | 3816 | 1/1 | 0.83 | 0.18 | 68,68,68,68 | 0 |
| 56 | MG | 2A | 3339 | 1/1 | 0.83 | 0.17 | 64,64,64,64 | 0 |
| 56 | MG | 1A | 3876 | 1/1 | 0.83 | 0.16 | 34,34,34,34 | 0 |
| 56 | MG | 2A | 3391 | 1/1 | 0.83 | 0.13 | 68,68,68,68 | 0 |
| 56 | MG | 2a | 3238 | 1/1 | 0.83 | 0.18 | 72,72,72,72 | 0 |
| 56 | MG | 1A | 3897 | 1/1 | 0.83 | 0.19 | 56,56,56,56 | 0 |
| 56 | MG | 2A | 3830 | 1/1 | 0.83 | 0.11 | 77,77,77,77 | 0 |
| 56 | MG | 2d | 301 | 1/1 | 0.83 | 0.13 | 65,65,65,65 | 0 |
| 56 | MG | 2A | 3869 | 1/1 | 0.83 | 0.13 | 45,45,45,45 | 0 |
| 56 | MG | 1a | 1654 | 1/1 | 0.83 | 0.25 | 71,71,71,71 | 0 |
| 56 | MG | 2B | 218 | 1/1 | 0.83 | 0.22 | 67,67,67,67 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 1A | 3224 | 1/1 | 0.84 | 0.14 | 45,45,45,45 | 0 |
| 56 | MG | 1a | 1609 | 1/1 | 0.84 | 0.17 | 65,65,65,65 | 0 |
| 56 | MG | 1a | 1611 | 1/1 | 0.84 | 0.13 | 68,68,68,68 | 0 |
| 56 | MG | 1B | 233 | 1/1 | 0.84 | 0.13 | 63,63,63,63 | 0 |
| 56 | MG | 2A | 3257 | 1/1 | 0.84 | 0.17 | 62,62,62,62 | 0 |
| 56 | MG | 2A | 3538 | 1/1 | 0.84 | 0.10 | 38,38,38,38 | 0 |
| 56 | MG | 2A | 3702 | 1/1 | 0.84 | 0.13 | 31,31,31,31 | 0 |
| 56 | MG | 2a | 3092 | 1/1 | 0.84 | 0.18 | 77,77,77,77 | 0 |
| 56 | MG | 1A | 3195 | 1/1 | 0.84 | 0.10 | 55,55,55,55 | 0 |
| 56 | MG | 2A | 3570 | 1/1 | 0.84 | 0.13 | 48,48,48,48 | 0 |
| 56 | MG | 2A | 3873 | 1/1 | 0.84 | 0.17 | 75,75,75,75 | 0 |
| 56 | MG | 2a | 3162 | 1/1 | 0.84 | 0.10 | 82,82,82,82 | 0 |
| 56 | MG | 2a | 3163 | 1/1 | 0.84 | 0.14 | 68,68,68,68 | 0 |
| 56 | MG | 2A | 3027 | 1/1 | 0.84 | 0.17 | 71,71,71,71 | 0 |
| 56 | MG | 2A | 3297 | 1/1 | 0.84 | 0.29 | 72,72,72,72 | 0 |
| 56 | MG | 2A | 3029 | 1/1 | 0.84 | 0.28 | 62,62,62,62 | 0 |
| 56 | MG | 2a | 3178 | 1/1 | 0.84 | 0.12 | 91,91,91,91 | 0 |
| 56 | MG | 1A | 3411 | 1/1 | 0.84 | 0.20 | 57,57,57,57 | 0 |
| 56 | MG | 1A | 3329 | 1/1 | 0.84 | 0.17 | 51,51,51,51 | 0 |
| 56 | MG | 2A | 3612 | 1/1 | 0.84 | 0.11 | 41,41,41,41 | 0 |
| 56 | MG | 1A | 3689 | 1/1 | 0.84 | 0.14 | 26,26,26,26 | 0 |
| 56 | MG | 2a | 3201 | 1/1 | 0.84 | 0.16 | 60,60,60,60 | 0 |
| 56 | MG | 1Y | 202 | 1/1 | 0.84 | 0.09 | 68,68,68,68 | 0 |
| 56 | MG | 2a | 3220 | 1/1 | 0.84 | 0.15 | 63,63,63,63 | 0 |
| 56 | MG | 2a | 3020 | 1/1 | 0.84 | 0.27 | 71,71,71,71 | 0 |
| 56 | MG | 1A | 3797 | 1/1 | 0.84 | 0.14 | 27,27,27,27 | 0 |
| 56 | MG | 2A | 3120 | 1/1 | 0.84 | 0.14 | 62,62,62,62 | 0 |
| 56 | MG | 2A | 3757 | 1/1 | 0.84 | 0.15 | 66,66,66,66 | 0 |
| 56 | MG | 2A | 3352 | 1/1 | 0.84 | 0.26 | 72,72,72,72 | 0 |
| 56 | MG | 2A | 3368 | 1/1 | 0.84 | 0.16 | 65,65,65,65 | 0 |
| 56 | MG | 2A | 3770 | 1/1 | 0.84 | 0.12 | 54,54,54,54 | 0 |
| 56 | MG | 1A | 3458 | 1/1 | 0.84 | 0.22 | 62,62,62,62 | 0 |
| 56 | MG | 2l | 203 | 1/1 | 0.84 | 0.21 | 61,61,61,61 | 0 |
| 56 | MG | 1e | 201 | 1/1 | 0.84 | 0.10 | 73,73,73,73 | 0 |
| 56 | MG | 1a | 1604 | 1/1 | 0.84 | 0.11 | 55,55,55,55 | 0 |
| 56 | MG | 2x | 105 | 1/1 | 0.84 | 0.20 | 67,67,67,67 | 0 |
| 56 | MG | 2A | 3191 | 1/1 | 0.85 | 0.18 | 70,70,70,70 | 0 |
| 56 | MG | 2A | 3353 | 1/1 | 0.85 | 0.10 | 71,71,71,71 | 0 |
| 56 | MG | 2A | 3624 | 1/1 | 0.85 | 0.17 | 40,40,40,40 | 0 |
| 56 | MG | 2A | 3364 | 1/1 | 0.85 | 0.33 | 66,66,66,66 | 0 |
| 56 | MG | 1A | 3665 | 1/1 | 0.85 | 0.09 | 30,30,30,30 | 0 |
| 56 | MG | 2A | 3210 | 1/1 | 0.85 | 0.12 | 61,61,61,61 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 1a | 1818 | 1/1 | 0.85 | 0.11 | 71,71,71,71 | 0 |
| 56 | MG | 1a | 1827 | 1/1 | 0.85 | 0.21 | 52,52,52,52 | 0 |
| 56 | MG | 2A | 3234 | 1/1 | 0.85 | 0.21 | 60,60,60,60 | 0 |
| 56 | MG | 2A | 3433 | 1/1 | 0.85 | 0.36 | 49,49,49,49 | 0 |
| 56 | MG | 2a | 3080 | 1/1 | 0.85 | 0.23 | 62,62,62,62 | 0 |
| 56 | MG | 2A | 3444 | 1/1 | 0.85 | 0.28 | 57,57,57,57 | 0 |
| 56 | MG | 2a | 3096 | 1/1 | 0.85 | 0.20 | 67,67,67,67 | 0 |
| 56 | MG | 1B | 207 | 1/1 | 0.85 | 0.31 | 70,70,70,70 | 0 |
| 56 | MG | 2A | 3467 | 1/1 | 0.85 | 0.22 | 74,74,74,74 | 0 |
| 56 | MG | 2A | 3679 | 1/1 | 0.85 | 0.11 | 52,52,52,52 | 0 |
| 56 | MG | 2a | 3135 | 1/1 | 0.85 | 0.18 | 59,59,59,59 | 0 |
| 56 | MG | 2A | 3686 | 1/1 | 0.85 | 0.14 | 53,53,53,53 | 0 |
| 56 | MG | 2A | 3853 | 1/1 | 0.85 | 0.13 | 49,49,49,49 | 0 |
| 56 | MG | 2A | 3858 | 1/1 | 0.85 | 0.12 | 64,64,64,64 | 0 |
| 56 | MG | 2A | 3484 | 1/1 | 0.85 | 0.12 | 58,58,58,58 | 0 |
| 56 | MG | 2A | 3491 | 1/1 | 0.85 | 0.18 | 50,50,50,50 | 0 |
| 56 | MG | 2A | 3881 | 1/1 | 0.85 | 0.16 | 62,62,62,62 | 0 |
| 56 | MG | 2a | 3188 | 1/1 | 0.85 | 0.15 | 59,59,59,59 | 0 |
| 56 | MG | 2A | 3058 | 1/1 | 0.85 | 0.13 | 52,52,52,52 | 0 |
| 56 | MG | 2B | 217 | 1/1 | 0.85 | 0.14 | 84,84,84,84 | 0 |
| 56 | MG | 2A | 3059 | 1/1 | 0.85 | 0.13 | 58,58,58,58 | 0 |
| 56 | MG | 2A | 3531 | 1/1 | 0.85 | 0.20 | 55,55,55,55 | 0 |
| 56 | MG | 2A | 3711 | 1/1 | 0.85 | 0.12 | 54,54,54,54 | 0 |
| 56 | MG | 2A | 3062 | 1/1 | 0.85 | 0.14 | 66,66,66,66 | 0 |
| 56 | MG | 2A | 3065 | 1/1 | 0.85 | 0.25 | 68,68,68,68 | 0 |
| 56 | MG | 20 | 101 | 1/1 | 0.85 | 0.24 | 67,67,67,67 | 0 |
| 56 | MG | 1A | 3739 | 1/1 | 0.85 | 0.13 | 51,51,51,51 | 0 |
| 56 | MG | 2a | 3228 | 1/1 | 0.85 | 0.29 | 62,62,62,62 | 0 |
| 56 | MG | 2a | 3005 | 1/1 | 0.85 | 0.25 | 66,66,66,66 | 0 |
| 56 | MG | 2a | 3012 | 1/1 | 0.85 | 0.25 | 70,70,70,70 | 0 |
| 56 | MG | 1A | 3766 | 1/1 | 0.85 | 0.10 | 26,26,26,26 | 0 |
| 56 | MG | 1A | 3512 | 1/1 | 0.85 | 0.17 | 60,60,60,60 | 0 |
| 56 | MG | 1A | 3270 | 1/1 | 0.85 | 0.12 | 55,55,55,55 | 0 |
| 56 | MG | 1a | 1780 | 1/1 | 0.85 | 0.10 | 58,58,58,58 | 0 |
| 56 | MG | 2A | 3601 | 1/1 | 0.85 | 0.17 | 58,58,58,58 | 0 |
| 56 | MG | 2q | 202 | 1/1 | 0.85 | 0.16 | 72,72,72,72 | 0 |
| 56 | MG | 1A | 3913 | 1/1 | 0.85 | 0.29 | 34,34,34,34 | 0 |
| 56 | MG | 2A | 3341 | 1/1 | 0.85 | 0.11 | 66,66,66,66 | 0 |
| 56 | MG | 2w | 104 | 1/1 | 0.85 | 0.10 | 69,69,69,69 | 0 |
| 56 | MG | 1A | 3921 | 1/1 | 0.85 | 0.12 | 41,41,41,41 | 0 |
| 56 | MG | 2A | 3718 | 1/1 | 0.86 | 0.09 | 41,41,41,41 | 0 |
| 56 | MG | 1B | 222 | 1/1 | 0.86 | 0.16 | 55,55,55,55 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 2A | 3502 | 1/1 | 0.86 | 0.12 | 55,55,55,55 | 0 |
| 56 | MG | 2A | 3514 | 1/1 | 0.86 | 0.18 | 67,67,67,67 | 0 |
| 56 | MG | 2a | 3043 | 1/1 | 0.86 | 0.28 | 66,66,66,66 | 0 |
| 56 | MG | 1B | 230 | 1/1 | 0.86 | 0.08 | 61,61,61,61 | 0 |
| 56 | MG | 2A | 3225 | 1/1 | 0.86 | 0.28 | 62,62,62,62 | 0 |
| 56 | MG | 1a | 1691 | 1/1 | 0.86 | 0.26 | 64,64,64,64 | 0 |
| 56 | MG | 1A | 3131 | 1/1 | 0.86 | 0.09 | 63,63,63,63 | 0 |
| 56 | MG | 1A | 3428 | 1/1 | 0.86 | 0.09 | 56,56,56,56 | 0 |
| 56 | MG | 1a | 1698 | 1/1 | 0.86 | 0.30 | 62,62,62,62 | 0 |
| 56 | MG | 1A | 3577 | 1/1 | 0.86 | 0.22 | 47,47,47,47 | 0 |
| 56 | MG | 2A | 3761 | 1/1 | 0.86 | 0.16 | 62,62,62,62 | 0 |
| 56 | MG | 1x | 112 | 1/1 | 0.86 | 0.16 | 58,58,58,58 | 0 |
| 56 | MG | 2A | 3596 | 1/1 | 0.86 | 0.09 | 40,40,40,40 | 0 |
| 56 | MG | 2A | 3287 | 1/1 | 0.86 | 0.24 | 67,67,67,67 | 0 |
| 56 | MG | 2a | 3082 | 1/1 | 0.86 | 0.20 | 65,65,65,65 | 0 |
| 56 | MG | 2a | 3085 | 1/1 | 0.86 | 0.32 | 73,73,73,73 | 0 |
| 56 | MG | 1x | 113 | 1/1 | 0.86 | 0.23 | 65,65,65,65 | 0 |
| 56 | MG | 2a | 3095 | 1/1 | 0.86 | 0.16 | 79,79,79,79 | 0 |
| 56 | MG | 2A | 3299 | 1/1 | 0.86 | 0.12 | 49,49,49,49 | 0 |
| 56 | MG | 1a | 1715 | 1/1 | 0.86 | 0.11 | 53,53,53,53 | 0 |
| 56 | MG | 2A | 3308 | 1/1 | 0.86 | 0.16 | 56,56,56,56 | 0 |
| 56 | MG | 2a | 3106 | 1/1 | 0.86 | 0.19 | 65,65,65,65 | 0 |
| 56 | MG | 2A | 3008 | 1/1 | 0.86 | 0.10 | 60,60,60,60 | 0 |
| 56 | MG | 2a | 3121 | 1/1 | 0.86 | 0.17 | 54,54,54,54 | 0 |
| 56 | MG | 1A | 3901 | 1/1 | 0.86 | 0.10 | 53,53,53,53 | 0 |
| 56 | MG | 2a | 3147 | 1/1 | 0.86 | 0.11 | 80,80,80,80 | 0 |
| 56 | MG | 2a | 3160 | 1/1 | 0.86 | 0.13 | 84,84,84,84 | 0 |
| 56 | MG | 2A | 3321 | 1/1 | 0.86 | 0.14 | 65,65,65,65 | 0 |
| 56 | MG | 1A | 3911 | 1/1 | 0.86 | 0.18 | 55,55,55,55 | 0 |
| 56 | MG | 2a | 3165 | 1/1 | 0.86 | 0.09 | 78,78,78,78 | 0 |
| 56 | MG | 1U | 201 | 1/1 | 0.86 | 0.18 | 51,51,51,51 | 0 |
| 56 | MG | 1A | 4039 | 1/1 | 0.86 | 0.11 | 61,61,61,61 | 0 |
| 56 | MG | 2A | 3831 | 1/1 | 0.86 | 0.15 | 56,56,56,56 | 0 |
| 56 | MG | 2A | 3645 | 1/1 | 0.86 | 0.10 | 37,37,37,37 | 0 |
| 56 | MG | 1A | 3798 | 1/1 | 0.86 | 0.10 | 39,39,39,39 | 0 |
| 56 | MG | 2A | 3347 | 1/1 | 0.86 | 0.13 | 66,66,66,66 | 0 |
| 56 | MG | 1a | 1763 | 1/1 | 0.86 | 0.18 | 62,62,62,62 | 0 |
| 56 | MG | 1A | 4047 | 1/1 | 0.86 | 0.12 | 47,47,47,47 | 0 |
| 56 | MG | 2B | 211 | 1/1 | 0.86 | 0.26 | 75,75,75,75 | 0 |
| 56 | MG | 1A | 4056 | 1/1 | 0.86 | 0.10 | 45,45,45,45 | 0 |
| 56 | MG | 1A | 3917 | 1/1 | 0.86 | 0.13 | 34,34,34,34 | 0 |
| 56 | MG | 2a | 3216 | 1/1 | 0.86 | 0.13 | 72,72,72,72 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 2A | 3086 | 1/1 | 0.86 | 0.23 | 66,66,66,66 | 0 |
| 56 | MG | 2A | 3377 | 1/1 | 0.86 | 0.10 | 65,65,65,65 | 0 |
| 56 | MG | 1A | 3446 | 1/1 | 0.86 | 0.11 | 52,52,52,52 | 0 |
| 56 | MG | 1A | 3004 | 1/1 | 0.86 | 0.10 | 22,22,22,22 | 0 |
| 56 | MG | 1a | 1634 | 1/1 | 0.86 | 0.29 | 66,66,66,66 | 0 |
| 56 | MG | 2a | 3235 | 1/1 | 0.86 | 0.12 | 66,66,66,66 | 0 |
| 56 | MG | 2a | 3236 | 1/1 | 0.86 | 0.28 | 73,73,73,73 | 0 |
| 56 | MG | 2R | 201 | 1/1 | 0.86 | 0.14 | 65,65,65,65 | 0 |
| 56 | MG | 2Z | 301 | 1/1 | 0.86 | 0.12 | 72,72,72,72 | 0 |
| 56 | MG | 2A | 3123 | 1/1 | 0.86 | 0.33 | 59,59,59,59 | 0 |
| 56 | MG | 27 | 101 | 1/1 | 0.86 | 0.11 | 46,46,46,46 | 0 |
| 56 | MG | 2f | 202 | 1/1 | 0.86 | 0.18 | 65,65,65,65 | 0 |
| 56 | MG | 2g | 201 | 1/1 | 0.86 | 0.11 | 81,81,81,81 | 0 |
| 56 | MG | 2A | 3124 | 1/1 | 0.86 | 0.09 | 66,66,66,66 | 0 |
| 56 | MG | 1a | 1793 | 1/1 | 0.86 | 0.10 | 78,78,78,78 | 0 |
| 56 | MG | 1A | 3214 | 1/1 | 0.86 | 0.15 | 57,57,57,57 | 0 |
| 56 | MG | 1A | 3121 | 1/1 | 0.86 | 0.13 | 46,46,46,46 | 0 |
| 56 | MG | 1a | 1826 | 1/1 | 0.86 | 0.19 | 58,58,58,58 | 0 |
| 56 | MG | 2A | 3714 | 1/1 | 0.86 | 0.11 | 57,57,57,57 | 0 |
| 56 | MG | 2x | 103 | 1/1 | 0.86 | 0.10 | 60,60,60,60 | 0 |
| 56 | MG | 2x | 104 | 1/1 | 0.86 | 0.17 | 62,62,62,62 | 0 |
| 56 | MG | 1A | 3422 | 1/1 | 0.86 | 0.12 | 58,58,58,58 | 0 |
| 56 | MG | 2y | 106 | 1/1 | 0.86 | 0.16 | 83,83,83,83 | 0 |
| 56 | MG | 1A | 3302 | 1/1 | 0.87 | 0.26 | 52,52,52,52 | 0 |
| 56 | MG | 2A | 3330 | 1/1 | 0.87 | 0.20 | 60,60,60,60 | 0 |
| 56 | MG | 2a | 3013 | 1/1 | 0.87 | 0.18 | 58,58,58,58 | 0 |
| 56 | MG | 1A | 3928 | 1/1 | 0.87 | 0.15 | 69,69,69,69 | 0 |
| 56 | MG | 1A | 3417 | 1/1 | 0.87 | 0.14 | 48,48,48,48 | 0 |
| 56 | MG | 1A | 3932 | 1/1 | 0.87 | 0.12 | 48,48,48,48 | 0 |
| 56 | MG | 1A | 3165 | 1/1 | 0.87 | 0.15 | 39,39,39,39 | 0 |
| 56 | MG | 2A | 3346 | 1/1 | 0.87 | 0.13 | 67,67,67,67 | 0 |
| 56 | MG | 1B | 234 | 1/1 | 0.87 | 0.16 | 56,56,56,56 | 0 |
| 56 | MG | 2A | 3349 | 1/1 | 0.87 | 0.19 | 59,59,59,59 | 0 |
| 56 | MG | 2a | 3039 | 1/1 | 0.87 | 0.22 | 55,55,55,55 | 0 |
| 56 | MG | 1A | 3817 | 1/1 | 0.87 | 0.46 | 39,39,39,39 | 0 |
| 56 | MG | 1D | 312 | 1/1 | 0.87 | 0.16 | 37,37,37,37 | 0 |
| 56 | MG | 1A | 3822 | 1/1 | 0.87 | 0.14 | 25,25,25,25 | 0 |
| 56 | MG | 2A | 3361 | 1/1 | 0.87 | 0.19 | 61,61,61,61 | 0 |
| 56 | MG | 1N | 205 | 1/1 | 0.87 | 0.10 | 57,57,57,57 | 0 |
| 56 | MG | 1O | 205 | 1/1 | 0.87 | 0.14 | 72,72,72,72 | 0 |
| 56 | MG | 1A | 3471 | 1/1 | 0.87 | 0.17 | 51,51,51,51 | 0 |
| 56 | MG | 2A | 3380 | 1/1 | 0.87 | 0.14 | 75,75,75,75 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 2a | 3062 | 1/1 | 0.87 | 0.23 | 71,71,71,71 | 0 |
| 56 | MG | 2A | 3089 | 1/1 | 0.87 | 0.27 | 61,61,61,61 | 0 |
| 56 | MG | 1Q | 208 | 1/1 | 0.87 | 0.16 | 47,47,47,47 | 0 |
| 56 | MG | 2A | 3397 | 1/1 | 0.87 | 0.16 | 72,72,72,72 | 0 |
| 56 | MG | 2A | 3099 | 1/1 | 0.87 | 0.28 | 68,68,68,68 | 0 |
| 56 | MG | 2A | 3721 | 1/1 | 0.87 | 0.13 | 62,62,62,62 | 0 |
| 56 | MG | 1A | 3483 | 1/1 | 0.87 | 0.18 | 59,59,59,59 | 0 |
| 56 | MG | 2A | 3416 | 1/1 | 0.87 | 0.16 | 64,64,64,64 | 0 |
| 56 | MG | 2A | 3418 | 1/1 | 0.87 | 0.10 | 66,66,66,66 | 0 |
| 56 | MG | 1A | 3993 | 1/1 | 0.87 | 0.09 | 27,27,27,27 | 0 |
| 56 | MG | 2A | 3737 | 1/1 | 0.87 | 0.08 | 70,70,70,70 | 0 |
| 56 | MG | 2A | 3440 | 1/1 | 0.87 | 0.21 | 61,61,61,61 | 0 |
| 56 | MG | 2A | 3443 | 1/1 | 0.87 | 0.22 | 59,59,59,59 | 0 |
| 56 | MG | 1A | 3643 | 1/1 | 0.87 | 0.14 | 56,56,56,56 | 0 |
| 56 | MG | 2A | 3753 | 1/1 | 0.87 | 0.12 | 42,42,42,42 | 0 |
| 56 | MG | 2a | 3112 | 1/1 | 0.87 | 0.20 | 62,62,62,62 | 0 |
| 56 | MG | 2a | 3117 | 1/1 | 0.87 | 0.19 | 65,65,65,65 | 0 |
| 56 | MG | 1A | 3866 | 1/1 | 0.87 | 0.09 | 22,22,22,22 | 0 |
| 56 | MG | 2A | 3155 | 1/1 | 0.87 | 0.16 | 55,55,55,55 | 0 |
| 56 | MG | 2a | 3136 | 1/1 | 0.87 | 0.15 | 78,78,78,78 | 0 |
| 56 | MG | 2A | 3474 | 1/1 | 0.87 | 0.07 | 61,61,61,61 | 0 |
| 56 | MG | 2a | 3150 | 1/1 | 0.87 | 0.10 | 76,76,76,76 | 0 |
| 56 | MG | 1A | 4028 | 1/1 | 0.87 | 0.09 | 61,61,61,61 | 0 |
| 56 | MG | 1A | 3869 | 1/1 | 0.87 | 0.17 | 45,45,45,45 | 0 |
| 56 | MG | 1A | 3360 | 1/1 | 0.87 | 0.17 | 65,65,65,65 | 0 |
| 56 | MG | 1A | 3888 | 1/1 | 0.87 | 0.18 | 44,44,44,44 | 0 |
| 56 | MG | 2A | 3205 | 1/1 | 0.87 | 0.09 | 63,63,63,63 | 0 |
| 56 | MG | 2A | 3802 | 1/1 | 0.87 | 0.11 | 57,57,57,57 | 0 |
| 56 | MG | 2A | 3207 | 1/1 | 0.87 | 0.19 | 64,64,64,64 | 0 |
| 56 | MG | 1a | 1832 | 1/1 | 0.87 | 0.15 | 55,55,55,55 | 0 |
| 56 | MG | 2a | 3186 | 1/1 | 0.87 | 0.16 | 54,54,54,54 | 0 |
| 56 | MG | 1a | 1833 | 1/1 | 0.87 | 0.19 | 43,43,43,43 | 0 |
| 56 | MG | 2A | 3533 | 1/1 | 0.87 | 0.10 | 60,60,60,60 | 0 |
| 56 | MG | 1A | 3894 | 1/1 | 0.87 | 0.07 | 21,21,21,21 | 0 |
| 56 | MG | 1d | 301 | 1/1 | 0.87 | 0.17 | 48,48,48,48 | 0 |
| 56 | MG | 2A | 3562 | 1/1 | 0.87 | 0.13 | 35,35,35,35 | 0 |
| 56 | MG | 2A | 3563 | 1/1 | 0.87 | 0.10 | 36,36,36,36 | 0 |
| 56 | MG | 2a | 3202 | 1/1 | 0.87 | 0.26 | 75,75,75,75 | 0 |
| 56 | MG | 2A | 3568 | 1/1 | 0.87 | 0.10 | 47,47,47,47 | 0 |
| 56 | MG | 1A | 4049 | 1/1 | 0.87 | 0.11 | 54,54,54,54 | 0 |
| 56 | MG | 2A | 3838 | 1/1 | 0.87 | 0.17 | 43,43,43,43 | 0 |
| 56 | MG | 1A | 3143 | 1/1 | 0.87 | 0.10 | 37,37,37,37 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 2A | 3586 | 1/1 | 0.87 | 0.11 | 60,60,60,60 | 0 |
| 56 | MG | 2A | 3860 | 1/1 | 0.87 | 0.11 | 73,73,73,73 | 0 |
| 56 | MG | 2A | 3254 | 1/1 | 0.87 | 0.28 | 63,63,63,63 | 0 |
| 56 | MG | 1A | 3514 | 1/1 | 0.87 | 0.21 | 64,64,64,64 | 0 |
| 56 | MG | 1A | 3793 | 1/1 | 0.87 | 0.14 | 56,56,56,56 | 0 |
| 56 | MG | 2A | 3884 | 1/1 | 0.87 | 0.38 | 61,61,61,61 | 0 |
| 56 | MG | 2A | 3886 | 1/1 | 0.87 | 0.17 | 71,71,71,71 | 0 |
| 56 | MG | 2A | 3280 | 1/1 | 0.87 | 0.15 | 57,57,57,57 | 0 |
| 56 | MG | 2B | 215 | 1/1 | 0.87 | 0.19 | 69,69,69,69 | 0 |
| 56 | MG | 1w | 106 | 1/1 | 0.87 | 0.12 | 61,61,61,61 | 0 |
| 56 | MG | 1x | 104 | 1/1 | 0.87 | 0.34 | 56,56,56,56 | 0 |
| 56 | MG | 1x | 109 | 1/1 | 0.87 | 0.17 | 61,61,61,61 | 0 |
| 56 | MG | 2A | 3614 | 1/1 | 0.87 | 0.14 | 45,45,45,45 | 0 |
| 56 | MG | 2m | 201 | 1/1 | 0.87 | 0.27 | 73,73,73,73 | 0 |
| 56 | MG | 2A | 3618 | 1/1 | 0.87 | 0.10 | 49,49,49,49 | 0 |
| 56 | MG | 1A | 3682 | 1/1 | 0.87 | 0.14 | 61,61,61,61 | 0 |
| 56 | MG | 2A | 3300 | 1/1 | 0.87 | 0.17 | 52,52,52,52 | 0 |
| 56 | MG | 1a | 1662 | 1/1 | 0.87 | 0.20 | 60,60,60,60 | 0 |
| 56 | MG | 1A | 3531 | 1/1 | 0.87 | 0.15 | 47,47,47,47 | 0 |
| 56 | MG | 1A | 4084 | 1/1 | 0.87 | 0.14 | 14,14,14,14 | 0 |
| 56 | MG | 1A | 4093 | 1/1 | 0.87 | 0.10 | 38,38,38,38 | 0 |
| 56 | MG | 2A | 3643 | 1/1 | 0.87 | 0.12 | 62,62,62,62 | 0 |
| 56 | MG | 1A | 4081 | 1/1 | 0.88 | 0.10 | 44,44,44,44 | 0 |
| 56 | MG | 1A | 3784 | 1/1 | 0.88 | 0.08 | 66,66,66,66 | 0 |
| 56 | MG | 2T | 202 | 1/1 | 0.88 | 0.14 | 61,61,61,61 | 0 |
| 56 | MG | 2U | 201 | 1/1 | 0.88 | 0.12 | 54,54,54,54 | 0 |
| 56 | MG | 2A | 3615 | 1/1 | 0.88 | 0.16 | 60,60,60,60 | 0 |
| 56 | MG | 2A | 3303 | 1/1 | 0.88 | 0.25 | 71,71,71,71 | 0 |
| 56 | MG | 1A | 3650 | 1/1 | 0.88 | 0.09 | 49,49,49,49 | 0 |
| 56 | MG | 1a | 1667 | 1/1 | 0.88 | 0.26 | 58,58,58,58 | 0 |
| 56 | MG | 1a | 1669 | 1/1 | 0.88 | 0.11 | 75,75,75,75 | 0 |
| 56 | MG | 2a | 3007 | 1/1 | 0.88 | 0.19 | 63,63,63,63 | 0 |
| 56 | MG | 1a | 1674 | 1/1 | 0.88 | 0.10 | 53,53,53,53 | 0 |
| 56 | MG | 2A | 3323 | 1/1 | 0.88 | 0.10 | 57,57,57,57 | 0 |
| 56 | MG | 2A | 3324 | 1/1 | 0.88 | 0.16 | 49,49,49,49 | 0 |
| 56 | MG | 2A | 3329 | 1/1 | 0.88 | 0.20 | 60,60,60,60 | 0 |
| 56 | MG | 1x | 115 | 1/1 | 0.88 | 0.24 | 64,64,64,64 | 0 |
| 56 | MG | 1a | 1688 | 1/1 | 0.88 | 0.27 | 63,63,63,63 | 0 |
| 56 | MG | 1A | 3399 | 1/1 | 0.88 | 0.09 | 48,48,48,48 | 0 |
| 56 | MG | 1A | 3513 | 1/1 | 0.88 | 0.23 | 63,63,63,63 | 0 |
| 56 | MG | 2a | 3032 | 1/1 | 0.88 | 0.43 | 65,65,65,65 | 0 |
| 56 | MG | 2a | 3034 | 1/1 | 0.88 | 0.12 | 72,72,72,72 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 1A | 3124 | 1/1 | 0.88 | 0.13 | 46,46,46,46 | 0 |
| 56 | MG | 2A | 3343 | 1/1 | 0.88 | 0.20 | 57,57,57,57 | 0 |
| 56 | MG | 2A | 3039 | 1/1 | 0.88 | 0.33 | 65,65,65,65 | 0 |
| 56 | MG | 1A | 3675 | 1/1 | 0.88 | 0.09 | 24,24,24,24 | 0 |
| 56 | MG | 2a | 3045 | 1/1 | 0.88 | 0.33 | 72,72,72,72 | 0 |
| 56 | MG | 1A | 3339 | 1/1 | 0.88 | 0.12 | 42,42,42,42 | 0 |
| 56 | MG | 2A | 3684 | 1/1 | 0.88 | 0.22 | 56,56,56,56 | 0 |
| 56 | MG | 1a | 1707 | 1/1 | 0.88 | 0.14 | 57,57,57,57 | 0 |
| 56 | MG | 1A | 3955 | 1/1 | 0.88 | 0.09 | 65,65,65,65 | 0 |
| 56 | MG | 1A | 3208 | 1/1 | 0.88 | 0.11 | 61,61,61,61 | 0 |
| 56 | MG | 1a | 1730 | 1/1 | 0.88 | 0.22 | 65,65,65,65 | 0 |
| 56 | MG | 2A | 3066 | 1/1 | 0.88 | 0.08 | 51,51,51,51 | 0 |
| 56 | MG | 2A | 3703 | 1/1 | 0.88 | 0.12 | 59,59,59,59 | 0 |
| 56 | MG | 1A | 3533 | 1/1 | 0.88 | 0.12 | 55,55,55,55 | 0 |
| 56 | MG | 2A | 3373 | 1/1 | 0.88 | 0.17 | 67,67,67,67 | 0 |
| 56 | MG | 1A | 3548 | 1/1 | 0.88 | 0.24 | 46,46,46,46 | 0 |
| 56 | MG | 1A | 3823 | 1/1 | 0.88 | 0.17 | 50,50,50,50 | 0 |
| 56 | MG | 2A | 3387 | 1/1 | 0.88 | 0.27 | 62,62,62,62 | 0 |
| 56 | MG | 1A | 3461 | 1/1 | 0.88 | 0.14 | 61,61,61,61 | 0 |
| 56 | MG | 1a | 1759 | 1/1 | 0.88 | 0.14 | 61,61,61,61 | 0 |
| 56 | MG | 1A | 3563 | 1/1 | 0.88 | 0.12 | 53,53,53,53 | 0 |
| 56 | MG | 1A | 3709 | 1/1 | 0.88 | 0.09 | 41,41,41,41 | 0 |
| 56 | MG | 2A | 3121 | 1/1 | 0.88 | 0.14 | 48,48,48,48 | 0 |
| 56 | MG | 1A | 4016 | 1/1 | 0.88 | 0.09 | 25,25,25,25 | 0 |
| 56 | MG | 2a | 3102 | 1/1 | 0.88 | 0.12 | 54,54,54,54 | 0 |
| 56 | MG | 1a | 1774 | 1/1 | 0.88 | 0.16 | 61,61,61,61 | 0 |
| 56 | MG | 1A | 4018 | 1/1 | 0.88 | 0.10 | 35,35,35,35 | 0 |
| 56 | MG | 1T | 201 | 1/1 | 0.88 | 0.09 | 47,47,47,47 | 0 |
| 56 | MG | 2a | 3113 | 1/1 | 0.88 | 0.10 | 56,56,56,56 | 0 |
| 56 | MG | 1A | 3855 | 1/1 | 0.88 | 0.10 | 20,20,20,20 | 0 |
| 56 | MG | 2a | 3120 | 1/1 | 0.88 | 0.25 | 66,66,66,66 | 0 |
| 56 | MG | 1X | 104 | 1/1 | 0.88 | 0.19 | 61,61,61,61 | 0 |
| 56 | MG | 2a | 3124 | 1/1 | 0.88 | 0.20 | 55,55,55,55 | 0 |
| 56 | MG | 2A | 3751 | 1/1 | 0.88 | 0.10 | 67,67,67,67 | 0 |
| 56 | MG | 1A | 3722 | 1/1 | 0.88 | 0.15 | 59,59,59,59 | 0 |
| 56 | MG | 2A | 3455 | 1/1 | 0.88 | 0.29 | 61,61,61,61 | 0 |
| 56 | MG | 2A | 3457 | 1/1 | 0.88 | 0.13 | 50,50,50,50 | 0 |
| 56 | MG | 2a | 3151 | 1/1 | 0.88 | 0.08 | 91,91,91,91 | 0 |
| 56 | MG | 2a | 3153 | 1/1 | 0.88 | 0.13 | 73,73,73,73 | 0 |
| 56 | MG | 2A | 3460 | 1/1 | 0.88 | 0.19 | 57,57,57,57 | 0 |
| 56 | MG | 10 | 102 | 1/1 | 0.88 | 0.08 | 41,41,41,41 | 0 |
| 56 | MG | 2A | 3204 | 1/1 | 0.88 | 0.12 | 47,47,47,47 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 2A | 3475 | 1/1 | 0.88 | 0.18 | 56,56,56,56 | 0 |
| 56 | MG | 10 | 104 | 1/1 | 0.88 | 0.14 | 59,59,59,59 | 0 |
| 56 | MG | 2A | 3490 | 1/1 | 0.88 | 0.28 | 53,53,53,53 | 0 |
| 56 | MG | 1A | 3725 | 1/1 | 0.88 | 0.15 | 66,66,66,66 | 0 |
| 56 | MG | 16 | 102 | 1/1 | 0.88 | 0.22 | 40,40,40,40 | 0 |
| 56 | MG | 2a | 3183 | 1/1 | 0.88 | 0.14 | 60,60,60,60 | 0 |
| 56 | MG | 2A | 3498 | 1/1 | 0.88 | 0.16 | 58,58,58,58 | 0 |
| 56 | MG | 1a | 1831 | 1/1 | 0.88 | 0.21 | 43,43,43,43 | 0 |
| 56 | MG | 2a | 3190 | 1/1 | 0.88 | 0.18 | 77,77,77,77 | 0 |
| 56 | MG | 2A | 3812 | 1/1 | 0.88 | 0.22 | 76,76,76,76 | 0 |
| 56 | MG | 2A | 3216 | 1/1 | 0.88 | 0.21 | 65,65,65,65 | 0 |
| 56 | MG | 2A | 3222 | 1/1 | 0.88 | 0.10 | 61,61,61,61 | 0 |
| 56 | MG | 2A | 3525 | 1/1 | 0.88 | 0.15 | 60,60,60,60 | 0 |
| 56 | MG | 2a | 3200 | 1/1 | 0.88 | 0.16 | 77,77,77,77 | 0 |
| 56 | MG | 1A | 3726 | 1/1 | 0.88 | 0.09 | 53,53,53,53 | 0 |
| 56 | MG | 2A | 3826 | 1/1 | 0.88 | 0.16 | 55,55,55,55 | 0 |
| 56 | MG | 1A | 3420 | 1/1 | 0.88 | 0.20 | 51,51,51,51 | 0 |
| 56 | MG | 1A | 3892 | 1/1 | 0.88 | 0.11 | 30,30,30,30 | 0 |
| 56 | MG | 2A | 3237 | 1/1 | 0.88 | 0.21 | 44,44,44,44 | 0 |
| 56 | MG | 2A | 3239 | 1/1 | 0.88 | 0.17 | 56,56,56,56 | 0 |
| 56 | MG | 1A | 4053 | 1/1 | 0.88 | 0.09 | 34,34,34,34 | 0 |
| 56 | MG | 2A | 3251 | 1/1 | 0.88 | 0.19 | 62,62,62,62 | 0 |
| 56 | MG | 2A | 3566 | 1/1 | 0.88 | 0.11 | 44,44,44,44 | 0 |
| 56 | MG | 2A | 3253 | 1/1 | 0.88 | 0.16 | 64,64,64,64 | 0 |
| 56 | MG | 1A | 3053 | 1/1 | 0.88 | 0.15 | 62,62,62,62 | 0 |
| 56 | MG | 2A | 3875 | 1/1 | 0.88 | 0.18 | 74,74,74,74 | 0 |
| 56 | MG | 2A | 3878 | 1/1 | 0.88 | 0.16 | 38,38,38,38 | 0 |
| 56 | MG | 2A | 3575 | 1/1 | 0.88 | 0.20 | 65,65,65,65 | 0 |
| 56 | MG | 2a | 3241 | 1/1 | 0.88 | 0.24 | 63,63,63,63 | 0 |
| 56 | MG | 1f | 202 | 1/1 | 0.88 | 0.21 | 70,70,70,70 | 0 |
| 56 | MG | 2A | 3259 | 1/1 | 0.88 | 0.09 | 60,60,60,60 | 0 |
| 56 | MG | 2B | 203 | 1/1 | 0.88 | 0.19 | 60,60,60,60 | 0 |
| 56 | MG | 2A | 3587 | 1/1 | 0.88 | 0.22 | 56,56,56,56 | 0 |
| 56 | MG | 2B | 212 | 1/1 | 0.88 | 0.14 | 57,57,57,57 | 0 |
| 56 | MG | 2B | 213 | 1/1 | 0.88 | 0.18 | 56,56,56,56 | 0 |
| 56 | MG | 2q | 201 | 1/1 | 0.88 | 0.16 | 68,68,68,68 | 0 |
| 56 | MG | 1A | 3494 | 1/1 | 0.88 | 0.13 | 56,56,56,56 | 0 |
| 56 | MG | 1A | 4059 | 1/1 | 0.88 | 0.12 | 27,27,27,27 | 0 |
| 56 | MG | 1A | 3372 | 1/1 | 0.88 | 0.14 | 43,43,43,43 | 0 |
| 56 | MG | 2w | 103 | 1/1 | 0.88 | 0.10 | 64,64,64,64 | 0 |
| 56 | MG | 2A | 3600 | 1/1 | 0.88 | 0.11 | 56,56,56,56 | 0 |
| 56 | MG | 1w | 105 | 1/1 | 0.88 | 0.15 | 62,62,62,62 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 2D | 308 | 1/1 | 0.88 | 0.08 | 39,39,39,39 | 0 |
| 56 | MG | 1A | 3772 | 1/1 | 0.88 | 0.09 | 28,28,28,28 | 0 |
| 56 | MG | 1w | 110 | 1/1 | 0.88 | 0.20 | 74,74,74,74 | 0 |
| 56 | MG | 2A | 3250 | 1/1 | 0.89 | 0.12 | 64,64,64,64 | 0 |
| 56 | MG | 1a | 1625 | 1/1 | 0.89 | 0.12 | 55,55,55,55 | 0 |
| 56 | MG | 2A | 3252 | 1/1 | 0.89 | 0.13 | 48,48,48,48 | 0 |
| 56 | MG | 1a | 1626 | 1/1 | 0.89 | 0.18 | 52,52,52,52 | 0 |
| 56 | MG | 2A | 3572 | 1/1 | 0.89 | 0.18 | 51,51,51,51 | 0 |
| 56 | MG | 1A | 3676 | 1/1 | 0.89 | 0.09 | 16,16,16,16 | 0 |
| 56 | MG | 1a | 1640 | 1/1 | 0.89 | 0.26 | 69,69,69,69 | 0 |
| 56 | MG | 1A | 3789 | 1/1 | 0.89 | 0.10 | 43,43,43,43 | 0 |
| 56 | MG | 1A | 3561 | 1/1 | 0.89 | 0.29 | 62,62,62,62 | 0 |
| 56 | MG | 2R | 202 | 1/1 | 0.89 | 0.12 | 47,47,47,47 | 0 |
| 56 | MG | 2A | 3594 | 1/1 | 0.89 | 0.18 | 66,66,66,66 | 0 |
| 56 | MG | 2A | 3262 | 1/1 | 0.89 | 0.11 | 60,60,60,60 | 0 |
| 56 | MG | 2W | 201 | 1/1 | 0.89 | 0.07 | 57,57,57,57 | 0 |
| 56 | MG | 1A | 4068 | 1/1 | 0.89 | 0.10 | 61,61,61,61 | 0 |
| 56 | MG | 2A | 3281 | 1/1 | 0.89 | 0.13 | 70,70,70,70 | 0 |
| 56 | MG | 1A | 4076 | 1/1 | 0.89 | 0.15 | 36,36,36,36 | 0 |
| 56 | MG | 2a | 3002 | 1/1 | 0.89 | 0.07 | 63,63,63,63 | 0 |
| 56 | MG | 1A | 3292 | 1/1 | 0.89 | 0.13 | 57,57,57,57 | 0 |
| 56 | MG | 2A | 3295 | 1/1 | 0.89 | 0.09 | 58,58,58,58 | 0 |
| 56 | MG | 2a | 3006 | 1/1 | 0.89 | 0.17 | 61,61,61,61 | 0 |
| 56 | MG | 2A | 3605 | 1/1 | 0.89 | 0.10 | 51,51,51,51 | 0 |
| 56 | MG | 2a | 3009 | 1/1 | 0.89 | 0.13 | 72,72,72,72 | 0 |
| 56 | MG | 2a | 3010 | 1/1 | 0.89 | 0.18 | 60,60,60,60 | 0 |
| 56 | MG | 2a | 3011 | 1/1 | 0.89 | 0.23 | 66,66,66,66 | 0 |
| 56 | MG | 2A | 3608 | 1/1 | 0.89 | 0.10 | 34,34,34,34 | 0 |
| 56 | MG | 1w | 109 | 1/1 | 0.89 | 0.24 | 77,77,77,77 | 0 |
| 56 | MG | 2a | 3015 | 1/1 | 0.89 | 0.32 | 69,69,69,69 | 0 |
| 56 | MG | 1A | 3796 | 1/1 | 0.89 | 0.15 | 20,20,20,20 | 0 |
| 56 | MG | 1w | 112 | 1/1 | 0.89 | 0.13 | 53,53,53,53 | 0 |
| 56 | MG | 1A | 3924 | 1/1 | 0.89 | 0.11 | 71,71,71,71 | 0 |
| 56 | MG | 1A | 3574 | 1/1 | 0.89 | 0.22 | 40,40,40,40 | 0 |
| 56 | MG | 1a | 1673 | 1/1 | 0.89 | 0.14 | 63,63,63,63 | 0 |
| 56 | MG | 1A | 3691 | 1/1 | 0.89 | 0.12 | 24,24,24,24 | 0 |
| 56 | MG | 1a | 1675 | 1/1 | 0.89 | 0.23 | 64,64,64,64 | 0 |
| 56 | MG | 1B | 202 | 1/1 | 0.89 | 0.18 | 47,47,47,47 | 0 |
| 56 | MG | 1A | 3331 | 1/1 | 0.89 | 0.10 | 43,43,43,43 | 0 |
| 56 | MG | 1B | 208 | 1/1 | 0.89 | 0.16 | 57,57,57,57 | 0 |
| 56 | MG | 2A | 3002 | 1/1 | 0.89 | 0.23 | 53,53,53,53 | 0 |
| 56 | MG | 1A | 3602 | 1/1 | 0.89 | 0.13 | 47,47,47,47 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 2a | 3044 | 1/1 | 0.89 | 0.22 | 56,56,56,56 | 0 |
| 56 | MG | 1A | 3251 | 1/1 | 0.89 | 0.17 | 69,69,69,69 | 0 |
| 56 | MG | 2A | 3652 | 1/1 | 0.89 | 0.13 | 50,50,50,50 | 0 |
| 56 | MG | 2A | 3657 | 1/1 | 0.89 | 0.12 | 84,84,84,84 | 0 |
| 56 | MG | 1A | 3966 | 1/1 | 0.89 | 0.12 | 36,36,36,36 | 0 |
| 56 | MG | 2A | 3337 | 1/1 | 0.89 | 0.10 | 49,49,49,49 | 0 |
| 56 | MG | 2A | 3034 | 1/1 | 0.89 | 0.11 | 56,56,56,56 | 0 |
| 56 | MG | 1A | 3703 | 1/1 | 0.89 | 0.14 | 48,48,48,48 | 0 |
| 56 | MG | 1a | 1709 | 1/1 | 0.89 | 0.20 | 50,50,50,50 | 0 |
| 56 | MG | 1A | 3971 | 1/1 | 0.89 | 0.15 | 32,32,32,32 | 0 |
| 56 | MG | 2A | 3054 | 1/1 | 0.89 | 0.19 | 63,63,63,63 | 0 |
| 56 | MG | 2A | 3680 | 1/1 | 0.89 | 0.12 | 54,54,54,54 | 0 |
| 56 | MG | 2A | 3348 | 1/1 | 0.89 | 0.08 | 65,65,65,65 | 0 |
| 56 | MG | 1A | 3706 | 1/1 | 0.89 | 0.12 | 53,53,53,53 | 0 |
| 56 | MG | 1A | 3708 | 1/1 | 0.89 | 0.09 | 45,45,45,45 | 0 |
| 56 | MG | 1F | 308 | 1/1 | 0.89 | 0.13 | 49,49,49,49 | 0 |
| 56 | MG | 2a | 3086 | 1/1 | 0.89 | 0.20 | 63,63,63,63 | 0 |
| 56 | MG | 2A | 3693 | 1/1 | 0.89 | 0.21 | 62,62,62,62 | 0 |
| 56 | MG | 1a | 1734 | 1/1 | 0.89 | 0.16 | 53,53,53,53 | 0 |
| 56 | MG | 1F | 309 | 1/1 | 0.89 | 0.12 | 53,53,53,53 | 0 |
| 56 | MG | 1a | 1746 | 1/1 | 0.89 | 0.11 | 59,59,59,59 | 0 |
| 56 | MG | 2A | 3704 | 1/1 | 0.89 | 0.13 | 44,44,44,44 | 0 |
| 56 | MG | 2A | 3365 | 1/1 | 0.89 | 0.11 | 54,54,54,54 | 0 |
| 56 | MG | 2A | 3710 | 1/1 | 0.89 | 0.13 | 42,42,42,42 | 0 |
| 56 | MG | 2A | 3367 | 1/1 | 0.89 | 0.15 | 54,54,54,54 | 0 |
| 56 | MG | 2a | 3108 | 1/1 | 0.89 | 0.30 | 65,65,65,65 | 0 |
| 56 | MG | 2A | 3085 | 1/1 | 0.89 | 0.18 | 55,55,55,55 | 0 |
| 56 | MG | 1a | 1751 | 1/1 | 0.89 | 0.15 | 52,52,52,52 | 0 |
| 56 | MG | 2a | 3116 | 1/1 | 0.89 | 0.23 | 53,53,53,53 | 0 |
| 56 | MG | 2A | 3087 | 1/1 | 0.89 | 0.13 | 48,48,48,48 | 0 |
| 56 | MG | 1A | 3988 | 1/1 | 0.89 | 0.15 | 21,21,21,21 | 0 |
| 56 | MG | 2A | 3383 | 1/1 | 0.89 | 0.16 | 66,66,66,66 | 0 |
| 56 | MG | 1A | 3989 | 1/1 | 0.89 | 0.12 | 31,31,31,31 | 0 |
| 56 | MG | 2a | 3127 | 1/1 | 0.89 | 0.19 | 63,63,63,63 | 0 |
| 56 | MG | 2a | 3132 | 1/1 | 0.89 | 0.10 | 54,54,54,54 | 0 |
| 56 | MG | 2a | 3133 | 1/1 | 0.89 | 0.20 | 66,66,66,66 | 0 |
| 56 | MG | 1A | 3826 | 1/1 | 0.89 | 0.11 | 45,45,45,45 | 0 |
| 56 | MG | 1A | 3835 | 1/1 | 0.89 | 0.09 | 33,33,33,33 | 0 |
| 56 | MG | 2A | 3108 | 1/1 | 0.89 | 0.29 | 65,65,65,65 | 0 |
| 56 | MG | 1a | 1766 | 1/1 | 0.89 | 0.08 | 61,61,61,61 | 0 |
| 56 | MG | 1A | 3098 | 1/1 | 0.89 | 0.09 | 44,44,44,44 | 0 |
| 56 | MG | 2A | 3408 | 1/1 | 0.89 | 0.27 | 52,52,52,52 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 2A | 3746 | 1/1 | 0.89 | 0.19 | 57,57,57,57 | 0 |
| 56 | MG | 2A | 3414 | 1/1 | 0.89 | 0.09 | 59,59,59,59 | 0 |
| 56 | MG | 1A | 3712 | 1/1 | 0.89 | 0.08 | 54,54,54,54 | 0 |
| 56 | MG | 2a | 3164 | 1/1 | 0.89 | 0.10 | 58,58,58,58 | 0 |
| 56 | MG | 1A | 3359 | 1/1 | 0.89 | 0.22 | 58,58,58,58 | 0 |
| 56 | MG | 2A | 3424 | 1/1 | 0.89 | 0.21 | 49,49,49,49 | 0 |
| 56 | MG | 2A | 3431 | 1/1 | 0.89 | 0.21 | 49,49,49,49 | 0 |
| 56 | MG | 2A | 3138 | 1/1 | 0.89 | 0.20 | 70,70,70,70 | 0 |
| 56 | MG | 2A | 3437 | 1/1 | 0.89 | 0.17 | 56,56,56,56 | 0 |
| 56 | MG | 2A | 3140 | 1/1 | 0.89 | 0.16 | 57,57,57,57 | 0 |
| 56 | MG | 1A | 4017 | 1/1 | 0.89 | 0.09 | 39,39,39,39 | 0 |
| 56 | MG | 1A | 3644 | 1/1 | 0.89 | 0.09 | 58,58,58,58 | 0 |
| 56 | MG | 2A | 3169 | 1/1 | 0.89 | 0.09 | 57,57,57,57 | 0 |
| 56 | MG | 2A | 3781 | 1/1 | 0.89 | 0.09 | 57,57,57,57 | 0 |
| 56 | MG | 1A | 3534 | 1/1 | 0.89 | 0.17 | 63,63,63,63 | 0 |
| 56 | MG | 2A | 3799 | 1/1 | 0.89 | 0.12 | 75,75,75,75 | 0 |
| 56 | MG | 2A | 3801 | 1/1 | 0.89 | 0.09 | 80,80,80,80 | 0 |
| 56 | MG | 1a | 1785 | 1/1 | 0.89 | 0.08 | 65,65,65,65 | 0 |
| 56 | MG | 2A | 3189 | 1/1 | 0.89 | 0.11 | 60,60,60,60 | 0 |
| 56 | MG | 2A | 3463 | 1/1 | 0.89 | 0.23 | 55,55,55,55 | 0 |
| 56 | MG | 2A | 3466 | 1/1 | 0.89 | 0.10 | 47,47,47,47 | 0 |
| 56 | MG | 2A | 3810 | 1/1 | 0.89 | 0.11 | 78,78,78,78 | 0 |
| 56 | MG | 1a | 1786 | 1/1 | 0.89 | 0.09 | 73,73,73,73 | 0 |
| 56 | MG | 2A | 3815 | 1/1 | 0.89 | 0.10 | 73,73,73,73 | 0 |
| 56 | MG | 2A | 3196 | 1/1 | 0.89 | 0.16 | 62,62,62,62 | 0 |
| 56 | MG | 1a | 1787 | 1/1 | 0.89 | 0.12 | 66,66,66,66 | 0 |
| 56 | MG | 1A | 3654 | 1/1 | 0.89 | 0.10 | 37,37,37,37 | 0 |
| 56 | MG | 2A | 3821 | 1/1 | 0.89 | 0.09 | 55,55,55,55 | 0 |
| 56 | MG | 2A | 3485 | 1/1 | 0.89 | 0.26 | 44,44,44,44 | 0 |
| 56 | MG | 1A | 3547 | 1/1 | 0.89 | 0.09 | 42,42,42,42 | 0 |
| 56 | MG | 1a | 1795 | 1/1 | 0.89 | 0.11 | 64,64,64,64 | 0 |
| 56 | MG | 1A | 3877 | 1/1 | 0.89 | 0.18 | 30,30,30,30 | 0 |
| 56 | MG | 2A | 3497 | 1/1 | 0.89 | 0.13 | 51,51,51,51 | 0 |
| 56 | MG | 2A | 3212 | 1/1 | 0.89 | 0.24 | 66,66,66,66 | 0 |
| 56 | MG | 1a | 1807 | 1/1 | 0.89 | 0.10 | 66,66,66,66 | 0 |
| 56 | MG | 2A | 3503 | 1/1 | 0.89 | 0.16 | 39,39,39,39 | 0 |
| 56 | MG | 2A | 3509 | 1/1 | 0.89 | 0.11 | 41,41,41,41 | 0 |
| 56 | MG | 1a | 1809 | 1/1 | 0.89 | 0.11 | 72,72,72,72 | 0 |
| 56 | MG | 1a | 1812 | 1/1 | 0.89 | 0.10 | 62,62,62,62 | 0 |
| 56 | MG | 1A | 3503 | 1/1 | 0.89 | 0.15 | 57,57,57,57 | 0 |
| 56 | MG | 1A | 3891 | 1/1 | 0.89 | 0.12 | 21,21,21,21 | 0 |
| 56 | MG | 1A | 3240 | 1/1 | 0.89 | 0.12 | 34,34,34,34 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 1A | 3559 | 1/1 | 0.89 | 0.21 | 54,54,54,54 | 0 |
| 56 | MG | 1A | 3774 | 1/1 | 0.89 | 0.10 | 19,19,19,19 | 0 |
| 56 | MG | 2A | 3540 | 1/1 | 0.89 | 0.10 | 35,35,35,35 | 0 |
| 56 | MG | 2A | 3541 | 1/1 | 0.89 | 0.12 | 49,49,49,49 | 0 |
| 56 | MG | 1a | 1617 | 1/1 | 0.89 | 0.09 | 53,53,53,53 | 0 |
| 56 | MG | 2A | 3556 | 1/1 | 0.89 | 0.22 | 50,50,50,50 | 0 |
| 56 | MG | 2A | 3248 | 1/1 | 0.89 | 0.23 | 65,65,65,65 | 0 |
| 56 | MG | 1a | 1799 | 1/1 | 0.90 | 0.15 | 46,46,46,46 | 0 |
| 56 | MG | 2B | 201 | 1/1 | 0.90 | 0.18 | 66,66,66,66 | 0 |
| 56 | MG | 2A | 3227 | 1/1 | 0.90 | 0.15 | 56,56,56,56 | 0 |
| 56 | MG | 2B | 204 | 1/1 | 0.90 | 0.10 | 61,61,61,61 | 0 |
| 56 | MG | 1A | 3238 | 1/1 | 0.90 | 0.29 | 56,56,56,56 | 0 |
| 56 | MG | 1Z | 301 | 1/1 | 0.90 | 0.11 | 48,48,48,48 | 0 |
| 56 | MG | 1Z | 302 | 1/1 | 0.90 | 0.08 | 60,60,60,60 | 0 |
| 56 | MG | 2B | 214 | 1/1 | 0.90 | 0.21 | 62,62,62,62 | 0 |
| 56 | MG | 1A | 3809 | 1/1 | 0.90 | 0.12 | 39,39,39,39 | 0 |
| 56 | MG | 2A | 3240 | 1/1 | 0.90 | 0.12 | 51,51,51,51 | 0 |
| 56 | MG | 2A | 3551 | 1/1 | 0.90 | 0.12 | 43,43,43,43 | 0 |
| 56 | MG | 1A | 3990 | 1/1 | 0.90 | 0.09 | 33,33,33,33 | 0 |
| 56 | MG | 1A | 3816 | 1/1 | 0.90 | 0.15 | 54,54,54,54 | 0 |
| 56 | MG | 1A | 3189 | 1/1 | 0.90 | 0.25 | 47,47,47,47 | 0 |
| 56 | MG | 2A | 3564 | 1/1 | 0.90 | 0.13 | 53,53,53,53 | 0 |
| 56 | MG | 1A | 3819 | 1/1 | 0.90 | 0.08 | 44,44,44,44 | 0 |
| 56 | MG | 1A | 3136 | 1/1 | 0.90 | 0.09 | 41,41,41,41 | 0 |
| 56 | MG | 1A | 3467 | 1/1 | 0.90 | 0.12 | 46,46,46,46 | 0 |
| 56 | MG | 1A | 3253 | 1/1 | 0.90 | 0.12 | 54,54,54,54 | 0 |
| 56 | MG | 1A | 3700 | 1/1 | 0.90 | 0.10 | 25,25,25,25 | 0 |
| 56 | MG | 1A | 3836 | 1/1 | 0.90 | 0.10 | 50,50,50,50 | 0 |
| 56 | MG | 1A | 3473 | 1/1 | 0.90 | 0.16 | 65,65,65,65 | 0 |
| 56 | MG | 1A | 3705 | 1/1 | 0.90 | 0.12 | 28,28,28,28 | 0 |
| 56 | MG | 2A | 3264 | 1/1 | 0.90 | 0.15 | 56,56,56,56 | 0 |
| 56 | MG | 25 | 104 | 1/1 | 0.90 | 0.14 | 54,54,54,54 | 0 |
| 56 | MG | 25 | 105 | 1/1 | 0.90 | 0.12 | 49,49,49,49 | 0 |
| 56 | MG | 2A | 3265 | 1/1 | 0.90 | 0.17 | 57,57,57,57 | 0 |
| 56 | MG | 2a | 3001 | 1/1 | 0.90 | 0.14 | 57,57,57,57 | 0 |
| 56 | MG | 2A | 3274 | 1/1 | 0.90 | 0.15 | 59,59,59,59 | 0 |
| 56 | MG | 2A | 3276 | 1/1 | 0.90 | 0.09 | 51,51,51,51 | 0 |
| 56 | MG | 2A | 3278 | 1/1 | 0.90 | 0.18 | 65,65,65,65 | 0 |
| 56 | MG | 1a | 1630 | 1/1 | 0.90 | 0.15 | 60,60,60,60 | 0 |
| 56 | MG | 1A | 3847 | 1/1 | 0.90 | 0.14 | 51,51,51,51 | 0 |
| 56 | MG | 1A | 3481 | 1/1 | 0.90 | 0.12 | 40,40,40,40 | 0 |
| 56 | MG | 2A | 3606 | 1/1 | 0.90 | 0.10 | 62,62,62,62 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 1A | 3575 | 1/1 | 0.90 | 0.24 | 55,55,55,55 | 0 |
| 56 | MG | 2A | 3291 | 1/1 | 0.90 | 0.15 | 57,57,57,57 | 0 |
| 56 | MG | 2A | 3610 | 1/1 | 0.90 | 0.09 | 41,41,41,41 | 0 |
| 56 | MG | 2a | 3014 | 1/1 | 0.90 | 0.19 | 63,63,63,63 | 0 |
| 56 | MG | 2A | 3294 | 1/1 | 0.90 | 0.09 | 67,67,67,67 | 0 |
| 56 | MG | 1A | 3858 | 1/1 | 0.90 | 0.09 | 43,43,43,43 | 0 |
| 56 | MG | 1A | 3083 | 1/1 | 0.90 | 0.23 | 37,37,37,37 | 0 |
| 56 | MG | 1a | 1657 | 1/1 | 0.90 | 0.09 | 68,68,68,68 | 0 |
| 56 | MG | 1A | 3867 | 1/1 | 0.90 | 0.13 | 55,55,55,55 | 0 |
| 56 | MG | 1a | 1660 | 1/1 | 0.90 | 0.20 | 72,72,72,72 | 0 |
| 56 | MG | 2a | 3030 | 1/1 | 0.90 | 0.38 | 63,63,63,63 | 0 |
| 56 | MG | 1A | 3404 | 1/1 | 0.90 | 0.25 | 60,60,60,60 | 0 |
| 56 | MG | 2A | 3630 | 1/1 | 0.90 | 0.20 | 42,42,42,42 | 0 |
| 56 | MG | 1A | 3018 | 1/1 | 0.90 | 0.09 | 30,30,30,30 | 0 |
| 56 | MG | 1A | 4061 | 1/1 | 0.90 | 0.17 | 68,68,68,68 | 0 |
| 56 | MG | 2A | 3314 | 1/1 | 0.90 | 0.08 | 60,60,60,60 | 0 |
| 56 | MG | 1A | 3724 | 1/1 | 0.90 | 0.14 | 53,53,53,53 | 0 |
| 56 | MG | 2a | 3042 | 1/1 | 0.90 | 0.20 | 60,60,60,60 | 0 |
| 56 | MG | 1A | 3885 | 1/1 | 0.90 | 0.07 | 25,25,25,25 | 0 |
| 56 | MG | 1A | 4075 | 1/1 | 0.90 | 0.15 | 48,48,48,48 | 0 |
| 56 | MG | 1A | 3609 | 1/1 | 0.90 | 0.14 | 25,25,25,25 | 0 |
| 56 | MG | 2A | 3003 | 1/1 | 0.90 | 0.24 | 44,44,44,44 | 0 |
| 56 | MG | 2A | 3006 | 1/1 | 0.90 | 0.27 | 54,54,54,54 | 0 |
| 56 | MG | 2A | 3662 | 1/1 | 0.90 | 0.08 | 59,59,59,59 | 0 |
| 56 | MG | 2A | 3664 | 1/1 | 0.90 | 0.15 | 57,57,57,57 | 0 |
| 56 | MG | 1a | 1687 | 1/1 | 0.90 | 0.14 | 50,50,50,50 | 0 |
| 56 | MG | 1A | 3611 | 1/1 | 0.90 | 0.12 | 36,36,36,36 | 0 |
| 56 | MG | 2A | 3673 | 1/1 | 0.90 | 0.12 | 57,57,57,57 | 0 |
| 56 | MG | 1A | 3624 | 1/1 | 0.90 | 0.17 | 46,46,46,46 | 0 |
| 56 | MG | 2a | 3066 | 1/1 | 0.90 | 0.17 | 60,60,60,60 | 0 |
| 56 | MG | 1A | 3741 | 1/1 | 0.90 | 0.12 | 37,37,37,37 | 0 |
| 56 | MG | 1A | 4088 | 1/1 | 0.90 | 0.12 | 21,21,21,21 | 0 |
| 56 | MG | 1a | 1694 | 1/1 | 0.90 | 0.06 | 56,56,56,56 | 0 |
| 56 | MG | 1a | 1697 | 1/1 | 0.90 | 0.25 | 49,49,49,49 | 0 |
| 56 | MG | 2A | 3681 | 1/1 | 0.90 | 0.10 | 54,54,54,54 | 0 |
| 56 | MG | 2A | 3049 | 1/1 | 0.90 | 0.13 | 54,54,54,54 | 0 |
| 56 | MG | 2A | 3052 | 1/1 | 0.90 | 0.21 | 63,63,63,63 | 0 |
| 56 | MG | 2A | 3053 | 1/1 | 0.90 | 0.36 | 64,64,64,64 | 0 |
| 56 | MG | 2a | 3094 | 1/1 | 0.90 | 0.26 | 62,62,62,62 | 0 |
| 56 | MG | 1A | 3748 | 1/1 | 0.90 | 0.10 | 47,47,47,47 | 0 |
| 56 | MG | 1A | 3756 | 1/1 | 0.90 | 0.14 | 45,45,45,45 | 0 |
| 56 | MG | 2A | 3697 | 1/1 | 0.90 | 0.16 | 72,72,72,72 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 1A | 3762 | 1/1 | 0.90 | 0.14 | 21,21,21,21 | 0 |
| 56 | MG | 2A | 3356 | 1/1 | 0.90 | 0.10 | 62,62,62,62 | 0 |
| 56 | MG | 2a | 3104 | 1/1 | 0.90 | 0.15 | 54,54,54,54 | 0 |
| 56 | MG | 2A | 3357 | 1/1 | 0.90 | 0.09 | 50,50,50,50 | 0 |
| 56 | MG | 1A | 3340 | 1/1 | 0.90 | 0.14 | 50,50,50,50 | 0 |
| 56 | MG | 1a | 1714 | 1/1 | 0.90 | 0.16 | 62,62,62,62 | 0 |
| 56 | MG | 1A | 3916 | 1/1 | 0.90 | 0.10 | 22,22,22,22 | 0 |
| 56 | MG | 1a | 1716 | 1/1 | 0.90 | 0.08 | 49,49,49,49 | 0 |
| 56 | MG | 2A | 3074 | 1/1 | 0.90 | 0.13 | 41,41,41,41 | 0 |
| 56 | MG | 2A | 3083 | 1/1 | 0.90 | 0.13 | 57,57,57,57 | 0 |
| 56 | MG | 1a | 1720 | 1/1 | 0.90 | 0.28 | 51,51,51,51 | 0 |
| 56 | MG | 2A | 3378 | 1/1 | 0.90 | 0.15 | 55,55,55,55 | 0 |
| 56 | MG | 1B | 221 | 1/1 | 0.90 | 0.12 | 56,56,56,56 | 0 |
| 56 | MG | 2A | 3381 | 1/1 | 0.90 | 0.10 | 57,57,57,57 | 0 |
| 56 | MG | 2A | 3722 | 1/1 | 0.90 | 0.11 | 40,40,40,40 | 0 |
| 56 | MG | 1a | 1728 | 1/1 | 0.90 | 0.26 | 51,51,51,51 | 0 |
| 56 | MG | 2A | 3730 | 1/1 | 0.90 | 0.07 | 41,41,41,41 | 0 |
| 56 | MG | 1A | 3632 | 1/1 | 0.90 | 0.08 | 34,34,34,34 | 0 |
| 56 | MG | 1A | 3188 | 1/1 | 0.90 | 0.06 | 37,37,37,37 | 0 |
| 56 | MG | 2A | 3735 | 1/1 | 0.90 | 0.09 | 62,62,62,62 | 0 |
| 56 | MG | 1a | 1732 | 1/1 | 0.90 | 0.25 | 64,64,64,64 | 0 |
| 56 | MG | 1A | 3344 | 1/1 | 0.90 | 0.13 | 53,53,53,53 | 0 |
| 56 | MG | 2a | 3154 | 1/1 | 0.90 | 0.09 | 69,69,69,69 | 0 |
| 56 | MG | 2A | 3107 | 1/1 | 0.90 | 0.09 | 65,65,65,65 | 0 |
| 56 | MG | 2A | 3742 | 1/1 | 0.90 | 0.08 | 72,72,72,72 | 0 |
| 56 | MG | 2A | 3743 | 1/1 | 0.90 | 0.11 | 59,59,59,59 | 0 |
| 56 | MG | 1A | 3349 | 1/1 | 0.90 | 0.15 | 56,56,56,56 | 0 |
| 56 | MG | 2A | 3406 | 1/1 | 0.90 | 0.11 | 66,66,66,66 | 0 |
| 56 | MG | 2A | 3112 | 1/1 | 0.90 | 0.16 | 51,51,51,51 | 0 |
| 56 | MG | 1a | 1743 | 1/1 | 0.90 | 0.14 | 61,61,61,61 | 0 |
| 56 | MG | 1A | 3515 | 1/1 | 0.90 | 0.09 | 47,47,47,47 | 0 |
| 56 | MG | 2a | 3175 | 1/1 | 0.90 | 0.08 | 73,73,73,73 | 0 |
| 56 | MG | 2a | 3176 | 1/1 | 0.90 | 0.09 | 72,72,72,72 | 0 |
| 56 | MG | 1A | 3522 | 1/1 | 0.90 | 0.18 | 53,53,53,53 | 0 |
| 56 | MG | 2A | 3421 | 1/1 | 0.90 | 0.29 | 69,69,69,69 | 0 |
| 56 | MG | 1A | 3937 | 1/1 | 0.90 | 0.10 | 60,60,60,60 | 0 |
| 56 | MG | 2A | 3131 | 1/1 | 0.90 | 0.21 | 75,75,75,75 | 0 |
| 56 | MG | 1A | 3942 | 1/1 | 0.90 | 0.09 | 51,51,51,51 | 0 |
| 56 | MG | 1A | 3524 | 1/1 | 0.90 | 0.12 | 51,51,51,51 | 0 |
| 56 | MG | 2A | 3771 | 1/1 | 0.90 | 0.11 | 62,62,62,62 | 0 |
| 56 | MG | 2A | 3439 | 1/1 | 0.90 | 0.32 | 55,55,55,55 | 0 |
| 56 | MG | 2A | 3149 | 1/1 | 0.90 | 0.17 | 63,63,63,63 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 2A | 3442 | 1/1 | 0.90 | 0.13 | 57,57,57,57 | 0 |
| 56 | MG | 2A | 3150 | 1/1 | 0.90 | 0.13 | 53,53,53,53 | 0 |
| 56 | MG | 2A | 3151 | 1/1 | 0.90 | 0.27 | 60,60,60,60 | 0 |
| 56 | MG | 2a | 3204 | 1/1 | 0.90 | 0.29 | 65,65,65,65 | 0 |
| 56 | MG | 2a | 3208 | 1/1 | 0.90 | 0.19 | 69,69,69,69 | 0 |
| 56 | MG | 2A | 3448 | 1/1 | 0.90 | 0.38 | 64,64,64,64 | 0 |
| 56 | MG | 1G | 203 | 1/1 | 0.90 | 0.07 | 63,63,63,63 | 0 |
| 56 | MG | 1A | 3526 | 1/1 | 0.90 | 0.32 | 42,42,42,42 | 0 |
| 56 | MG | 2a | 3224 | 1/1 | 0.90 | 0.16 | 61,61,61,61 | 0 |
| 56 | MG | 2A | 3808 | 1/1 | 0.90 | 0.15 | 63,63,63,63 | 0 |
| 56 | MG | 1A | 3962 | 1/1 | 0.90 | 0.11 | 48,48,48,48 | 0 |
| 56 | MG | 1A | 3964 | 1/1 | 0.90 | 0.09 | 33,33,33,33 | 0 |
| 56 | MG | 2a | 3229 | 1/1 | 0.90 | 0.10 | 61,61,61,61 | 0 |
| 56 | MG | 2A | 3462 | 1/1 | 0.90 | 0.33 | 60,60,60,60 | 0 |
| 56 | MG | 1A | 3353 | 1/1 | 0.90 | 0.16 | 33,33,33,33 | 0 |
| 56 | MG | 2A | 3176 | 1/1 | 0.90 | 0.11 | 59,59,59,59 | 0 |
| 56 | MG | 2a | 3237 | 1/1 | 0.90 | 0.23 | 61,61,61,61 | 0 |
| 56 | MG | 2A | 3179 | 1/1 | 0.90 | 0.18 | 65,65,65,65 | 0 |
| 56 | MG | 2A | 3469 | 1/1 | 0.90 | 0.28 | 64,64,64,64 | 0 |
| 56 | MG | 2A | 3472 | 1/1 | 0.90 | 0.10 | 64,64,64,64 | 0 |
| 56 | MG | 1a | 1775 | 1/1 | 0.90 | 0.12 | 65,65,65,65 | 0 |
| 56 | MG | 2A | 3190 | 1/1 | 0.90 | 0.37 | 67,67,67,67 | 0 |
| 56 | MG | 1A | 3438 | 1/1 | 0.90 | 0.10 | 50,50,50,50 | 0 |
| 56 | MG | 2A | 3194 | 1/1 | 0.90 | 0.09 | 60,60,60,60 | 0 |
| 56 | MG | 1S | 202 | 1/1 | 0.90 | 0.16 | 51,51,51,51 | 0 |
| 56 | MG | 2k | 201 | 1/1 | 0.90 | 0.16 | 55,55,55,55 | 0 |
| 56 | MG | 1a | 1782 | 1/1 | 0.90 | 0.07 | 79,79,79,79 | 0 |
| 56 | MG | 2A | 3839 | 1/1 | 0.90 | 0.10 | 35,35,35,35 | 0 |
| 56 | MG | 1S | 203 | 1/1 | 0.90 | 0.09 | 66,66,66,66 | 0 |
| 56 | MG | 1A | 3356 | 1/1 | 0.90 | 0.09 | 53,53,53,53 | 0 |
| 56 | MG | 1T | 204 | 1/1 | 0.90 | 0.13 | 59,59,59,59 | 0 |
| 56 | MG | 2A | 3868 | 1/1 | 0.90 | 0.16 | 70,70,70,70 | 0 |
| 56 | MG | 1A | 3685 | 1/1 | 0.90 | 0.17 | 31,31,31,31 | 0 |
| 56 | MG | 1a | 1789 | 1/1 | 0.90 | 0.16 | 77,77,77,77 | 0 |
| 56 | MG | 2x | 102 | 1/1 | 0.90 | 0.19 | 70,70,70,70 | 0 |
| 56 | MG | 1V | 202 | 1/1 | 0.90 | 0.14 | 39,39,39,39 | 0 |
| 56 | MG | 1A | 3450 | 1/1 | 0.90 | 0.14 | 50,50,50,50 | 0 |
| 56 | MG | 2A | 3217 | 1/1 | 0.90 | 0.28 | 67,67,67,67 | 0 |
| 56 | MG | 2y | 102 | 1/1 | 0.90 | 0.10 | 74,74,74,74 | 0 |
| 56 | MG | 2y | 103 | 1/1 | 0.90 | 0.11 | 76,76,76,76 | 0 |
| 56 | MG | 1Y | 201 | 1/1 | 0.90 | 0.09 | 32,32,32,32 | 0 |
| 56 | MG | 2A | 3293 | 1/1 | 0.91 | 0.07 | 52,52,52,52 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 2A | 3046 | 1/1 | 0.91 | 0.12 | 48,48,48,48 | 0 |
| 56 | MG | 1A | 3039 | 1/1 | 0.91 | 0.14 | 54,54,54,54 | 0 |
| 56 | MG | 1A | 3380 | 1/1 | 0.91 | 0.09 | 48,48,48,48 | 0 |
| 56 | MG | 2A | 3051 | 1/1 | 0.91 | 0.30 | 72,72,72,72 | 0 |
| 56 | MG | 1A | 3844 | 1/1 | 0.91 | 0.08 | 57,57,57,57 | 0 |
| 56 | MG | 2A | 3301 | 1/1 | 0.91 | 0.08 | 57,57,57,57 | 0 |
| 56 | MG | 1A | 3394 | 1/1 | 0.91 | 0.11 | 50,50,50,50 | 0 |
| 56 | MG | 2P | 202 | 1/1 | 0.91 | 0.07 | 47,47,47,47 | 0 |
| 56 | MG | 2Q | 203 | 1/1 | 0.91 | 0.11 | 56,56,56,56 | 0 |
| 56 | MG | 1a | 1722 | 1/1 | 0.91 | 0.16 | 50,50,50,50 | 0 |
| 56 | MG | 2A | 3597 | 1/1 | 0.91 | 0.18 | 58,58,58,58 | 0 |
| 56 | MG | 1a | 1726 | 1/1 | 0.91 | 0.15 | 61,61,61,61 | 0 |
| 56 | MG | 1A | 3733 | 1/1 | 0.91 | 0.11 | 45,45,45,45 | 0 |
| 56 | MG | 2A | 3311 | 1/1 | 0.91 | 0.16 | 59,59,59,59 | 0 |
| 56 | MG | 2V | 202 | 1/1 | 0.91 | 0.27 | 48,48,48,48 | 0 |
| 56 | MG | 1a | 1729 | 1/1 | 0.91 | 0.25 | 54,54,54,54 | 0 |
| 56 | MG | 1A | 3191 | 1/1 | 0.91 | 0.09 | 43,43,43,43 | 0 |
| 56 | MG | 1A | 3646 | 1/1 | 0.91 | 0.09 | 30,30,30,30 | 0 |
| 56 | MG | 1A | 3254 | 1/1 | 0.91 | 0.11 | 36,36,36,36 | 0 |
| 56 | MG | 2A | 3071 | 1/1 | 0.91 | 0.07 | 40,40,40,40 | 0 |
| 56 | MG | 1a | 1733 | 1/1 | 0.91 | 0.31 | 53,53,53,53 | 0 |
| 56 | MG | 2A | 3611 | 1/1 | 0.91 | 0.11 | 51,51,51,51 | 0 |
| 56 | MG | 1A | 3992 | 1/1 | 0.91 | 0.08 | 25,25,25,25 | 0 |
| 56 | MG | 1A | 3865 | 1/1 | 0.91 | 0.11 | 65,65,65,65 | 0 |
| 56 | MG | 1A | 3998 | 1/1 | 0.91 | 0.18 | 67,67,67,67 | 0 |
| 56 | MG | 1A | 3346 | 1/1 | 0.91 | 0.12 | 52,52,52,52 | 0 |
| 56 | MG | 1A | 4005 | 1/1 | 0.91 | 0.07 | 26,26,26,26 | 0 |
| 56 | MG | 2a | 3008 | 1/1 | 0.91 | 0.14 | 57,57,57,57 | 0 |
| 56 | MG | 1A | 3759 | 1/1 | 0.91 | 0.08 | 15,15,15,15 | 0 |
| 56 | MG | 1A | 3324 | 1/1 | 0.91 | 0.10 | 39,39,39,39 | 0 |
| 56 | MG | 2A | 3095 | 1/1 | 0.91 | 0.08 | 59,59,59,59 | 0 |
| 56 | MG | 2A | 3631 | 1/1 | 0.91 | 0.12 | 39,39,39,39 | 0 |
| 56 | MG | 2A | 3634 | 1/1 | 0.91 | 0.14 | 56,56,56,56 | 0 |
| 56 | MG | 2A | 3096 | 1/1 | 0.91 | 0.13 | 52,52,52,52 | 0 |
| 56 | MG | 2A | 3097 | 1/1 | 0.91 | 0.11 | 45,45,45,45 | 0 |
| 56 | MG | 2A | 3098 | 1/1 | 0.91 | 0.20 | 61,61,61,61 | 0 |
| 56 | MG | 1A | 3662 | 1/1 | 0.91 | 0.09 | 19,19,19,19 | 0 |
| 56 | MG | 1A | 3538 | 1/1 | 0.91 | 0.10 | 50,50,50,50 | 0 |
| 56 | MG | 1A | 3880 | 1/1 | 0.91 | 0.16 | 60,60,60,60 | 0 |
| 56 | MG | 1A | 3883 | 1/1 | 0.91 | 0.28 | 66,66,66,66 | 0 |
| 56 | MG | 2A | 3113 | 1/1 | 0.91 | 0.24 | 59,59,59,59 | 0 |
| 56 | MG | 2A | 3359 | 1/1 | 0.91 | 0.11 | 51,51,51,51 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 2A | 3116 | 1/1 | 0.91 | 0.30 | 60,60,60,60 | 0 |
| 56 | MG | 1A | 3541 | 1/1 | 0.91 | 0.14 | 43,43,43,43 | 0 |
| 56 | MG | 1A | 4042 | 1/1 | 0.91 | 0.10 | 40,40,40,40 | 0 |
| 56 | MG | 2a | 3037 | 1/1 | 0.91 | 0.18 | 48,48,48,48 | 0 |
| 56 | MG | 1A | 3414 | 1/1 | 0.91 | 0.15 | 43,43,43,43 | 0 |
| 56 | MG | 11 | 104 | 1/1 | 0.91 | 0.14 | 48,48,48,48 | 0 |
| 56 | MG | 2A | 3372 | 1/1 | 0.91 | 0.12 | 50,50,50,50 | 0 |
| 56 | MG | 12 | 101 | 1/1 | 0.91 | 0.09 | 54,54,54,54 | 0 |
| 56 | MG | 2A | 3376 | 1/1 | 0.91 | 0.10 | 53,53,53,53 | 0 |
| 56 | MG | 1A | 3477 | 1/1 | 0.91 | 0.09 | 53,53,53,53 | 0 |
| 56 | MG | 15 | 103 | 1/1 | 0.91 | 0.16 | 33,33,33,33 | 0 |
| 56 | MG | 1A | 3680 | 1/1 | 0.91 | 0.14 | 38,38,38,38 | 0 |
| 56 | MG | 2A | 3683 | 1/1 | 0.91 | 0.16 | 64,64,64,64 | 0 |
| 56 | MG | 1A | 4052 | 1/1 | 0.91 | 0.12 | 48,48,48,48 | 0 |
| 56 | MG | 2A | 3382 | 1/1 | 0.91 | 0.23 | 47,47,47,47 | 0 |
| 56 | MG | 2a | 3059 | 1/1 | 0.91 | 0.18 | 80,80,80,80 | 0 |
| 56 | MG | 18 | 107 | 1/1 | 0.91 | 0.14 | 56,56,56,56 | 0 |
| 56 | MG | 1A | 3480 | 1/1 | 0.91 | 0.12 | 54,54,54,54 | 0 |
| 56 | MG | 2a | 3063 | 1/1 | 0.91 | 0.10 | 63,63,63,63 | 0 |
| 56 | MG | 1A | 3232 | 1/1 | 0.91 | 0.25 | 56,56,56,56 | 0 |
| 56 | MG | 2a | 3065 | 1/1 | 0.91 | 0.10 | 77,77,77,77 | 0 |
| 56 | MG | 2A | 3395 | 1/1 | 0.91 | 0.24 | 66,66,66,66 | 0 |
| 56 | MG | 2A | 3156 | 1/1 | 0.91 | 0.28 | 54,54,54,54 | 0 |
| 56 | MG | 2A | 3699 | 1/1 | 0.91 | 0.11 | 70,70,70,70 | 0 |
| 56 | MG | 2A | 3160 | 1/1 | 0.91 | 0.15 | 57,57,57,57 | 0 |
| 56 | MG | 2A | 3399 | 1/1 | 0.91 | 0.18 | 69,69,69,69 | 0 |
| 56 | MG | 2A | 3166 | 1/1 | 0.91 | 0.18 | 50,50,50,50 | 0 |
| 56 | MG | 2a | 3083 | 1/1 | 0.91 | 0.22 | 65,65,65,65 | 0 |
| 56 | MG | 1a | 1607 | 1/1 | 0.91 | 0.09 | 55,55,55,55 | 0 |
| 56 | MG | 2A | 3170 | 1/1 | 0.91 | 0.14 | 52,52,52,52 | 0 |
| 56 | MG | 2a | 3089 | 1/1 | 0.91 | 0.15 | 69,69,69,69 | 0 |
| 56 | MG | 1A | 4057 | 1/1 | 0.91 | 0.10 | 23,23,23,23 | 0 |
| 56 | MG | 2A | 3410 | 1/1 | 0.91 | 0.11 | 70,70,70,70 | 0 |
| 56 | MG | 2A | 3412 | 1/1 | 0.91 | 0.10 | 53,53,53,53 | 0 |
| 56 | MG | 1A | 3898 | 1/1 | 0.91 | 0.14 | 32,32,32,32 | 0 |
| 56 | MG | 1A | 3418 | 1/1 | 0.91 | 0.11 | 55,55,55,55 | 0 |
| 56 | MG | 1a | 1619 | 1/1 | 0.91 | 0.19 | 52,52,52,52 | 0 |
| 56 | MG | 2A | 3419 | 1/1 | 0.91 | 0.13 | 62,62,62,62 | 0 |
| 56 | MG | 2A | 3420 | 1/1 | 0.91 | 0.12 | 60,60,60,60 | 0 |
| 56 | MG | 2A | 3723 | 1/1 | 0.91 | 0.12 | 51,51,51,51 | 0 |
| 56 | MG | 2A | 3182 | 1/1 | 0.91 | 0.15 | 49,49,49,49 | 0 |
| 56 | MG | 2A | 3186 | 1/1 | 0.91 | 0.24 | 53,53,53,53 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 2A | 3428 | 1/1 | 0.91 | 0.21 | 50,50,50,50 | 0 |
| 56 | MG | 1A | 3904 | 1/1 | 0.91 | 0.10 | 32,32,32,32 | 0 |
| 56 | MG | 2a | 3115 | 1/1 | 0.91 | 0.20 | 61,61,61,61 | 0 |
| 56 | MG | 2A | 3432 | 1/1 | 0.91 | 0.26 | 40,40,40,40 | 0 |
| 56 | MG | 1A | 3909 | 1/1 | 0.91 | 0.13 | 49,49,49,49 | 0 |
| 56 | MG | 1A | 3486 | 1/1 | 0.91 | 0.13 | 44,44,44,44 | 0 |
| 56 | MG | 2A | 3438 | 1/1 | 0.91 | 0.31 | 56,56,56,56 | 0 |
| 56 | MG | 2a | 3122 | 1/1 | 0.91 | 0.33 | 73,73,73,73 | 0 |
| 56 | MG | 2a | 3123 | 1/1 | 0.91 | 0.27 | 68,68,68,68 | 0 |
| 56 | MG | 2A | 3741 | 1/1 | 0.91 | 0.12 | 42,42,42,42 | 0 |
| 56 | MG | 1A | 3690 | 1/1 | 0.91 | 0.12 | 19,19,19,19 | 0 |
| 56 | MG | 1A | 3565 | 1/1 | 0.91 | 0.10 | 58,58,58,58 | 0 |
| 56 | MG | 2A | 3745 | 1/1 | 0.91 | 0.07 | 50,50,50,50 | 0 |
| 56 | MG | 2a | 3134 | 1/1 | 0.91 | 0.18 | 58,58,58,58 | 0 |
| 56 | MG | 2A | 3441 | 1/1 | 0.91 | 0.19 | 60,60,60,60 | 0 |
| 56 | MG | 1a | 1641 | 1/1 | 0.91 | 0.09 | 57,57,57,57 | 0 |
| 56 | MG | 2a | 3138 | 1/1 | 0.91 | 0.09 | 67,67,67,67 | 0 |
| 56 | MG | 2A | 3201 | 1/1 | 0.91 | 0.32 | 70,70,70,70 | 0 |
| 56 | MG | 1A | 3572 | 1/1 | 0.91 | 0.25 | 39,39,39,39 | 0 |
| 56 | MG | 2A | 3447 | 1/1 | 0.91 | 0.28 | 55,55,55,55 | 0 |
| 56 | MG | 1A | 4078 | 1/1 | 0.91 | 0.07 | 24,24,24,24 | 0 |
| 56 | MG | 1A | 3491 | 1/1 | 0.91 | 0.09 | 38,38,38,38 | 0 |
| 56 | MG | 2a | 3155 | 1/1 | 0.91 | 0.07 | 70,70,70,70 | 0 |
| 56 | MG | 1A | 3807 | 1/1 | 0.91 | 0.32 | 27,27,27,27 | 0 |
| 56 | MG | 1A | 3133 | 1/1 | 0.91 | 0.14 | 35,35,35,35 | 0 |
| 56 | MG | 2A | 3458 | 1/1 | 0.91 | 0.08 | 53,53,53,53 | 0 |
| 56 | MG | 2A | 3764 | 1/1 | 0.91 | 0.10 | 44,44,44,44 | 0 |
| 56 | MG | 2A | 3765 | 1/1 | 0.91 | 0.13 | 53,53,53,53 | 0 |
| 56 | MG | 2A | 3768 | 1/1 | 0.91 | 0.08 | 42,42,42,42 | 0 |
| 56 | MG | 1A | 3357 | 1/1 | 0.91 | 0.20 | 48,48,48,48 | 0 |
| 56 | MG | 1a | 1661 | 1/1 | 0.91 | 0.12 | 58,58,58,58 | 0 |
| 56 | MG | 1t | 201 | 1/1 | 0.91 | 0.13 | 59,59,59,59 | 0 |
| 56 | MG | 2A | 3775 | 1/1 | 0.91 | 0.16 | 66,66,66,66 | 0 |
| 56 | MG | 1A | 4089 | 1/1 | 0.91 | 0.15 | 65,65,65,65 | 0 |
| 56 | MG | 2A | 3792 | 1/1 | 0.91 | 0.14 | 63,63,63,63 | 0 |
| 56 | MG | 2A | 3795 | 1/1 | 0.91 | 0.09 | 55,55,55,55 | 0 |
| 56 | MG | 1w | 103 | 1/1 | 0.91 | 0.24 | 64,64,64,64 | 0 |
| 56 | MG | 1A | 3815 | 1/1 | 0.91 | 0.08 | 28,28,28,28 | 0 |
| 56 | MG | 2a | 3192 | 1/1 | 0.91 | 0.11 | 56,56,56,56 | 0 |
| 56 | MG | 1A | 3933 | 1/1 | 0.91 | 0.08 | 49,49,49,49 | 0 |
| 56 | MG | 1A | 3585 | 1/1 | 0.91 | 0.16 | 35,35,35,35 | 0 |
| 56 | MG | 1w | 107 | 1/1 | 0.91 | 0.20 | 69,69,69,69 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 2A | 3479 | 1/1 | 0.91 | 0.13 | 52,52,52,52 | 0 |
| 56 | MG | 2A | 3806 | 1/1 | 0.91 | 0.12 | 50,50,50,50 | 0 |
| 56 | MG | 1A | 3601 | 1/1 | 0.91 | 0.23 | 43,43,43,43 | 0 |
| 56 | MG | 1A | 3947 | 1/1 | 0.91 | 0.08 | 27,27,27,27 | 0 |
| 56 | MG | 1B | 212 | 1/1 | 0.91 | 0.09 | 40,40,40,40 | 0 |
| 56 | MG | 1a | 1676 | 1/1 | 0.91 | 0.17 | 72,72,72,72 | 0 |
| 56 | MG | 1x | 108 | 1/1 | 0.91 | 0.26 | 62,62,62,62 | 0 |
| 56 | MG | 2A | 3495 | 1/1 | 0.91 | 0.10 | 57,57,57,57 | 0 |
| 56 | MG | 2a | 3217 | 1/1 | 0.91 | 0.13 | 72,72,72,72 | 0 |
| 56 | MG | 1a | 1685 | 1/1 | 0.91 | 0.28 | 65,65,65,65 | 0 |
| 56 | MG | 1a | 1686 | 1/1 | 0.91 | 0.14 | 62,62,62,62 | 0 |
| 56 | MG | 1A | 3358 | 1/1 | 0.91 | 0.08 | 45,45,45,45 | 0 |
| 56 | MG | 1A | 3336 | 1/1 | 0.91 | 0.12 | 60,60,60,60 | 0 |
| 56 | MG | 2A | 3255 | 1/1 | 0.91 | 0.13 | 69,69,69,69 | 0 |
| 56 | MG | 2A | 3513 | 1/1 | 0.91 | 0.10 | 50,50,50,50 | 0 |
| 56 | MG | 2a | 3231 | 1/1 | 0.91 | 0.10 | 58,58,58,58 | 0 |
| 56 | MG | 1a | 1690 | 1/1 | 0.91 | 0.08 | 56,56,56,56 | 0 |
| 56 | MG | 1B | 226 | 1/1 | 0.91 | 0.08 | 69,69,69,69 | 0 |
| 56 | MG | 2A | 3517 | 1/1 | 0.91 | 0.08 | 46,46,46,46 | 0 |
| 56 | MG | 2A | 3524 | 1/1 | 0.91 | 0.18 | 69,69,69,69 | 0 |
| 56 | MG | 1B | 229 | 1/1 | 0.91 | 0.07 | 38,38,38,38 | 0 |
| 56 | MG | 2A | 3527 | 1/1 | 0.91 | 0.12 | 44,44,44,44 | 0 |
| 56 | MG | 2A | 3859 | 1/1 | 0.91 | 0.09 | 60,60,60,60 | 0 |
| 56 | MG | 1A | 3958 | 1/1 | 0.91 | 0.09 | 50,50,50,50 | 0 |
| 56 | MG | 2A | 3864 | 1/1 | 0.91 | 0.11 | 69,69,69,69 | 0 |
| 56 | MG | 1A | 3431 | 1/1 | 0.91 | 0.14 | 54,54,54,54 | 0 |
| 56 | MG | 1a | 1695 | 1/1 | 0.91 | 0.20 | 52,52,52,52 | 0 |
| 56 | MG | 2A | 3267 | 1/1 | 0.91 | 0.17 | 67,67,67,67 | 0 |
| 56 | MG | 2A | 3271 | 1/1 | 0.91 | 0.20 | 58,58,58,58 | 0 |
| 56 | MG | 1A | 3963 | 1/1 | 0.91 | 0.09 | 33,33,33,33 | 0 |
| 56 | MG | 1B | 236 | 1/1 | 0.91 | 0.10 | 49,49,49,49 | 0 |
| 56 | MG | 2A | 3547 | 1/1 | 0.91 | 0.11 | 34,34,34,34 | 0 |
| 56 | MG | 2A | 3550 | 1/1 | 0.91 | 0.15 | 57,57,57,57 | 0 |
| 56 | MG | 2t | 201 | 1/1 | 0.91 | 0.14 | 47,47,47,47 | 0 |
| 56 | MG | 2A | 3887 | 1/1 | 0.91 | 0.11 | 56,56,56,56 | 0 |
| 56 | MG | 2w | 101 | 1/1 | 0.91 | 0.32 | 69,69,69,69 | 0 |
| 56 | MG | 1A | 3433 | 1/1 | 0.91 | 0.07 | 31,31,31,31 | 0 |
| 56 | MG | 2B | 202 | 1/1 | 0.91 | 0.08 | 63,63,63,63 | 0 |
| 56 | MG | 2A | 3033 | 1/1 | 0.91 | 0.13 | 36,36,36,36 | 0 |
| 56 | MG | 1A | 3091 | 1/1 | 0.91 | 0.26 | 50,50,50,50 | 0 |
| 56 | MG | 2B | 205 | 1/1 | 0.91 | 0.11 | 66,66,66,66 | 0 |
| 56 | MG | 2B | 207 | 1/1 | 0.91 | 0.12 | 61,61,61,61 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 2A | 3282 | 1/1 | 0.91 | 0.14 | 63,63,63,63 | 0 |
| 56 | MG | 2A | 3037 | 1/1 | 0.91 | 0.29 | 68,68,68,68 | 0 |
| 56 | MG | 1E | 303 | 1/1 | 0.91 | 0.13 | 38,38,38,38 | 0 |
| 56 | MG | 1E | 309 | 1/1 | 0.91 | 0.13 | 47,47,47,47 | 0 |
| 56 | MG | 1a | 1710 | 1/1 | 0.92 | 0.15 | 53,53,53,53 | 0 |
| 56 | MG | 1A | 3123 | 1/1 | 0.92 | 0.12 | 41,41,41,41 | 0 |
| 56 | MG | 2D | 302 | 1/1 | 0.92 | 0.19 | 55,55,55,55 | 0 |
| 56 | MG | 2D | 304 | 1/1 | 0.92 | 0.18 | 57,57,57,57 | 0 |
| 56 | MG | 2A | 3326 | 1/1 | 0.92 | 0.12 | 61,61,61,61 | 0 |
| 56 | MG | 1A | 3954 | 1/1 | 0.92 | 0.11 | 75,75,75,75 | 0 |
| 56 | MG | 1A | 3663 | 1/1 | 0.92 | 0.07 | 21,21,21,21 | 0 |
| 56 | MG | 1F | 304 | 1/1 | 0.92 | 0.07 | 34,34,34,34 | 0 |
| 56 | MG | 1A | 3002 | 1/1 | 0.92 | 0.13 | 51,51,51,51 | 0 |
| 56 | MG | 1A | 3342 | 1/1 | 0.92 | 0.25 | 60,60,60,60 | 0 |
| 56 | MG | 1A | 3089 | 1/1 | 0.92 | 0.10 | 41,41,41,41 | 0 |
| 56 | MG | 1G | 204 | 1/1 | 0.92 | 0.07 | 52,52,52,52 | 0 |
| 56 | MG | 1N | 201 | 1/1 | 0.92 | 0.30 | 51,51,51,51 | 0 |
| 56 | MG | 2A | 3613 | 1/1 | 0.92 | 0.10 | 46,46,46,46 | 0 |
| 56 | MG | 2U | 203 | 1/1 | 0.92 | 0.14 | 54,54,54,54 | 0 |
| 56 | MG | 1A | 3530 | 1/1 | 0.92 | 0.09 | 40,40,40,40 | 0 |
| 56 | MG | 1O | 201 | 1/1 | 0.92 | 0.08 | 57,57,57,57 | 0 |
| 56 | MG | 2A | 3617 | 1/1 | 0.92 | 0.22 | 59,59,59,59 | 0 |
| 56 | MG | 1A | 3813 | 1/1 | 0.92 | 0.13 | 40,40,40,40 | 0 |
| 56 | MG | 20 | 103 | 1/1 | 0.92 | 0.14 | 66,66,66,66 | 0 |
| 56 | MG | 2A | 3619 | 1/1 | 0.92 | 0.08 | 36,36,36,36 | 0 |
| 56 | MG | 1A | 3814 | 1/1 | 0.92 | 0.16 | 63,63,63,63 | 0 |
| 56 | MG | 2A | 3621 | 1/1 | 0.92 | 0.19 | 63,63,63,63 | 0 |
| 56 | MG | 2A | 3622 | 1/1 | 0.92 | 0.08 | 38,38,38,38 | 0 |
| 56 | MG | 1P | 209 | 1/1 | 0.92 | 0.09 | 40,40,40,40 | 0 |
| 56 | MG | 1a | 1736 | 1/1 | 0.92 | 0.20 | 46,46,46,46 | 0 |
| 56 | MG | 1a | 1737 | 1/1 | 0.92 | 0.31 | 62,62,62,62 | 0 |
| 56 | MG | 2A | 3110 | 1/1 | 0.92 | 0.21 | 61,61,61,61 | 0 |
| 56 | MG | 1A | 3345 | 1/1 | 0.92 | 0.08 | 46,46,46,46 | 0 |
| 56 | MG | 1A | 3973 | 1/1 | 0.92 | 0.11 | 50,50,50,50 | 0 |
| 56 | MG | 1A | 3256 | 1/1 | 0.92 | 0.10 | 53,53,53,53 | 0 |
| 56 | MG | 1A | 3684 | 1/1 | 0.92 | 0.09 | 36,36,36,36 | 0 |
| 56 | MG | 1A | 3986 | 1/1 | 0.92 | 0.16 | 70,70,70,70 | 0 |
| 56 | MG | 1A | 3261 | 1/1 | 0.92 | 0.15 | 52,52,52,52 | 0 |
| 56 | MG | 2A | 3648 | 1/1 | 0.92 | 0.21 | 47,47,47,47 | 0 |
| 56 | MG | 1A | 3444 | 1/1 | 0.92 | 0.14 | 43,43,43,43 | 0 |
| 56 | MG | 2A | 3371 | 1/1 | 0.92 | 0.16 | 64,64,64,64 | 0 |
| 56 | MG | 1a | 1760 | 1/1 | 0.92 | 0.11 | 56,56,56,56 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 2A | 3658 | 1/1 | 0.92 | 0.19 | 69,69,69,69 | 0 |
| 56 | MG | 2A | 3135 | 1/1 | 0.92 | 0.19 | 51,51,51,51 | 0 |
| 56 | MG | 1A | 3535 | 1/1 | 0.92 | 0.15 | 57,57,57,57 | 0 |
| 56 | MG | 1W | 204 | 1/1 | 0.92 | 0.11 | 34,34,34,34 | 0 |
| 56 | MG | 2a | 3028 | 1/1 | 0.92 | 0.13 | 62,62,62,62 | 0 |
| 56 | MG | 1A | 3536 | 1/1 | 0.92 | 0.13 | 69,69,69,69 | 0 |
| 56 | MG | 1A | 3832 | 1/1 | 0.92 | 0.21 | 59,59,59,59 | 0 |
| 56 | MG | 1A | 3834 | 1/1 | 0.92 | 0.18 | 32,32,32,32 | 0 |
| 56 | MG | 1A | 3048 | 1/1 | 0.92 | 0.08 | 20,20,20,20 | 0 |
| 56 | MG | 1A | 3205 | 1/1 | 0.92 | 0.10 | 46,46,46,46 | 0 |
| 56 | MG | 1A | 3696 | 1/1 | 0.92 | 0.06 | 20,20,20,20 | 0 |
| 56 | MG | 2A | 3390 | 1/1 | 0.92 | 0.18 | 54,54,54,54 | 0 |
| 56 | MG | 2a | 3040 | 1/1 | 0.92 | 0.12 | 77,77,77,77 | 0 |
| 56 | MG | 2A | 3159 | 1/1 | 0.92 | 0.17 | 66,66,66,66 | 0 |
| 56 | MG | 1A | 3840 | 1/1 | 0.92 | 0.07 | 22,22,22,22 | 0 |
| 56 | MG | 2A | 3164 | 1/1 | 0.92 | 0.13 | 48,48,48,48 | 0 |
| 56 | MG | 1A | 3283 | 1/1 | 0.92 | 0.21 | 33,33,33,33 | 0 |
| 56 | MG | 1A | 3207 | 1/1 | 0.92 | 0.10 | 47,47,47,47 | 0 |
| 56 | MG | 1A | 3062 | 1/1 | 0.92 | 0.25 | 51,51,51,51 | 0 |
| 56 | MG | 2a | 3048 | 1/1 | 0.92 | 0.19 | 58,58,58,58 | 0 |
| 56 | MG | 2A | 3404 | 1/1 | 0.92 | 0.15 | 45,45,45,45 | 0 |
| 56 | MG | 2a | 3050 | 1/1 | 0.92 | 0.10 | 47,47,47,47 | 0 |
| 56 | MG | 2a | 3052 | 1/1 | 0.92 | 0.17 | 56,56,56,56 | 0 |
| 56 | MG | 15 | 102 | 1/1 | 0.92 | 0.14 | 42,42,42,42 | 0 |
| 56 | MG | 2A | 3172 | 1/1 | 0.92 | 0.12 | 50,50,50,50 | 0 |
| 56 | MG | 1A | 3848 | 1/1 | 0.92 | 0.15 | 54,54,54,54 | 0 |
| 56 | MG | 2a | 3058 | 1/1 | 0.92 | 0.12 | 74,74,74,74 | 0 |
| 56 | MG | 2A | 3175 | 1/1 | 0.92 | 0.13 | 50,50,50,50 | 0 |
| 56 | MG | 15 | 105 | 1/1 | 0.92 | 0.11 | 49,49,49,49 | 0 |
| 56 | MG | 1A | 4030 | 1/1 | 0.92 | 0.10 | 61,61,61,61 | 0 |
| 56 | MG | 2A | 3181 | 1/1 | 0.92 | 0.15 | 44,44,44,44 | 0 |
| 56 | MG | 2A | 3417 | 1/1 | 0.92 | 0.20 | 68,68,68,68 | 0 |
| 56 | MG | 18 | 103 | 1/1 | 0.92 | 0.07 | 22,22,22,22 | 0 |
| 56 | MG | 1A | 3463 | 1/1 | 0.92 | 0.12 | 47,47,47,47 | 0 |
| 56 | MG | 1A | 4033 | 1/1 | 0.92 | 0.14 | 55,55,55,55 | 0 |
| 56 | MG | 1a | 1602 | 1/1 | 0.92 | 0.16 | 61,61,61,61 | 0 |
| 56 | MG | 2a | 3071 | 1/1 | 0.92 | 0.21 | 62,62,62,62 | 0 |
| 56 | MG | 2a | 3072 | 1/1 | 0.92 | 0.17 | 51,51,51,51 | 0 |
| 56 | MG | 1A | 3464 | 1/1 | 0.92 | 0.07 | 46,46,46,46 | 0 |
| 56 | MG | 2A | 3425 | 1/1 | 0.92 | 0.20 | 43,43,43,43 | 0 |
| 56 | MG | 1a | 1605 | 1/1 | 0.92 | 0.10 | 55,55,55,55 | 0 |
| 56 | MG | 2A | 3429 | 1/1 | 0.92 | 0.29 | 53,53,53,53 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 1A | 3065 | 1/1 | 0.92 | 0.10 | 51,51,51,51 | 0 |
| 56 | MG | 1A | 3468 | 1/1 | 0.92 | 0.17 | 57,57,57,57 | 0 |
| 56 | MG | 2A | 3724 | 1/1 | 0.92 | 0.20 | 56,56,56,56 | 0 |
| 56 | MG | 1A | 3367 | 1/1 | 0.92 | 0.16 | 57,57,57,57 | 0 |
| 56 | MG | 2a | 3093 | 1/1 | 0.92 | 0.18 | 53,53,53,53 | 0 |
| 56 | MG | 2A | 3202 | 1/1 | 0.92 | 0.12 | 47,47,47,47 | 0 |
| 56 | MG | 1A | 3711 | 1/1 | 0.92 | 0.15 | 48,48,48,48 | 0 |
| 56 | MG | 1a | 1616 | 1/1 | 0.92 | 0.07 | 55,55,55,55 | 0 |
| 56 | MG | 2a | 3098 | 1/1 | 0.92 | 0.22 | 62,62,62,62 | 0 |
| 56 | MG | 2A | 3206 | 1/1 | 0.92 | 0.15 | 53,53,53,53 | 0 |
| 56 | MG | 1A | 3162 | 1/1 | 0.92 | 0.38 | 31,31,31,31 | 0 |
| 56 | MG | 1b | 301 | 1/1 | 0.92 | 0.07 | 74,74,74,74 | 0 |
| 56 | MG | 2A | 3738 | 1/1 | 0.92 | 0.08 | 48,48,48,48 | 0 |
| 56 | MG | 1A | 3713 | 1/1 | 0.92 | 0.17 | 63,63,63,63 | 0 |
| 56 | MG | 2A | 3213 | 1/1 | 0.92 | 0.21 | 61,61,61,61 | 0 |
| 56 | MG | 1A | 3714 | 1/1 | 0.92 | 0.06 | 14,14,14,14 | 0 |
| 56 | MG | 2a | 3109 | 1/1 | 0.92 | 0.08 | 72,72,72,72 | 0 |
| 56 | MG | 1A | 3323 | 1/1 | 0.92 | 0.10 | 50,50,50,50 | 0 |
| 56 | MG | 2A | 3744 | 1/1 | 0.92 | 0.10 | 44,44,44,44 | 0 |
| 56 | MG | 2A | 3449 | 1/1 | 0.92 | 0.22 | 56,56,56,56 | 0 |
| 56 | MG | 1a | 1627 | 1/1 | 0.92 | 0.08 | 55,55,55,55 | 0 |
| 56 | MG | 1A | 3478 | 1/1 | 0.92 | 0.15 | 41,41,41,41 | 0 |
| 56 | MG | 2A | 3749 | 1/1 | 0.92 | 0.10 | 58,58,58,58 | 0 |
| 56 | MG | 1a | 1632 | 1/1 | 0.92 | 0.15 | 58,58,58,58 | 0 |
| 56 | MG | 1a | 1633 | 1/1 | 0.92 | 0.14 | 52,52,52,52 | 0 |
| 56 | MG | 1A | 3479 | 1/1 | 0.92 | 0.11 | 53,53,53,53 | 0 |
| 56 | MG | 2A | 3461 | 1/1 | 0.92 | 0.18 | 44,44,44,44 | 0 |
| 56 | MG | 2a | 3126 | 1/1 | 0.92 | 0.26 | 66,66,66,66 | 0 |
| 56 | MG | 2A | 3755 | 1/1 | 0.92 | 0.19 | 54,54,54,54 | 0 |
| 56 | MG | 1A | 3592 | 1/1 | 0.92 | 0.10 | 22,22,22,22 | 0 |
| 56 | MG | 2A | 3758 | 1/1 | 0.92 | 0.18 | 64,64,64,64 | 0 |
| 56 | MG | 1A | 3382 | 1/1 | 0.92 | 0.12 | 46,46,46,46 | 0 |
| 56 | MG | 1A | 3163 | 1/1 | 0.92 | 0.27 | 48,48,48,48 | 0 |
| 56 | MG | 1a | 1651 | 1/1 | 0.92 | 0.12 | 61,61,61,61 | 0 |
| 56 | MG | 2A | 3243 | 1/1 | 0.92 | 0.15 | 64,64,64,64 | 0 |
| 56 | MG | 2a | 3145 | 1/1 | 0.92 | 0.09 | 79,79,79,79 | 0 |
| 56 | MG | 1A | 3893 | 1/1 | 0.92 | 0.10 | 21,21,21,21 | 0 |
| 56 | MG | 2A | 3766 | 1/1 | 0.92 | 0.13 | 68,68,68,68 | 0 |
| 56 | MG | 2A | 3767 | 1/1 | 0.92 | 0.15 | 51,51,51,51 | 0 |
| 56 | MG | 1A | 4073 | 1/1 | 0.92 | 0.15 | 59,59,59,59 | 0 |
| 56 | MG | 1a | 1656 | 1/1 | 0.92 | 0.15 | 62,62,62,62 | 0 |
| 56 | MG | 2A | 3476 | 1/1 | 0.92 | 0.10 | 62,62,62,62 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 2A | 3478 | 1/1 | 0.92 | 0.08 | 43,43,43,43 | 0 |
| 56 | MG | 1A | 3482 | 1/1 | 0.92 | 0.08 | 43,43,43,43 | 0 |
| 56 | MG | 2A | 3483 | 1/1 | 0.92 | 0.12 | 68,68,68,68 | 0 |
| 56 | MG | 2A | 3788 | 1/1 | 0.92 | 0.07 | 51,51,51,51 | 0 |
| 56 | MG | 2A | 3789 | 1/1 | 0.92 | 0.10 | 44,44,44,44 | 0 |
| 56 | MG | 1A | 3895 | 1/1 | 0.92 | 0.08 | 18,18,18,18 | 0 |
| 56 | MG | 1A | 3742 | 1/1 | 0.92 | 0.10 | 17,17,17,17 | 0 |
| 56 | MG | 2A | 3486 | 1/1 | 0.92 | 0.13 | 62,62,62,62 | 0 |
| 56 | MG | 2A | 3489 | 1/1 | 0.92 | 0.34 | 62,62,62,62 | 0 |
| 56 | MG | 1A | 3397 | 1/1 | 0.92 | 0.20 | 30,30,30,30 | 0 |
| 56 | MG | 1A | 3398 | 1/1 | 0.92 | 0.22 | 23,23,23,23 | 0 |
| 56 | MG | 2a | 3179 | 1/1 | 0.92 | 0.07 | 69,69,69,69 | 0 |
| 56 | MG | 2A | 3492 | 1/1 | 0.92 | 0.34 | 58,58,58,58 | 0 |
| 56 | MG | 2A | 3256 | 1/1 | 0.92 | 0.21 | 68,68,68,68 | 0 |
| 56 | MG | 1a | 1664 | 1/1 | 0.92 | 0.08 | 60,60,60,60 | 0 |
| 56 | MG | 1A | 3613 | 1/1 | 0.92 | 0.14 | 42,42,42,42 | 0 |
| 56 | MG | 1A | 3905 | 1/1 | 0.92 | 0.23 | 23,23,23,23 | 0 |
| 56 | MG | 1A | 3623 | 1/1 | 0.92 | 0.09 | 26,26,26,26 | 0 |
| 56 | MG | 2a | 3194 | 1/1 | 0.92 | 0.09 | 55,55,55,55 | 0 |
| 56 | MG | 2A | 3811 | 1/1 | 0.92 | 0.09 | 54,54,54,54 | 0 |
| 56 | MG | 1a | 1671 | 1/1 | 0.92 | 0.08 | 49,49,49,49 | 0 |
| 56 | MG | 2a | 3198 | 1/1 | 0.92 | 0.12 | 62,62,62,62 | 0 |
| 56 | MG | 1A | 3074 | 1/1 | 0.92 | 0.25 | 55,55,55,55 | 0 |
| 56 | MG | 2A | 3511 | 1/1 | 0.92 | 0.10 | 58,58,58,58 | 0 |
| 56 | MG | 1A | 4099 | 1/1 | 0.92 | 0.10 | 40,40,40,40 | 0 |
| 56 | MG | 2A | 3269 | 1/1 | 0.92 | 0.12 | 53,53,53,53 | 0 |
| 56 | MG | 2A | 3515 | 1/1 | 0.92 | 0.10 | 36,36,36,36 | 0 |
| 56 | MG | 1A | 3493 | 1/1 | 0.92 | 0.10 | 48,48,48,48 | 0 |
| 56 | MG | 2A | 3011 | 1/1 | 0.92 | 0.10 | 53,53,53,53 | 0 |
| 56 | MG | 2a | 3215 | 1/1 | 0.92 | 0.12 | 59,59,59,59 | 0 |
| 56 | MG | 2A | 3016 | 1/1 | 0.92 | 0.29 | 57,57,57,57 | 0 |
| 56 | MG | 1A | 3770 | 1/1 | 0.92 | 0.06 | 32,32,32,32 | 0 |
| 56 | MG | 2a | 3218 | 1/1 | 0.92 | 0.20 | 74,74,74,74 | 0 |
| 56 | MG | 1a | 1678 | 1/1 | 0.92 | 0.08 | 59,59,59,59 | 0 |
| 56 | MG | 2A | 3833 | 1/1 | 0.92 | 0.11 | 53,53,53,53 | 0 |
| 56 | MG | 1A | 3184 | 1/1 | 0.92 | 0.15 | 64,64,64,64 | 0 |
| 56 | MG | 1A | 3918 | 1/1 | 0.92 | 0.11 | 28,28,28,28 | 0 |
| 56 | MG | 2A | 3844 | 1/1 | 0.92 | 0.09 | 72,72,72,72 | 0 |
| 56 | MG | 1A | 3640 | 1/1 | 0.92 | 0.15 | 49,49,49,49 | 0 |
| 56 | MG | 2A | 3855 | 1/1 | 0.92 | 0.11 | 74,74,74,74 | 0 |
| 56 | MG | 2A | 3536 | 1/1 | 0.92 | 0.09 | 57,57,57,57 | 0 |
| 56 | MG | 1B | 215 | 1/1 | 0.92 | 0.10 | 55,55,55,55 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 1A | 3332 | 1/1 | 0.92 | 0.09 | 57,57,57,57 | 0 |
| 56 | MG | 1A | 3775 | 1/1 | 0.92 | 0.09 | 21,21,21,21 | 0 |
| 56 | MG | 2A | 3867 | 1/1 | 0.92 | 0.10 | 35,35,35,35 | 0 |
| 56 | MG | 2A | 3047 | 1/1 | 0.92 | 0.06 | 24,24,24,24 | 0 |
| 56 | MG | 1B | 224 | 1/1 | 0.92 | 0.13 | 52,52,52,52 | 0 |
| 56 | MG | 1A | 3929 | 1/1 | 0.92 | 0.09 | 39,39,39,39 | 0 |
| 56 | MG | 2A | 3050 | 1/1 | 0.92 | 0.14 | 57,57,57,57 | 0 |
| 56 | MG | 2e | 201 | 1/1 | 0.92 | 0.12 | 64,64,64,64 | 0 |
| 56 | MG | 1A | 3333 | 1/1 | 0.92 | 0.27 | 56,56,56,56 | 0 |
| 56 | MG | 1A | 3504 | 1/1 | 0.92 | 0.12 | 54,54,54,54 | 0 |
| 56 | MG | 1A | 3647 | 1/1 | 0.92 | 0.09 | 30,30,30,30 | 0 |
| 56 | MG | 2A | 3885 | 1/1 | 0.92 | 0.08 | 59,59,59,59 | 0 |
| 56 | MG | 1A | 3934 | 1/1 | 0.92 | 0.09 | 55,55,55,55 | 0 |
| 56 | MG | 2l | 204 | 1/1 | 0.92 | 0.16 | 72,72,72,72 | 0 |
| 56 | MG | 2A | 3304 | 1/1 | 0.92 | 0.11 | 44,44,44,44 | 0 |
| 56 | MG | 2A | 3306 | 1/1 | 0.92 | 0.14 | 50,50,50,50 | 0 |
| 56 | MG | 2A | 3569 | 1/1 | 0.92 | 0.09 | 46,46,46,46 | 0 |
| 56 | MG | 1A | 3245 | 1/1 | 0.92 | 0.09 | 43,43,43,43 | 0 |
| 56 | MG | 1a | 1701 | 1/1 | 0.92 | 0.29 | 53,53,53,53 | 0 |
| 56 | MG | 1a | 1703 | 1/1 | 0.92 | 0.28 | 60,60,60,60 | 0 |
| 56 | MG | 2B | 206 | 1/1 | 0.92 | 0.17 | 60,60,60,60 | 0 |
| 56 | MG | 2A | 3583 | 1/1 | 0.92 | 0.08 | 61,61,61,61 | 0 |
| 56 | MG | 2B | 210 | 1/1 | 0.92 | 0.14 | 67,67,67,67 | 0 |
| 56 | MG | 2A | 3313 | 1/1 | 0.92 | 0.09 | 57,57,57,57 | 0 |
| 56 | MG | 2A | 3063 | 1/1 | 0.92 | 0.15 | 58,58,58,58 | 0 |
| 56 | MG | 1A | 3338 | 1/1 | 0.92 | 0.17 | 48,48,48,48 | 0 |
| 56 | MG | 2A | 3317 | 1/1 | 0.92 | 0.24 | 49,49,49,49 | 0 |
| 56 | MG | 2A | 3318 | 1/1 | 0.92 | 0.15 | 50,50,50,50 | 0 |
| 56 | MG | 2A | 3319 | 1/1 | 0.92 | 0.16 | 53,53,53,53 | 0 |
| 56 | MG | 1A | 3247 | 1/1 | 0.92 | 0.12 | 53,53,53,53 | 0 |
| 56 | MG | 2A | 3529 | 1/1 | 0.93 | 0.20 | 52,52,52,52 | 0 |
| 56 | MG | 1a | 1646 | 1/1 | 0.93 | 0.14 | 56,56,56,56 | 0 |
| 56 | MG | 1A | 3499 | 1/1 | 0.93 | 0.07 | 44,44,44,44 | 0 |
| 56 | MG | 2A | 3268 | 1/1 | 0.93 | 0.27 | 57,57,57,57 | 0 |
| 56 | MG | 1A | 3116 | 1/1 | 0.93 | 0.08 | 36,36,36,36 | 0 |
| 56 | MG | 1A | 3289 | 1/1 | 0.93 | 0.06 | 49,49,49,49 | 0 |
| 56 | MG | 1A | 3506 | 1/1 | 0.93 | 0.08 | 47,47,47,47 | 0 |
| 56 | MG | 2A | 3275 | 1/1 | 0.93 | 0.08 | 59,59,59,59 | 0 |
| 56 | MG | 2A | 3542 | 1/1 | 0.93 | 0.07 | 46,46,46,46 | 0 |
| 56 | MG | 2B | 208 | 1/1 | 0.93 | 0.11 | 59,59,59,59 | 0 |
| 56 | MG | 1A | 3760 | 1/1 | 0.93 | 0.18 | 45,45,45,45 | 0 |
| 56 | MG | 1A | 3117 | 1/1 | 0.93 | 0.10 | 35,35,35,35 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 2A | 3279 | 1/1 | 0.93 | 0.16 | 62,62,62,62 | 0 |
| 56 | MG | 1A | 4090 | 1/1 | 0.93 | 0.12 | 53,53,53,53 | 0 |
| 56 | MG | 1A | 3296 | 1/1 | 0.93 | 0.06 | 32,32,32,32 | 0 |
| 56 | MG | 2A | 3005 | 1/1 | 0.93 | 0.22 | 55,55,55,55 | 0 |
| 56 | MG | 2A | 3283 | 1/1 | 0.93 | 0.07 | 57,57,57,57 | 0 |
| 56 | MG | 1A | 3297 | 1/1 | 0.93 | 0.10 | 50,50,50,50 | 0 |
| 56 | MG | 2A | 3565 | 1/1 | 0.93 | 0.20 | 68,68,68,68 | 0 |
| 56 | MG | 2B | 219 | 1/1 | 0.93 | 0.13 | 62,62,62,62 | 0 |
| 56 | MG | 2A | 3286 | 1/1 | 0.93 | 0.19 | 56,56,56,56 | 0 |
| 56 | MG | 2A | 3567 | 1/1 | 0.93 | 0.08 | 54,54,54,54 | 0 |
| 56 | MG | 1A | 3768 | 1/1 | 0.93 | 0.09 | 38,38,38,38 | 0 |
| 56 | MG | 2A | 3289 | 1/1 | 0.93 | 0.14 | 61,61,61,61 | 0 |
| 56 | MG | 1a | 1665 | 1/1 | 0.93 | 0.16 | 51,51,51,51 | 0 |
| 56 | MG | 2D | 310 | 1/1 | 0.93 | 0.09 | 56,56,56,56 | 0 |
| 56 | MG | 2F | 304 | 1/1 | 0.93 | 0.10 | 54,54,54,54 | 0 |
| 56 | MG | 2A | 3014 | 1/1 | 0.93 | 0.13 | 55,55,55,55 | 0 |
| 56 | MG | 2O | 8400 | 1/1 | 0.93 | 0.11 | 64,64,64,64 | 0 |
| 56 | MG | 1B | 201 | 1/1 | 0.93 | 0.20 | 48,48,48,48 | 0 |
| 56 | MG | 2P | 203 | 1/1 | 0.93 | 0.08 | 38,38,38,38 | 0 |
| 56 | MG | 2P | 204 | 1/1 | 0.93 | 0.13 | 57,57,57,57 | 0 |
| 56 | MG | 2A | 3576 | 1/1 | 0.93 | 0.07 | 26,26,26,26 | 0 |
| 56 | MG | 2A | 3578 | 1/1 | 0.93 | 0.18 | 54,54,54,54 | 0 |
| 56 | MG | 2A | 3020 | 1/1 | 0.93 | 0.18 | 39,39,39,39 | 0 |
| 56 | MG | 2A | 3022 | 1/1 | 0.93 | 0.10 | 56,56,56,56 | 0 |
| 56 | MG | 2T | 201 | 1/1 | 0.93 | 0.12 | 54,54,54,54 | 0 |
| 56 | MG | 1A | 3769 | 1/1 | 0.93 | 0.09 | 25,25,25,25 | 0 |
| 56 | MG | 2T | 204 | 1/1 | 0.93 | 0.13 | 54,54,54,54 | 0 |
| 56 | MG | 1a | 1668 | 1/1 | 0.93 | 0.09 | 66,66,66,66 | 0 |
| 56 | MG | 1B | 203 | 1/1 | 0.93 | 0.06 | 33,33,33,33 | 0 |
| 56 | MG | 2V | 201 | 1/1 | 0.93 | 0.21 | 69,69,69,69 | 0 |
| 56 | MG | 1a | 1670 | 1/1 | 0.93 | 0.20 | 60,60,60,60 | 0 |
| 56 | MG | 2V | 203 | 1/1 | 0.93 | 0.07 | 57,57,57,57 | 0 |
| 56 | MG | 1A | 3634 | 1/1 | 0.93 | 0.09 | 52,52,52,52 | 0 |
| 56 | MG | 1A | 3639 | 1/1 | 0.93 | 0.07 | 36,36,36,36 | 0 |
| 56 | MG | 2A | 3305 | 1/1 | 0.93 | 0.10 | 54,54,54,54 | 0 |
| 56 | MG | 1B | 211 | 1/1 | 0.93 | 0.17 | 51,51,51,51 | 0 |
| 56 | MG | 25 | 103 | 1/1 | 0.93 | 0.11 | 45,45,45,45 | 0 |
| 56 | MG | 2A | 3043 | 1/1 | 0.93 | 0.15 | 57,57,57,57 | 0 |
| 56 | MG | 2A | 3309 | 1/1 | 0.93 | 0.35 | 55,55,55,55 | 0 |
| 56 | MG | 1A | 3440 | 1/1 | 0.93 | 0.06 | 36,36,36,36 | 0 |
| 56 | MG | 28 | 101 | 1/1 | 0.93 | 0.13 | 66,66,66,66 | 0 |
| 56 | MG | 1B | 213 | 1/1 | 0.93 | 0.09 | 56,56,56,56 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 1a | 1677 | 1/1 | 0.93 | 0.15 | 57,57,57,57 | 0 |
| 56 | MG | 1A | 3920 | 1/1 | 0.93 | 0.22 | 65,65,65,65 | 0 |
| 56 | MG | 1a | 1679 | 1/1 | 0.93 | 0.18 | 66,66,66,66 | 0 |
| 56 | MG | 2A | 3316 | 1/1 | 0.93 | 0.18 | 53,53,53,53 | 0 |
| 56 | MG | 1A | 3518 | 1/1 | 0.93 | 0.12 | 54,54,54,54 | 0 |
| 56 | MG | 1A | 3234 | 1/1 | 0.93 | 0.12 | 54,54,54,54 | 0 |
| 56 | MG | 1B | 223 | 1/1 | 0.93 | 0.15 | 51,51,51,51 | 0 |
| 56 | MG | 1A | 3776 | 1/1 | 0.93 | 0.06 | 31,31,31,31 | 0 |
| 56 | MG | 1B | 225 | 1/1 | 0.93 | 0.10 | 53,53,53,53 | 0 |
| 56 | MG | 1A | 3783 | 1/1 | 0.93 | 0.07 | 17,17,17,17 | 0 |
| 56 | MG | 2A | 3325 | 1/1 | 0.93 | 0.11 | 57,57,57,57 | 0 |
| 56 | MG | 2A | 3060 | 1/1 | 0.93 | 0.10 | 46,46,46,46 | 0 |
| 56 | MG | 2A | 3327 | 1/1 | 0.93 | 0.07 | 51,51,51,51 | 0 |
| 56 | MG | 1A | 3303 | 1/1 | 0.93 | 0.29 | 55,55,55,55 | 0 |
| 56 | MG | 2a | 3018 | 1/1 | 0.93 | 0.30 | 61,61,61,61 | 0 |
| 56 | MG | 1A | 3931 | 1/1 | 0.93 | 0.07 | 40,40,40,40 | 0 |
| 56 | MG | 2A | 3331 | 1/1 | 0.93 | 0.14 | 72,72,72,72 | 0 |
| 56 | MG | 2A | 3628 | 1/1 | 0.93 | 0.14 | 55,55,55,55 | 0 |
| 56 | MG | 2a | 3024 | 1/1 | 0.93 | 0.19 | 59,59,59,59 | 0 |
| 56 | MG | 2a | 3025 | 1/1 | 0.93 | 0.12 | 59,59,59,59 | 0 |
| 56 | MG | 2a | 3026 | 1/1 | 0.93 | 0.15 | 60,60,60,60 | 0 |
| 56 | MG | 2A | 3332 | 1/1 | 0.93 | 0.07 | 46,46,46,46 | 0 |
| 56 | MG | 1B | 232 | 1/1 | 0.93 | 0.09 | 50,50,50,50 | 0 |
| 56 | MG | 1A | 3447 | 1/1 | 0.93 | 0.17 | 51,51,51,51 | 0 |
| 56 | MG | 2A | 3068 | 1/1 | 0.93 | 0.18 | 61,61,61,61 | 0 |
| 56 | MG | 1A | 3528 | 1/1 | 0.93 | 0.11 | 47,47,47,47 | 0 |
| 56 | MG | 2A | 3639 | 1/1 | 0.93 | 0.13 | 42,42,42,42 | 0 |
| 56 | MG | 1A | 3651 | 1/1 | 0.93 | 0.08 | 37,37,37,37 | 0 |
| 56 | MG | 2A | 3072 | 1/1 | 0.93 | 0.09 | 61,61,61,61 | 0 |
| 56 | MG | 2A | 3644 | 1/1 | 0.93 | 0.20 | 43,43,43,43 | 0 |
| 56 | MG | 1A | 3653 | 1/1 | 0.93 | 0.10 | 35,35,35,35 | 0 |
| 56 | MG | 2A | 3075 | 1/1 | 0.93 | 0.07 | 48,48,48,48 | 0 |
| 56 | MG | 2A | 3649 | 1/1 | 0.93 | 0.12 | 68,68,68,68 | 0 |
| 56 | MG | 2A | 3077 | 1/1 | 0.93 | 0.10 | 57,57,57,57 | 0 |
| 56 | MG | 2A | 3078 | 1/1 | 0.93 | 0.24 | 59,59,59,59 | 0 |
| 56 | MG | 2A | 3656 | 1/1 | 0.93 | 0.14 | 59,59,59,59 | 0 |
| 56 | MG | 1A | 3941 | 1/1 | 0.93 | 0.06 | 35,35,35,35 | 0 |
| 56 | MG | 1A | 3096 | 1/1 | 0.93 | 0.13 | 57,57,57,57 | 0 |
| 56 | MG | 1A | 3945 | 1/1 | 0.93 | 0.12 | 56,56,56,56 | 0 |
| 56 | MG | 1a | 1708 | 1/1 | 0.93 | 0.24 | 58,58,58,58 | 0 |
| 56 | MG | 1E | 310 | 1/1 | 0.93 | 0.21 | 61,61,61,61 | 0 |
| 56 | MG | 1A | 3309 | 1/1 | 0.93 | 0.11 | 38,38,38,38 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 2A | 3093 | 1/1 | 0.93 | 0.08 | 37,37,37,37 | 0 |
| 56 | MG | 1A | 3312 | 1/1 | 0.93 | 0.07 | 34,34,34,34 | 0 |
| 56 | MG | 1A | 3361 | 1/1 | 0.93 | 0.12 | 56,56,56,56 | 0 |
| 56 | MG | 1A | 3802 | 1/1 | 0.93 | 0.10 | 60,60,60,60 | 0 |
| 56 | MG | 1a | 1718 | 1/1 | 0.93 | 0.16 | 53,53,53,53 | 0 |
| 56 | MG | 1A | 3365 | 1/1 | 0.93 | 0.16 | 55,55,55,55 | 0 |
| 56 | MG | 1A | 3366 | 1/1 | 0.93 | 0.09 | 40,40,40,40 | 0 |
| 56 | MG | 1A | 3674 | 1/1 | 0.93 | 0.08 | 22,22,22,22 | 0 |
| 56 | MG | 1A | 3314 | 1/1 | 0.93 | 0.17 | 48,48,48,48 | 0 |
| 56 | MG | 1A | 3537 | 1/1 | 0.93 | 0.08 | 61,61,61,61 | 0 |
| 56 | MG | 2a | 3067 | 1/1 | 0.93 | 0.12 | 47,47,47,47 | 0 |
| 56 | MG | 1A | 3678 | 1/1 | 0.93 | 0.08 | 23,23,23,23 | 0 |
| 56 | MG | 2a | 3069 | 1/1 | 0.93 | 0.09 | 62,62,62,62 | 0 |
| 56 | MG | 1A | 3969 | 1/1 | 0.93 | 0.10 | 42,42,42,42 | 0 |
| 56 | MG | 2A | 3114 | 1/1 | 0.93 | 0.37 | 64,64,64,64 | 0 |
| 56 | MG | 1P | 207 | 1/1 | 0.93 | 0.11 | 51,51,51,51 | 0 |
| 56 | MG | 2a | 3074 | 1/1 | 0.93 | 0.21 | 52,52,52,52 | 0 |
| 56 | MG | 2A | 3694 | 1/1 | 0.93 | 0.12 | 50,50,50,50 | 0 |
| 56 | MG | 2a | 3078 | 1/1 | 0.93 | 0.18 | 50,50,50,50 | 0 |
| 56 | MG | 2A | 3695 | 1/1 | 0.93 | 0.07 | 60,60,60,60 | 0 |
| 56 | MG | 2a | 3081 | 1/1 | 0.93 | 0.28 | 60,60,60,60 | 0 |
| 56 | MG | 2A | 3696 | 1/1 | 0.93 | 0.08 | 55,55,55,55 | 0 |
| 56 | MG | 2A | 3117 | 1/1 | 0.93 | 0.10 | 55,55,55,55 | 0 |
| 56 | MG | 2a | 3084 | 1/1 | 0.93 | 0.28 | 58,58,58,58 | 0 |
| 56 | MG | 2A | 3384 | 1/1 | 0.93 | 0.09 | 62,62,62,62 | 0 |
| 56 | MG | 1A | 3016 | 1/1 | 0.93 | 0.16 | 45,45,45,45 | 0 |
| 56 | MG | 2a | 3088 | 1/1 | 0.93 | 0.11 | 55,55,55,55 | 0 |
| 56 | MG | 2A | 3701 | 1/1 | 0.93 | 0.08 | 58,58,58,58 | 0 |
| 56 | MG | 1Q | 205 | 1/1 | 0.93 | 0.06 | 55,55,55,55 | 0 |
| 56 | MG | 1A | 3539 | 1/1 | 0.93 | 0.22 | 45,45,45,45 | 0 |
| 56 | MG | 2A | 3392 | 1/1 | 0.93 | 0.15 | 58,58,58,58 | 0 |
| 56 | MG | 1a | 1735 | 1/1 | 0.93 | 0.22 | 53,53,53,53 | 0 |
| 56 | MG | 1R | 203 | 1/1 | 0.93 | 0.23 | 46,46,46,46 | 0 |
| 56 | MG | 2a | 3097 | 1/1 | 0.93 | 0.29 | 49,49,49,49 | 0 |
| 56 | MG | 1A | 3320 | 1/1 | 0.93 | 0.18 | 46,46,46,46 | 0 |
| 56 | MG | 1A | 3544 | 1/1 | 0.93 | 0.14 | 37,37,37,37 | 0 |
| 56 | MG | 2A | 3400 | 1/1 | 0.93 | 0.13 | 59,59,59,59 | 0 |
| 56 | MG | 1A | 3984 | 1/1 | 0.93 | 0.08 | 71,71,71,71 | 0 |
| 56 | MG | 2A | 3148 | 1/1 | 0.93 | 0.13 | 51,51,51,51 | 0 |
| 56 | MG | 2a | 3105 | 1/1 | 0.93 | 0.12 | 45,45,45,45 | 0 |
| 56 | MG | 2A | 3717 | 1/1 | 0.93 | 0.07 | 51,51,51,51 | 0 |
| 56 | MG | 1A | 3546 | 1/1 | 0.93 | 0.17 | 43,43,43,43 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 1a | 1748 | 1/1 | 0.93 | 0.06 | 36,36,36,36 | 0 |
| 56 | MG | 1A | 3194 | 1/1 | 0.93 | 0.25 | 33,33,33,33 | 0 |
| 56 | MG | 2a | 3110 | 1/1 | 0.93 | 0.15 | 62,62,62,62 | 0 |
| 56 | MG | 2a | 3111 | 1/1 | 0.93 | 0.13 | 63,63,63,63 | 0 |
| 56 | MG | 1a | 1752 | 1/1 | 0.93 | 0.10 | 74,74,74,74 | 0 |
| 56 | MG | 2A | 3154 | 1/1 | 0.93 | 0.17 | 52,52,52,52 | 0 |
| 56 | MG | 2a | 3114 | 1/1 | 0.93 | 0.12 | 65,65,65,65 | 0 |
| 56 | MG | 1A | 3026 | 1/1 | 0.93 | 0.07 | 45,45,45,45 | 0 |
| 56 | MG | 2A | 3415 | 1/1 | 0.93 | 0.15 | 62,62,62,62 | 0 |
| 56 | MG | 1a | 1754 | 1/1 | 0.93 | 0.11 | 57,57,57,57 | 0 |
| 56 | MG | 2a | 3118 | 1/1 | 0.93 | 0.28 | 62,62,62,62 | 0 |
| 56 | MG | 2A | 3732 | 1/1 | 0.93 | 0.19 | 72,72,72,72 | 0 |
| 56 | MG | 1A | 3202 | 1/1 | 0.93 | 0.08 | 40,40,40,40 | 0 |
| 56 | MG | 1V | 205 | 1/1 | 0.93 | 0.07 | 29,29,29,29 | 0 |
| 56 | MG | 2A | 3163 | 1/1 | 0.93 | 0.14 | 57,57,57,57 | 0 |
| 56 | MG | 1V | 207 | 1/1 | 0.93 | 0.07 | 52,52,52,52 | 0 |
| 56 | MG | 1A | 3556 | 1/1 | 0.93 | 0.21 | 41,41,41,41 | 0 |
| 56 | MG | 2A | 3422 | 1/1 | 0.93 | 0.07 | 42,42,42,42 | 0 |
| 56 | MG | 2A | 3167 | 1/1 | 0.93 | 0.08 | 39,39,39,39 | 0 |
| 56 | MG | 1a | 1765 | 1/1 | 0.93 | 0.13 | 51,51,51,51 | 0 |
| 56 | MG | 2A | 3426 | 1/1 | 0.93 | 0.23 | 42,42,42,42 | 0 |
| 56 | MG | 2A | 3427 | 1/1 | 0.93 | 0.20 | 42,42,42,42 | 0 |
| 56 | MG | 1A | 3330 | 1/1 | 0.93 | 0.12 | 46,46,46,46 | 0 |
| 56 | MG | 1A | 3164 | 1/1 | 0.93 | 0.15 | 52,52,52,52 | 0 |
| 56 | MG | 2a | 3140 | 1/1 | 0.93 | 0.08 | 57,57,57,57 | 0 |
| 56 | MG | 1a | 1768 | 1/1 | 0.93 | 0.17 | 64,64,64,64 | 0 |
| 56 | MG | 1A | 3996 | 1/1 | 0.93 | 0.16 | 51,51,51,51 | 0 |
| 56 | MG | 1A | 3107 | 1/1 | 0.93 | 0.07 | 27,27,27,27 | 0 |
| 56 | MG | 1A | 3843 | 1/1 | 0.93 | 0.07 | 51,51,51,51 | 0 |
| 56 | MG | 1a | 1776 | 1/1 | 0.93 | 0.12 | 58,58,58,58 | 0 |
| 56 | MG | 10 | 101 | 1/1 | 0.93 | 0.07 | 38,38,38,38 | 0 |
| 56 | MG | 1A | 4001 | 1/1 | 0.93 | 0.12 | 48,48,48,48 | 0 |
| 56 | MG | 1A | 3180 | 1/1 | 0.93 | 0.12 | 35,35,35,35 | 0 |
| 56 | MG | 2A | 3187 | 1/1 | 0.93 | 0.19 | 56,56,56,56 | 0 |
| 56 | MG | 11 | 102 | 1/1 | 0.93 | 0.12 | 42,42,42,42 | 0 |
| 56 | MG | 1A | 3566 | 1/1 | 0.93 | 0.22 | 52,52,52,52 | 0 |
| 56 | MG | 2A | 3446 | 1/1 | 0.93 | 0.30 | 63,63,63,63 | 0 |
| 56 | MG | 2A | 3763 | 1/1 | 0.93 | 0.12 | 60,60,60,60 | 0 |
| 56 | MG | 11 | 105 | 1/1 | 0.93 | 0.09 | 53,53,53,53 | 0 |
| 56 | MG | 1A | 4008 | 1/1 | 0.93 | 0.33 | 33,33,33,33 | 0 |
| 56 | MG | 1A | 3212 | 1/1 | 0.93 | 0.08 | 35,35,35,35 | 0 |
| 56 | MG | 2A | 3450 | 1/1 | 0.93 | 0.21 | 56,56,56,56 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 1A | 3484 | 1/1 | 0.93 | 0.13 | 59,59,59,59 | 0 |
| 56 | MG | 2A | 3453 | 1/1 | 0.93 | 0.14 | 52,52,52,52 | 0 |
| 56 | MG | 2a | 3182 | 1/1 | 0.93 | 0.09 | 83,83,83,83 | 0 |
| 56 | MG | 2A | 3454 | 1/1 | 0.93 | 0.24 | 50,50,50,50 | 0 |
| 56 | MG | 2a | 3185 | 1/1 | 0.93 | 0.14 | 52,52,52,52 | 0 |
| 56 | MG | 2A | 3200 | 1/1 | 0.93 | 0.23 | 48,48,48,48 | 0 |
| 56 | MG | 1A | 3183 | 1/1 | 0.93 | 0.08 | 48,48,48,48 | 0 |
| 56 | MG | 2A | 3777 | 1/1 | 0.93 | 0.09 | 47,47,47,47 | 0 |
| 56 | MG | 1A | 3853 | 1/1 | 0.93 | 0.13 | 55,55,55,55 | 0 |
| 56 | MG | 2A | 3784 | 1/1 | 0.93 | 0.11 | 64,64,64,64 | 0 |
| 56 | MG | 2A | 3785 | 1/1 | 0.93 | 0.08 | 53,53,53,53 | 0 |
| 56 | MG | 1a | 1797 | 1/1 | 0.93 | 0.08 | 65,65,65,65 | 0 |
| 56 | MG | 1a | 1798 | 1/1 | 0.93 | 0.09 | 76,76,76,76 | 0 |
| 56 | MG | 2A | 3791 | 1/1 | 0.93 | 0.13 | 56,56,56,56 | 0 |
| 56 | MG | 1A | 3576 | 1/1 | 0.93 | 0.20 | 43,43,43,43 | 0 |
| 56 | MG | 1A | 3487 | 1/1 | 0.93 | 0.10 | 44,44,44,44 | 0 |
| 56 | MG | 1A | 3861 | 1/1 | 0.93 | 0.10 | 61,61,61,61 | 0 |
| 56 | MG | 2A | 3798 | 1/1 | 0.93 | 0.09 | 51,51,51,51 | 0 |
| 56 | MG | 2a | 3203 | 1/1 | 0.93 | 0.07 | 63,63,63,63 | 0 |
| 56 | MG | 1A | 3864 | 1/1 | 0.93 | 0.13 | 52,52,52,52 | 0 |
| 56 | MG | 1A | 3584 | 1/1 | 0.93 | 0.07 | 32,32,32,32 | 0 |
| 56 | MG | 2A | 3470 | 1/1 | 0.93 | 0.16 | 62,62,62,62 | 0 |
| 56 | MG | 2A | 3803 | 1/1 | 0.93 | 0.08 | 81,81,81,81 | 0 |
| 56 | MG | 1a | 1603 | 1/1 | 0.93 | 0.08 | 61,61,61,61 | 0 |
| 56 | MG | 2A | 3215 | 1/1 | 0.93 | 0.15 | 56,56,56,56 | 0 |
| 56 | MG | 1A | 3265 | 1/1 | 0.93 | 0.12 | 43,43,43,43 | 0 |
| 56 | MG | 2a | 3219 | 1/1 | 0.93 | 0.14 | 68,68,68,68 | 0 |
| 56 | MG | 1A | 3587 | 1/1 | 0.93 | 0.23 | 35,35,35,35 | 0 |
| 56 | MG | 2a | 3223 | 1/1 | 0.93 | 0.15 | 64,64,64,64 | 0 |
| 56 | MG | 2A | 3221 | 1/1 | 0.93 | 0.10 | 57,57,57,57 | 0 |
| 56 | MG | 1a | 1830 | 1/1 | 0.93 | 0.17 | 42,42,42,42 | 0 |
| 56 | MG | 1A | 3589 | 1/1 | 0.93 | 0.10 | 35,35,35,35 | 0 |
| 56 | MG | 1A | 4051 | 1/1 | 0.93 | 0.13 | 58,58,58,58 | 0 |
| 56 | MG | 1A | 3871 | 1/1 | 0.93 | 0.07 | 32,32,32,32 | 0 |
| 56 | MG | 2a | 3230 | 1/1 | 0.93 | 0.09 | 65,65,65,65 | 0 |
| 56 | MG | 2A | 3230 | 1/1 | 0.93 | 0.16 | 67,67,67,67 | 0 |
| 56 | MG | 2a | 3232 | 1/1 | 0.93 | 0.07 | 63,63,63,63 | 0 |
| 56 | MG | 2A | 3487 | 1/1 | 0.93 | 0.27 | 48,48,48,48 | 0 |
| 56 | MG | 2A | 3818 | 1/1 | 0.93 | 0.08 | 64,64,64,64 | 0 |
| 56 | MG | 1A | 3221 | 1/1 | 0.93 | 0.09 | 46,46,46,46 | 0 |
| 56 | MG | 1a | 1613 | 1/1 | 0.93 | 0.15 | 49,49,49,49 | 0 |
| 56 | MG | 1A | 4054 | 1/1 | 0.93 | 0.17 | 53,53,53,53 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 1A | 3594 | 1/1 | 0.93 | 0.15 | 55,55,55,55 | 0 |
| 56 | MG | 2A | 3241 | 1/1 | 0.93 | 0.23 | 62,62,62,62 | 0 |
| 56 | MG | 1a | 1618 | 1/1 | 0.93 | 0.10 | 49,49,49,49 | 0 |
| 56 | MG | 1A | 3271 | 1/1 | 0.93 | 0.23 | 44,44,44,44 | 0 |
| 56 | MG | 2A | 3832 | 1/1 | 0.93 | 0.09 | 38,38,38,38 | 0 |
| 56 | MG | 1A | 3881 | 1/1 | 0.93 | 0.13 | 36,36,36,36 | 0 |
| 56 | MG | 2A | 3834 | 1/1 | 0.93 | 0.12 | 48,48,48,48 | 0 |
| 56 | MG | 2i | 201 | 1/1 | 0.93 | 0.08 | 62,62,62,62 | 0 |
| 56 | MG | 2A | 3836 | 1/1 | 0.93 | 0.10 | 62,62,62,62 | 0 |
| 56 | MG | 2A | 3499 | 1/1 | 0.93 | 0.09 | 47,47,47,47 | 0 |
| 56 | MG | 2A | 3501 | 1/1 | 0.93 | 0.07 | 58,58,58,58 | 0 |
| 56 | MG | 1w | 101 | 1/1 | 0.93 | 0.21 | 65,65,65,65 | 0 |
| 56 | MG | 1A | 3727 | 1/1 | 0.93 | 0.07 | 39,39,39,39 | 0 |
| 56 | MG | 2A | 3505 | 1/1 | 0.93 | 0.21 | 57,57,57,57 | 0 |
| 56 | MG | 1A | 3884 | 1/1 | 0.93 | 0.17 | 28,28,28,28 | 0 |
| 56 | MG | 1a | 1629 | 1/1 | 0.93 | 0.19 | 54,54,54,54 | 0 |
| 56 | MG | 2A | 3512 | 1/1 | 0.93 | 0.16 | 58,58,58,58 | 0 |
| 56 | MG | 1A | 3728 | 1/1 | 0.93 | 0.10 | 44,44,44,44 | 0 |
| 56 | MG | 1A | 3887 | 1/1 | 0.93 | 0.09 | 31,31,31,31 | 0 |
| 56 | MG | 1A | 3497 | 1/1 | 0.93 | 0.09 | 50,50,50,50 | 0 |
| 56 | MG | 1A | 3734 | 1/1 | 0.93 | 0.10 | 49,49,49,49 | 0 |
| 56 | MG | 2x | 101 | 1/1 | 0.93 | 0.10 | 60,60,60,60 | 0 |
| 56 | MG | 1a | 1638 | 1/1 | 0.93 | 0.19 | 61,61,61,61 | 0 |
| 56 | MG | 2A | 3518 | 1/1 | 0.93 | 0.11 | 53,53,53,53 | 0 |
| 56 | MG | 1A | 4074 | 1/1 | 0.93 | 0.08 | 48,48,48,48 | 0 |
| 56 | MG | 2A | 3880 | 1/1 | 0.93 | 0.11 | 52,52,52,52 | 0 |
| 56 | MG | 1A | 3279 | 1/1 | 0.93 | 0.18 | 39,39,39,39 | 0 |
| 56 | MG | 2A | 3526 | 1/1 | 0.93 | 0.08 | 30,30,30,30 | 0 |
| 56 | MG | 2y | 104 | 1/1 | 0.93 | 0.08 | 50,50,50,50 | 0 |
| 56 | MG | 1A | 3607 | 1/1 | 0.93 | 0.10 | 27,27,27,27 | 0 |
| 56 | MG | 1A | 3704 | 1/1 | 0.94 | 0.06 | 21,21,21,21 | 0 |
| 56 | MG | 1x | 118 | 1/1 | 0.94 | 0.09 | 58,58,58,58 | 0 |
| 56 | MG | 1A | 3558 | 1/1 | 0.94 | 0.21 | 54,54,54,54 | 0 |
| 56 | MG | 2A | 3292 | 1/1 | 0.94 | 0.22 | 57,57,57,57 | 0 |
| 56 | MG | 2A | 3571 | 1/1 | 0.94 | 0.09 | 42,42,42,42 | 0 |
| 56 | MG | 1A | 3868 | 1/1 | 0.94 | 0.08 | 35,35,35,35 | 0 |
| 56 | MG | 2A | 3573 | 1/1 | 0.94 | 0.10 | 62,62,62,62 | 0 |
| 56 | MG | 2D | 306 | 1/1 | 0.94 | 0.32 | 47,47,47,47 | 0 |
| 56 | MG | 2D | 307 | 1/1 | 0.94 | 0.27 | 47,47,47,47 | 0 |
| 56 | MG | 2A | 3574 | 1/1 | 0.94 | 0.13 | 46,46,46,46 | 0 |
| 56 | MG | 1A | 3462 | 1/1 | 0.94 | 0.14 | 54,54,54,54 | 0 |
| 56 | MG | 1a | 1643 | 1/1 | 0.94 | 0.07 | 51,51,51,51 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 2E | 301 | 1/1 | 0.94 | 0.10 | 49,49,49,49 | 0 |
| 56 | MG | 2E | 302 | 1/1 | 0.94 | 0.13 | 61,61,61,61 | 0 |
| 56 | MG | 2F | 302 | 1/1 | 0.94 | 0.17 | 64,64,64,64 | 0 |
| 56 | MG | 1A | 3870 | 1/1 | 0.94 | 0.10 | 30,30,30,30 | 0 |
| 56 | MG | 2A | 3298 | 1/1 | 0.94 | 0.16 | 57,57,57,57 | 0 |
| 56 | MG | 1a | 1647 | 1/1 | 0.94 | 0.20 | 55,55,55,55 | 0 |
| 56 | MG | 1A | 3111 | 1/1 | 0.94 | 0.10 | 37,37,37,37 | 0 |
| 56 | MG | 1A | 3304 | 1/1 | 0.94 | 0.15 | 21,21,21,21 | 0 |
| 56 | MG | 2A | 3590 | 1/1 | 0.94 | 0.10 | 64,64,64,64 | 0 |
| 56 | MG | 2Q | 201 | 1/1 | 0.94 | 0.06 | 49,49,49,49 | 0 |
| 56 | MG | 2Q | 202 | 1/1 | 0.94 | 0.10 | 53,53,53,53 | 0 |
| 56 | MG | 2A | 3592 | 1/1 | 0.94 | 0.09 | 46,46,46,46 | 0 |
| 56 | MG | 1A | 3564 | 1/1 | 0.94 | 0.12 | 49,49,49,49 | 0 |
| 56 | MG | 2A | 3021 | 1/1 | 0.94 | 0.24 | 55,55,55,55 | 0 |
| 56 | MG | 1A | 3050 | 1/1 | 0.94 | 0.09 | 21,21,21,21 | 0 |
| 56 | MG | 2A | 3024 | 1/1 | 0.94 | 0.18 | 48,48,48,48 | 0 |
| 56 | MG | 2A | 3025 | 1/1 | 0.94 | 0.06 | 44,44,44,44 | 0 |
| 56 | MG | 2A | 3026 | 1/1 | 0.94 | 0.23 | 53,53,53,53 | 0 |
| 56 | MG | 1A | 3182 | 1/1 | 0.94 | 0.16 | 49,49,49,49 | 0 |
| 56 | MG | 2U | 202 | 1/1 | 0.94 | 0.28 | 58,58,58,58 | 0 |
| 56 | MG | 1a | 1658 | 1/1 | 0.94 | 0.10 | 63,63,63,63 | 0 |
| 56 | MG | 1A | 3470 | 1/1 | 0.94 | 0.18 | 49,49,49,49 | 0 |
| 56 | MG | 2A | 3312 | 1/1 | 0.94 | 0.10 | 50,50,50,50 | 0 |
| 56 | MG | 1A | 3717 | 1/1 | 0.94 | 0.08 | 41,41,41,41 | 0 |
| 56 | MG | 1A | 3310 | 1/1 | 0.94 | 0.24 | 40,40,40,40 | 0 |
| 56 | MG | 2W | 202 | 1/1 | 0.94 | 0.08 | 45,45,45,45 | 0 |
| 56 | MG | 2W | 203 | 1/1 | 0.94 | 0.08 | 51,51,51,51 | 0 |
| 56 | MG | 2X | 101 | 1/1 | 0.94 | 0.08 | 56,56,56,56 | 0 |
| 56 | MG | 1A | 3243 | 1/1 | 0.94 | 0.17 | 33,33,33,33 | 0 |
| 56 | MG | 1A | 3474 | 1/1 | 0.94 | 0.23 | 32,32,32,32 | 0 |
| 56 | MG | 1A | 3889 | 1/1 | 0.94 | 0.10 | 44,44,44,44 | 0 |
| 56 | MG | 21 | 101 | 1/1 | 0.94 | 0.28 | 55,55,55,55 | 0 |
| 56 | MG | 23 | 101 | 1/1 | 0.94 | 0.10 | 54,54,54,54 | 0 |
| 56 | MG | 23 | 102 | 1/1 | 0.94 | 0.09 | 45,45,45,45 | 0 |
| 56 | MG | 25 | 101 | 1/1 | 0.94 | 0.37 | 58,58,58,58 | 0 |
| 56 | MG | 1A | 3051 | 1/1 | 0.94 | 0.15 | 31,31,31,31 | 0 |
| 56 | MG | 1A | 3578 | 1/1 | 0.94 | 0.08 | 43,43,43,43 | 0 |
| 56 | MG | 2A | 3320 | 1/1 | 0.94 | 0.22 | 54,54,54,54 | 0 |
| 56 | MG | 1A | 4092 | 1/1 | 0.94 | 0.10 | 54,54,54,54 | 0 |
| 56 | MG | 27 | 102 | 1/1 | 0.94 | 0.16 | 34,34,34,34 | 0 |
| 56 | MG | 1A | 3581 | 1/1 | 0.94 | 0.06 | 15,15,15,15 | 0 |
| 56 | MG | 28 | 102 | 1/1 | 0.94 | 0.10 | 48,48,48,48 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 1A | 3378 | 1/1 | 0.94 | 0.10 | 42,42,42,42 | 0 |
| 56 | MG | 1A | 3379 | 1/1 | 0.94 | 0.13 | 48,48,48,48 | 0 |
| 56 | MG | 1a | 1672 | 1/1 | 0.94 | 0.07 | 44,44,44,44 | 0 |
| 56 | MG | 1A | 3896 | 1/1 | 0.94 | 0.08 | 60,60,60,60 | 0 |
| 56 | MG | 1A | 3737 | 1/1 | 0.94 | 0.06 | 41,41,41,41 | 0 |
| 56 | MG | 1A | 3084 | 1/1 | 0.94 | 0.11 | 33,33,33,33 | 0 |
| 56 | MG | 1B | 206 | 1/1 | 0.94 | 0.12 | 40,40,40,40 | 0 |
| 56 | MG | 2A | 3629 | 1/1 | 0.94 | 0.10 | 36,36,36,36 | 0 |
| 56 | MG | 1A | 3381 | 1/1 | 0.94 | 0.19 | 52,52,52,52 | 0 |
| 56 | MG | 1A | 3318 | 1/1 | 0.94 | 0.20 | 43,43,43,43 | 0 |
| 56 | MG | 2A | 3633 | 1/1 | 0.94 | 0.12 | 40,40,40,40 | 0 |
| 56 | MG | 1A | 3746 | 1/1 | 0.94 | 0.12 | 46,46,46,46 | 0 |
| 56 | MG | 1a | 1680 | 1/1 | 0.94 | 0.20 | 63,63,63,63 | 0 |
| 56 | MG | 2A | 3338 | 1/1 | 0.94 | 0.14 | 62,62,62,62 | 0 |
| 56 | MG | 2A | 3638 | 1/1 | 0.94 | 0.15 | 55,55,55,55 | 0 |
| 56 | MG | 1a | 1683 | 1/1 | 0.94 | 0.10 | 43,43,43,43 | 0 |
| 56 | MG | 1a | 1684 | 1/1 | 0.94 | 0.28 | 63,63,63,63 | 0 |
| 56 | MG | 2A | 3641 | 1/1 | 0.94 | 0.09 | 38,38,38,38 | 0 |
| 56 | MG | 1A | 3906 | 1/1 | 0.94 | 0.10 | 49,49,49,49 | 0 |
| 56 | MG | 1A | 3747 | 1/1 | 0.94 | 0.06 | 54,54,54,54 | 0 |
| 56 | MG | 1A | 3910 | 1/1 | 0.94 | 0.11 | 51,51,51,51 | 0 |
| 56 | MG | 1A | 3388 | 1/1 | 0.94 | 0.12 | 44,44,44,44 | 0 |
| 56 | MG | 1a | 1689 | 1/1 | 0.94 | 0.07 | 59,59,59,59 | 0 |
| 56 | MG | 2A | 3076 | 1/1 | 0.94 | 0.12 | 31,31,31,31 | 0 |
| 56 | MG | 1A | 3600 | 1/1 | 0.94 | 0.12 | 39,39,39,39 | 0 |
| 56 | MG | 2A | 3653 | 1/1 | 0.94 | 0.17 | 61,61,61,61 | 0 |
| 56 | MG | 1A | 3757 | 1/1 | 0.94 | 0.11 | 50,50,50,50 | 0 |
| 56 | MG | 2A | 3079 | 1/1 | 0.94 | 0.12 | 46,46,46,46 | 0 |
| 56 | MG | 1A | 3390 | 1/1 | 0.94 | 0.13 | 36,36,36,36 | 0 |
| 56 | MG | 2A | 3358 | 1/1 | 0.94 | 0.17 | 56,56,56,56 | 0 |
| 56 | MG | 1A | 3391 | 1/1 | 0.94 | 0.07 | 42,42,42,42 | 0 |
| 56 | MG | 1A | 3392 | 1/1 | 0.94 | 0.08 | 45,45,45,45 | 0 |
| 56 | MG | 2A | 3363 | 1/1 | 0.94 | 0.11 | 51,51,51,51 | 0 |
| 56 | MG | 2A | 3668 | 1/1 | 0.94 | 0.15 | 54,54,54,54 | 0 |
| 56 | MG | 2A | 3670 | 1/1 | 0.94 | 0.16 | 47,47,47,47 | 0 |
| 56 | MG | 1A | 3763 | 1/1 | 0.94 | 0.08 | 22,22,22,22 | 0 |
| 56 | MG | 1a | 1696 | 1/1 | 0.94 | 0.23 | 44,44,44,44 | 0 |
| 56 | MG | 1A | 3923 | 1/1 | 0.94 | 0.11 | 59,59,59,59 | 0 |
| 56 | MG | 2a | 3047 | 1/1 | 0.94 | 0.14 | 55,55,55,55 | 0 |
| 56 | MG | 2A | 3675 | 1/1 | 0.94 | 0.12 | 57,57,57,57 | 0 |
| 56 | MG | 1A | 3490 | 1/1 | 0.94 | 0.09 | 35,35,35,35 | 0 |
| 56 | MG | 2A | 3369 | 1/1 | 0.94 | 0.12 | 64,64,64,64 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 2a | 3051 | 1/1 | 0.94 | 0.13 | 62,62,62,62 | 0 |
| 56 | MG | 2A | 3370 | 1/1 | 0.94 | 0.16 | 64,64,64,64 | 0 |
| 56 | MG | 1a | 1699 | 1/1 | 0.94 | 0.29 | 47,47,47,47 | 0 |
| 56 | MG | 1A | 3052 | 1/1 | 0.94 | 0.08 | 40,40,40,40 | 0 |
| 56 | MG | 2A | 3682 | 1/1 | 0.94 | 0.15 | 74,74,74,74 | 0 |
| 56 | MG | 1A | 3034 | 1/1 | 0.94 | 0.20 | 23,23,23,23 | 0 |
| 56 | MG | 1A | 3130 | 1/1 | 0.94 | 0.09 | 29,29,29,29 | 0 |
| 56 | MG | 1a | 1706 | 1/1 | 0.94 | 0.23 | 59,59,59,59 | 0 |
| 56 | MG | 1A | 3621 | 1/1 | 0.94 | 0.09 | 27,27,27,27 | 0 |
| 56 | MG | 2A | 3379 | 1/1 | 0.94 | 0.15 | 56,56,56,56 | 0 |
| 56 | MG | 2A | 3690 | 1/1 | 0.94 | 0.07 | 40,40,40,40 | 0 |
| 56 | MG | 1B | 239 | 1/1 | 0.94 | 0.07 | 30,30,30,30 | 0 |
| 56 | MG | 1D | 306 | 1/1 | 0.94 | 0.12 | 33,33,33,33 | 0 |
| 56 | MG | 1D | 310 | 1/1 | 0.94 | 0.09 | 24,24,24,24 | 0 |
| 56 | MG | 1a | 1712 | 1/1 | 0.94 | 0.09 | 53,53,53,53 | 0 |
| 56 | MG | 1A | 3328 | 1/1 | 0.94 | 0.15 | 48,48,48,48 | 0 |
| 56 | MG | 1D | 313 | 1/1 | 0.94 | 0.18 | 34,34,34,34 | 0 |
| 56 | MG | 2A | 3115 | 1/1 | 0.94 | 0.08 | 41,41,41,41 | 0 |
| 56 | MG | 1A | 3400 | 1/1 | 0.94 | 0.33 | 42,42,42,42 | 0 |
| 56 | MG | 1a | 1717 | 1/1 | 0.94 | 0.15 | 64,64,64,64 | 0 |
| 56 | MG | 2a | 3075 | 1/1 | 0.94 | 0.16 | 57,57,57,57 | 0 |
| 56 | MG | 2a | 3076 | 1/1 | 0.94 | 0.07 | 53,53,53,53 | 0 |
| 56 | MG | 2A | 3394 | 1/1 | 0.94 | 0.25 | 51,51,51,51 | 0 |
| 56 | MG | 2A | 3118 | 1/1 | 0.94 | 0.15 | 43,43,43,43 | 0 |
| 56 | MG | 2A | 3706 | 1/1 | 0.94 | 0.08 | 68,68,68,68 | 0 |
| 56 | MG | 1E | 308 | 1/1 | 0.94 | 0.06 | 31,31,31,31 | 0 |
| 56 | MG | 1A | 3401 | 1/1 | 0.94 | 0.20 | 35,35,35,35 | 0 |
| 56 | MG | 2A | 3122 | 1/1 | 0.94 | 0.24 | 53,53,53,53 | 0 |
| 56 | MG | 1A | 3627 | 1/1 | 0.94 | 0.08 | 18,18,18,18 | 0 |
| 56 | MG | 2A | 3401 | 1/1 | 0.94 | 0.10 | 54,54,54,54 | 0 |
| 56 | MG | 1A | 3095 | 1/1 | 0.94 | 0.18 | 44,44,44,44 | 0 |
| 56 | MG | 2A | 3403 | 1/1 | 0.94 | 0.09 | 57,57,57,57 | 0 |
| 56 | MG | 1a | 1724 | 1/1 | 0.94 | 0.21 | 49,49,49,49 | 0 |
| 56 | MG | 2a | 3090 | 1/1 | 0.94 | 0.15 | 66,66,66,66 | 0 |
| 56 | MG | 1A | 3780 | 1/1 | 0.94 | 0.09 | 34,34,34,34 | 0 |
| 56 | MG | 1F | 305 | 1/1 | 0.94 | 0.07 | 45,45,45,45 | 0 |
| 56 | MG | 1A | 3781 | 1/1 | 0.94 | 0.07 | 41,41,41,41 | 0 |
| 56 | MG | 2A | 3409 | 1/1 | 0.94 | 0.26 | 66,66,66,66 | 0 |
| 56 | MG | 2A | 3144 | 1/1 | 0.94 | 0.19 | 54,54,54,54 | 0 |
| 56 | MG | 2A | 3726 | 1/1 | 0.94 | 0.07 | 50,50,50,50 | 0 |
| 56 | MG | 1A | 3403 | 1/1 | 0.94 | 0.08 | 53,53,53,53 | 0 |
| 56 | MG | 1A | 3635 | 1/1 | 0.94 | 0.11 | 33,33,33,33 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 1A | 3505 | 1/1 | 0.94 | 0.08 | 39,39,39,39 | 0 |
| 56 | MG | 1A | 3257 | 1/1 | 0.94 | 0.15 | 58,58,58,58 | 0 |
| 56 | MG | 1N | 204 | 1/1 | 0.94 | 0.17 | 42,42,42,42 | 0 |
| 56 | MG | 1A | 3641 | 1/1 | 0.94 | 0.07 | 22,22,22,22 | 0 |
| 56 | MG | 1A | 3961 | 1/1 | 0.94 | 0.07 | 56,56,56,56 | 0 |
| 56 | MG | 1A | 3794 | 1/1 | 0.94 | 0.16 | 48,48,48,48 | 0 |
| 56 | MG | 2A | 3158 | 1/1 | 0.94 | 0.28 | 56,56,56,56 | 0 |
| 56 | MG | 1P | 202 | 1/1 | 0.94 | 0.14 | 23,23,23,23 | 0 |
| 56 | MG | 1P | 205 | 1/1 | 0.94 | 0.07 | 16,16,16,16 | 0 |
| 56 | MG | 2A | 3161 | 1/1 | 0.94 | 0.15 | 64,64,64,64 | 0 |
| 56 | MG | 2A | 3162 | 1/1 | 0.94 | 0.19 | 64,64,64,64 | 0 |
| 56 | MG | 1a | 1744 | 1/1 | 0.94 | 0.15 | 54,54,54,54 | 0 |
| 56 | MG | 1A | 3642 | 1/1 | 0.94 | 0.06 | 14,14,14,14 | 0 |
| 56 | MG | 2A | 3165 | 1/1 | 0.94 | 0.30 | 65,65,65,65 | 0 |
| 56 | MG | 1A | 3510 | 1/1 | 0.94 | 0.06 | 41,41,41,41 | 0 |
| 56 | MG | 1A | 3408 | 1/1 | 0.94 | 0.18 | 32,32,32,32 | 0 |
| 56 | MG | 1Q | 204 | 1/1 | 0.94 | 0.08 | 44,44,44,44 | 0 |
| 56 | MG | 2a | 3119 | 1/1 | 0.94 | 0.11 | 69,69,69,69 | 0 |
| 56 | MG | 1A | 3258 | 1/1 | 0.94 | 0.17 | 25,25,25,25 | 0 |
| 56 | MG | 1A | 3054 | 1/1 | 0.94 | 0.07 | 42,42,42,42 | 0 |
| 56 | MG | 1A | 3416 | 1/1 | 0.94 | 0.12 | 36,36,36,36 | 0 |
| 56 | MG | 1A | 3972 | 1/1 | 0.94 | 0.08 | 43,43,43,43 | 0 |
| 56 | MG | 1A | 3020 | 1/1 | 0.94 | 0.07 | 33,33,33,33 | 0 |
| 56 | MG | 1a | 1762 | 1/1 | 0.94 | 0.10 | 61,61,61,61 | 0 |
| 56 | MG | 2A | 3178 | 1/1 | 0.94 | 0.14 | 48,48,48,48 | 0 |
| 56 | MG | 2a | 3129 | 1/1 | 0.94 | 0.07 | 49,49,49,49 | 0 |
| 56 | MG | 1A | 3976 | 1/1 | 0.94 | 0.09 | 47,47,47,47 | 0 |
| 56 | MG | 1A | 3519 | 1/1 | 0.94 | 0.10 | 45,45,45,45 | 0 |
| 56 | MG | 1A | 3980 | 1/1 | 0.94 | 0.08 | 62,62,62,62 | 0 |
| 56 | MG | 1A | 3981 | 1/1 | 0.94 | 0.08 | 60,60,60,60 | 0 |
| 56 | MG | 1U | 209 | 1/1 | 0.94 | 0.30 | 44,44,44,44 | 0 |
| 56 | MG | 1A | 3100 | 1/1 | 0.94 | 0.15 | 41,41,41,41 | 0 |
| 56 | MG | 1A | 3660 | 1/1 | 0.94 | 0.06 | 31,31,31,31 | 0 |
| 56 | MG | 2a | 3144 | 1/1 | 0.94 | 0.09 | 65,65,65,65 | 0 |
| 56 | MG | 1A | 3985 | 1/1 | 0.94 | 0.11 | 61,61,61,61 | 0 |
| 56 | MG | 1A | 3523 | 1/1 | 0.94 | 0.11 | 53,53,53,53 | 0 |
| 56 | MG | 1a | 1777 | 1/1 | 0.94 | 0.11 | 59,59,59,59 | 0 |
| 56 | MG | 2A | 3772 | 1/1 | 0.94 | 0.12 | 66,66,66,66 | 0 |
| 56 | MG | 1A | 3268 | 1/1 | 0.94 | 0.15 | 35,35,35,35 | 0 |
| 56 | MG | 1A | 3147 | 1/1 | 0.94 | 0.11 | 39,39,39,39 | 0 |
| 56 | MG | 2A | 3459 | 1/1 | 0.94 | 0.13 | 41,41,41,41 | 0 |
| 56 | MG | 2A | 3779 | 1/1 | 0.94 | 0.07 | 71,71,71,71 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 1A | 3664 | 1/1 | 0.94 | 0.07 | 40,40,40,40 | 0 |
| 56 | MG | 1A | 3424 | 1/1 | 0.94 | 0.09 | 48,48,48,48 | 0 |
| 56 | MG | 2A | 3203 | 1/1 | 0.94 | 0.20 | 48,48,48,48 | 0 |
| 56 | MG | 1A | 3148 | 1/1 | 0.94 | 0.16 | 35,35,35,35 | 0 |
| 56 | MG | 2a | 3167 | 1/1 | 0.94 | 0.06 | 75,75,75,75 | 0 |
| 56 | MG | 1A | 3668 | 1/1 | 0.94 | 0.06 | 21,21,21,21 | 0 |
| 56 | MG | 2a | 3172 | 1/1 | 0.94 | 0.08 | 62,62,62,62 | 0 |
| 56 | MG | 1A | 3825 | 1/1 | 0.94 | 0.12 | 34,34,34,34 | 0 |
| 56 | MG | 2A | 3468 | 1/1 | 0.94 | 0.32 | 51,51,51,51 | 0 |
| 56 | MG | 2A | 3793 | 1/1 | 0.94 | 0.15 | 77,77,77,77 | 0 |
| 56 | MG | 1a | 1788 | 1/1 | 0.94 | 0.07 | 61,61,61,61 | 0 |
| 56 | MG | 2a | 3177 | 1/1 | 0.94 | 0.14 | 65,65,65,65 | 0 |
| 56 | MG | 1A | 3997 | 1/1 | 0.94 | 0.15 | 45,45,45,45 | 0 |
| 56 | MG | 1A | 3276 | 1/1 | 0.94 | 0.09 | 45,45,45,45 | 0 |
| 56 | MG | 2a | 3180 | 1/1 | 0.94 | 0.08 | 71,71,71,71 | 0 |
| 56 | MG | 2a | 3181 | 1/1 | 0.94 | 0.12 | 64,64,64,64 | 0 |
| 56 | MG | 2A | 3473 | 1/1 | 0.94 | 0.21 | 60,60,60,60 | 0 |
| 56 | MG | 11 | 103 | 1/1 | 0.94 | 0.07 | 36,36,36,36 | 0 |
| 56 | MG | 1A | 3999 | 1/1 | 0.94 | 0.08 | 39,39,39,39 | 0 |
| 56 | MG | 1A | 3278 | 1/1 | 0.94 | 0.07 | 41,41,41,41 | 0 |
| 56 | MG | 1A | 3209 | 1/1 | 0.94 | 0.10 | 38,38,38,38 | 0 |
| 56 | MG | 12 | 102 | 1/1 | 0.94 | 0.09 | 39,39,39,39 | 0 |
| 56 | MG | 2A | 3480 | 1/1 | 0.94 | 0.11 | 46,46,46,46 | 0 |
| 56 | MG | 2A | 3219 | 1/1 | 0.94 | 0.16 | 52,52,52,52 | 0 |
| 56 | MG | 13 | 103 | 1/1 | 0.94 | 0.06 | 39,39,39,39 | 0 |
| 56 | MG | 1a | 1803 | 1/1 | 0.94 | 0.09 | 61,61,61,61 | 0 |
| 56 | MG | 1A | 4002 | 1/1 | 0.94 | 0.07 | 31,31,31,31 | 0 |
| 56 | MG | 2A | 3226 | 1/1 | 0.94 | 0.10 | 57,57,57,57 | 0 |
| 56 | MG | 1A | 3435 | 1/1 | 0.94 | 0.08 | 42,42,42,42 | 0 |
| 56 | MG | 1A | 3436 | 1/1 | 0.94 | 0.07 | 49,49,49,49 | 0 |
| 56 | MG | 1A | 4007 | 1/1 | 0.94 | 0.07 | 15,15,15,15 | 0 |
| 56 | MG | 1A | 3837 | 1/1 | 0.94 | 0.11 | 51,51,51,51 | 0 |
| 56 | MG | 2A | 3235 | 1/1 | 0.94 | 0.12 | 44,44,44,44 | 0 |
| 56 | MG | 2A | 3236 | 1/1 | 0.94 | 0.10 | 45,45,45,45 | 0 |
| 56 | MG | 2a | 3206 | 1/1 | 0.94 | 0.15 | 62,62,62,62 | 0 |
| 56 | MG | 17 | 104 | 1/1 | 0.94 | 0.07 | 37,37,37,37 | 0 |
| 56 | MG | 2A | 3824 | 1/1 | 0.94 | 0.11 | 66,66,66,66 | 0 |
| 56 | MG | 1a | 1829 | 1/1 | 0.94 | 0.14 | 43,43,43,43 | 0 |
| 56 | MG | 2A | 3827 | 1/1 | 0.94 | 0.07 | 62,62,62,62 | 0 |
| 56 | MG | 18 | 101 | 1/1 | 0.94 | 0.11 | 37,37,37,37 | 0 |
| 56 | MG | 1A | 4009 | 1/1 | 0.94 | 0.16 | 23,23,23,23 | 0 |
| 56 | MG | 2A | 3242 | 1/1 | 0.94 | 0.08 | 64,64,64,64 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 18 | 104 | 1/1 | 0.94 | 0.12 | 49,49,49,49 | 0 |
| 56 | MG | 2a | 3221 | 1/1 | 0.94 | 0.10 | 55,55,55,55 | 0 |
| 56 | MG | 2A | 3245 | 1/1 | 0.94 | 0.09 | 47,47,47,47 | 0 |
| 56 | MG | 1A | 4011 | 1/1 | 0.94 | 0.08 | 65,65,65,65 | 0 |
| 56 | MG | 1A | 4012 | 1/1 | 0.94 | 0.09 | 68,68,68,68 | 0 |
| 56 | MG | 1A | 4015 | 1/1 | 0.94 | 0.05 | 29,29,29,29 | 0 |
| 56 | MG | 1A | 3437 | 1/1 | 0.94 | 0.18 | 53,53,53,53 | 0 |
| 56 | MG | 2A | 3841 | 1/1 | 0.94 | 0.09 | 47,47,47,47 | 0 |
| 56 | MG | 1A | 3151 | 1/1 | 0.94 | 0.12 | 42,42,42,42 | 0 |
| 56 | MG | 2A | 3848 | 1/1 | 0.94 | 0.07 | 74,74,74,74 | 0 |
| 56 | MG | 1e | 202 | 1/1 | 0.94 | 0.14 | 59,59,59,59 | 0 |
| 56 | MG | 1A | 3155 | 1/1 | 0.94 | 0.11 | 43,43,43,43 | 0 |
| 56 | MG | 2a | 3234 | 1/1 | 0.94 | 0.11 | 60,60,60,60 | 0 |
| 56 | MG | 1A | 4019 | 1/1 | 0.94 | 0.06 | 22,22,22,22 | 0 |
| 56 | MG | 1A | 4022 | 1/1 | 0.94 | 0.08 | 31,31,31,31 | 0 |
| 56 | MG | 1v | 101 | 1/1 | 0.94 | 0.12 | 65,65,65,65 | 0 |
| 56 | MG | 1A | 3291 | 1/1 | 0.94 | 0.09 | 32,32,32,32 | 0 |
| 56 | MG | 1A | 3350 | 1/1 | 0.94 | 0.23 | 51,51,51,51 | 0 |
| 56 | MG | 1A | 3846 | 1/1 | 0.94 | 0.07 | 39,39,39,39 | 0 |
| 56 | MG | 1A | 3351 | 1/1 | 0.94 | 0.30 | 47,47,47,47 | 0 |
| 56 | MG | 1A | 4037 | 1/1 | 0.94 | 0.07 | 68,68,68,68 | 0 |
| 56 | MG | 2A | 3874 | 1/1 | 0.94 | 0.12 | 66,66,66,66 | 0 |
| 56 | MG | 2f | 201 | 1/1 | 0.94 | 0.10 | 48,48,48,48 | 0 |
| 56 | MG | 1A | 3545 | 1/1 | 0.94 | 0.09 | 46,46,46,46 | 0 |
| 56 | MG | 2A | 3876 | 1/1 | 0.94 | 0.14 | 47,47,47,47 | 0 |
| 56 | MG | 1A | 3217 | 1/1 | 0.94 | 0.06 | 39,39,39,39 | 0 |
| 56 | MG | 1a | 1621 | 1/1 | 0.94 | 0.13 | 51,51,51,51 | 0 |
| 56 | MG | 1a | 1622 | 1/1 | 0.94 | 0.07 | 40,40,40,40 | 0 |
| 56 | MG | 2A | 3883 | 1/1 | 0.94 | 0.11 | 68,68,68,68 | 0 |
| 56 | MG | 2A | 3272 | 1/1 | 0.94 | 0.12 | 56,56,56,56 | 0 |
| 56 | MG | 1a | 1623 | 1/1 | 0.94 | 0.17 | 55,55,55,55 | 0 |
| 56 | MG | 1x | 101 | 1/1 | 0.94 | 0.12 | 38,38,38,38 | 0 |
| 56 | MG | 1A | 3454 | 1/1 | 0.94 | 0.19 | 39,39,39,39 | 0 |
| 56 | MG | 2r | 101 | 1/1 | 0.94 | 0.09 | 65,65,65,65 | 0 |
| 56 | MG | 2A | 3546 | 1/1 | 0.94 | 0.12 | 65,65,65,65 | 0 |
| 56 | MG | 1x | 107 | 1/1 | 0.94 | 0.15 | 49,49,49,49 | 0 |
| 56 | MG | 2A | 3549 | 1/1 | 0.94 | 0.17 | 47,47,47,47 | 0 |
| 56 | MG | 1A | 3854 | 1/1 | 0.94 | 0.07 | 60,60,60,60 | 0 |
| 56 | MG | 1A | 3101 | 1/1 | 0.94 | 0.18 | 56,56,56,56 | 0 |
| 56 | MG | 2A | 3552 | 1/1 | 0.94 | 0.10 | 43,43,43,43 | 0 |
| 56 | MG | 2A | 3555 | 1/1 | 0.94 | 0.09 | 27,27,27,27 | 0 |
| 56 | MG | 1A | 3857 | 1/1 | 0.94 | 0.15 | 36,36,36,36 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 2B | 209 | 1/1 | 0.94 | 0.23 | 59,59,59,59 | 0 |
| 56 | MG | 2A | 3557 | 1/1 | 0.94 | 0.10 | 59,59,59,59 | 0 |
| 56 | MG | 1A | 3046 | 1/1 | 0.94 | 0.10 | 28,28,28,28 | 0 |
| 56 | MG | 1A | 3019 | 1/1 | 0.94 | 0.15 | 41,41,41,41 | 0 |
| 56 | MG | 2A | 3284 | 1/1 | 0.94 | 0.07 | 59,59,59,59 | 0 |
| 56 | MG | 1A | 3701 | 1/1 | 0.94 | 0.08 | 23,23,23,23 | 0 |
| 56 | MG | 1A | 3557 | 1/1 | 0.94 | 0.08 | 47,47,47,47 | 0 |
| 59 | ZN | 24 | 501 | 1/1 | 0.94 | 0.07 | 117,117,117,117 | 0 |
| 56 | MG | 2A | 3001 | 1/1 | 0.95 | 0.23 | 55,55,55,55 | 0 |
| 56 | MG | 1A | 4064 | 1/1 | 0.95 | 0.06 | 34,34,34,34 | 0 |
| 56 | MG | 2E | 304 | 1/1 | 0.95 | 0.09 | 43,43,43,43 | 0 |
| 56 | MG | 2A | 3581 | 1/1 | 0.95 | 0.10 | 46,46,46,46 | 0 |
| 56 | MG | 2F | 303 | 1/1 | 0.95 | 0.09 | 48,48,48,48 | 0 |
| 56 | MG | 1A | 3873 | 1/1 | 0.95 | 0.10 | 35,35,35,35 | 0 |
| 56 | MG | 2A | 3004 | 1/1 | 0.95 | 0.24 | 58,58,58,58 | 0 |
| 56 | MG | 1a | 1635 | 1/1 | 0.95 | 0.09 | 55,55,55,55 | 0 |
| 56 | MG | 2P | 201 | 1/1 | 0.95 | 0.23 | 58,58,58,58 | 0 |
| 56 | MG | 1A | 3041 | 1/1 | 0.95 | 0.30 | 34,34,34,34 | 0 |
| 56 | MG | 2A | 3007 | 1/1 | 0.95 | 0.15 | 49,49,49,49 | 0 |
| 56 | MG | 1a | 1639 | 1/1 | 0.95 | 0.19 | 56,56,56,56 | 0 |
| 56 | MG | 1A | 4071 | 1/1 | 0.95 | 0.07 | 51,51,51,51 | 0 |
| 56 | MG | 2A | 3012 | 1/1 | 0.95 | 0.06 | 40,40,40,40 | 0 |
| 56 | MG | 1A | 3448 | 1/1 | 0.95 | 0.07 | 36,36,36,36 | 0 |
| 56 | MG | 2A | 3015 | 1/1 | 0.95 | 0.11 | 39,39,39,39 | 0 |
| 56 | MG | 2A | 3598 | 1/1 | 0.95 | 0.08 | 42,42,42,42 | 0 |
| 56 | MG | 1A | 3707 | 1/1 | 0.95 | 0.08 | 25,25,25,25 | 0 |
| 56 | MG | 2A | 3018 | 1/1 | 0.95 | 0.11 | 49,49,49,49 | 0 |
| 56 | MG | 1A | 3449 | 1/1 | 0.95 | 0.15 | 32,32,32,32 | 0 |
| 56 | MG | 1A | 3882 | 1/1 | 0.95 | 0.12 | 44,44,44,44 | 0 |
| 56 | MG | 1A | 3262 | 1/1 | 0.95 | 0.18 | 59,59,59,59 | 0 |
| 56 | MG | 1a | 1650 | 1/1 | 0.95 | 0.07 | 56,56,56,56 | 0 |
| 56 | MG | 1A | 4079 | 1/1 | 0.95 | 0.08 | 53,53,53,53 | 0 |
| 56 | MG | 1A | 3710 | 1/1 | 0.95 | 0.10 | 51,51,51,51 | 0 |
| 56 | MG | 1A | 3348 | 1/1 | 0.95 | 0.14 | 41,41,41,41 | 0 |
| 56 | MG | 1A | 3456 | 1/1 | 0.95 | 0.09 | 49,49,49,49 | 0 |
| 56 | MG | 2A | 3030 | 1/1 | 0.95 | 0.07 | 46,46,46,46 | 0 |
| 56 | MG | 1A | 4087 | 1/1 | 0.95 | 0.10 | 53,53,53,53 | 0 |
| 56 | MG | 1A | 3192 | 1/1 | 0.95 | 0.11 | 25,25,25,25 | 0 |
| 56 | MG | 1A | 3193 | 1/1 | 0.95 | 0.27 | 30,30,30,30 | 0 |
| 56 | MG | 2A | 3616 | 1/1 | 0.95 | 0.07 | 63,63,63,63 | 0 |
| 56 | MG | 2A | 3038 | 1/1 | 0.95 | 0.06 | 48,48,48,48 | 0 |
| 56 | MG | 20 | 102 | 1/1 | 0.95 | 0.06 | 65,65,65,65 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 1A | 3460 | 1/1 | 0.95 | 0.07 | 40,40,40,40 | 0 |
| 56 | MG | 1A | 3718 | 1/1 | 0.95 | 0.06 | 31,31,31,31 | 0 |
| 56 | MG | 2A | 3041 | 1/1 | 0.95 | 0.12 | 70,70,70,70 | 0 |
| 56 | MG | 1A | 3088 | 1/1 | 0.95 | 0.13 | 37,37,37,37 | 0 |
| 56 | MG | 1A | 4095 | 1/1 | 0.95 | 0.06 | 38,38,38,38 | 0 |
| 56 | MG | 1A | 4096 | 1/1 | 0.95 | 0.09 | 46,46,46,46 | 0 |
| 56 | MG | 1A | 4098 | 1/1 | 0.95 | 0.06 | 50,50,50,50 | 0 |
| 56 | MG | 2A | 3627 | 1/1 | 0.95 | 0.06 | 44,44,44,44 | 0 |
| 56 | MG | 1A | 3573 | 1/1 | 0.95 | 0.09 | 34,34,34,34 | 0 |
| 56 | MG | 1A | 3044 | 1/1 | 0.95 | 0.06 | 29,29,29,29 | 0 |
| 56 | MG | 1A | 3198 | 1/1 | 0.95 | 0.12 | 35,35,35,35 | 0 |
| 56 | MG | 1A | 3055 | 1/1 | 0.95 | 0.05 | 23,23,23,23 | 0 |
| 56 | MG | 28 | 103 | 1/1 | 0.95 | 0.08 | 42,42,42,42 | 0 |
| 56 | MG | 2A | 3632 | 1/1 | 0.95 | 0.13 | 39,39,39,39 | 0 |
| 56 | MG | 1A | 3465 | 1/1 | 0.95 | 0.28 | 48,48,48,48 | 0 |
| 56 | MG | 1A | 3277 | 1/1 | 0.95 | 0.18 | 44,44,44,44 | 0 |
| 56 | MG | 1A | 3580 | 1/1 | 0.95 | 0.19 | 29,29,29,29 | 0 |
| 56 | MG | 1A | 3735 | 1/1 | 0.95 | 0.07 | 45,45,45,45 | 0 |
| 56 | MG | 1B | 209 | 1/1 | 0.95 | 0.09 | 47,47,47,47 | 0 |
| 56 | MG | 1A | 3203 | 1/1 | 0.95 | 0.12 | 24,24,24,24 | 0 |
| 56 | MG | 1A | 3907 | 1/1 | 0.95 | 0.05 | 48,48,48,48 | 0 |
| 56 | MG | 2A | 3335 | 1/1 | 0.95 | 0.19 | 47,47,47,47 | 0 |
| 56 | MG | 2A | 3064 | 1/1 | 0.95 | 0.16 | 48,48,48,48 | 0 |
| 56 | MG | 1A | 3582 | 1/1 | 0.95 | 0.10 | 30,30,30,30 | 0 |
| 56 | MG | 1B | 214 | 1/1 | 0.95 | 0.08 | 46,46,46,46 | 0 |
| 56 | MG | 2A | 3646 | 1/1 | 0.95 | 0.07 | 59,59,59,59 | 0 |
| 56 | MG | 1A | 3092 | 1/1 | 0.95 | 0.17 | 45,45,45,45 | 0 |
| 56 | MG | 1B | 219 | 1/1 | 0.95 | 0.14 | 34,34,34,34 | 0 |
| 56 | MG | 2A | 3070 | 1/1 | 0.95 | 0.06 | 56,56,56,56 | 0 |
| 56 | MG | 2a | 3019 | 1/1 | 0.95 | 0.13 | 54,54,54,54 | 0 |
| 56 | MG | 1A | 3093 | 1/1 | 0.95 | 0.14 | 51,51,51,51 | 0 |
| 56 | MG | 1A | 3472 | 1/1 | 0.95 | 0.13 | 33,33,33,33 | 0 |
| 56 | MG | 2A | 3654 | 1/1 | 0.95 | 0.17 | 57,57,57,57 | 0 |
| 56 | MG | 2A | 3073 | 1/1 | 0.95 | 0.14 | 52,52,52,52 | 0 |
| 56 | MG | 1A | 3363 | 1/1 | 0.95 | 0.08 | 51,51,51,51 | 0 |
| 56 | MG | 2A | 3351 | 1/1 | 0.95 | 0.26 | 59,59,59,59 | 0 |
| 56 | MG | 1A | 3591 | 1/1 | 0.95 | 0.17 | 35,35,35,35 | 0 |
| 56 | MG | 1A | 3364 | 1/1 | 0.95 | 0.08 | 37,37,37,37 | 0 |
| 56 | MG | 2a | 3029 | 1/1 | 0.95 | 0.09 | 40,40,40,40 | 0 |
| 56 | MG | 2A | 3354 | 1/1 | 0.95 | 0.09 | 62,62,62,62 | 0 |
| 56 | MG | 1A | 3919 | 1/1 | 0.95 | 0.11 | 30,30,30,30 | 0 |
| 56 | MG | 1B | 227 | 1/1 | 0.95 | 0.07 | 60,60,60,60 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 2a | 3033 | 1/1 | 0.95 | 0.09 | 81,81,81,81 | 0 |
| 56 | MG | 1A | 3475 | 1/1 | 0.95 | 0.10 | 48,48,48,48 | 0 |
| 56 | MG | 2a | 3035 | 1/1 | 0.95 | 0.08 | 76,76,76,76 | 0 |
| 56 | MG | 2A | 3081 | 1/1 | 0.95 | 0.16 | 52,52,52,52 | 0 |
| 56 | MG | 2A | 3360 | 1/1 | 0.95 | 0.06 | 56,56,56,56 | 0 |
| 56 | MG | 2a | 3038 | 1/1 | 0.95 | 0.23 | 53,53,53,53 | 0 |
| 56 | MG | 1A | 3596 | 1/1 | 0.95 | 0.06 | 29,29,29,29 | 0 |
| 56 | MG | 1A | 3597 | 1/1 | 0.95 | 0.07 | 49,49,49,49 | 0 |
| 56 | MG | 1A | 3284 | 1/1 | 0.95 | 0.39 | 35,35,35,35 | 0 |
| 56 | MG | 1A | 3926 | 1/1 | 0.95 | 0.05 | 28,28,28,28 | 0 |
| 56 | MG | 1B | 235 | 1/1 | 0.95 | 0.12 | 47,47,47,47 | 0 |
| 56 | MG | 1A | 3288 | 1/1 | 0.95 | 0.11 | 34,34,34,34 | 0 |
| 56 | MG | 2A | 3090 | 1/1 | 0.95 | 0.09 | 45,45,45,45 | 0 |
| 56 | MG | 2A | 3091 | 1/1 | 0.95 | 0.11 | 48,48,48,48 | 0 |
| 56 | MG | 1A | 3765 | 1/1 | 0.95 | 0.12 | 43,43,43,43 | 0 |
| 56 | MG | 1A | 3140 | 1/1 | 0.95 | 0.14 | 40,40,40,40 | 0 |
| 56 | MG | 1A | 3370 | 1/1 | 0.95 | 0.11 | 40,40,40,40 | 0 |
| 56 | MG | 2A | 3374 | 1/1 | 0.95 | 0.24 | 57,57,57,57 | 0 |
| 56 | MG | 1D | 308 | 1/1 | 0.95 | 0.05 | 36,36,36,36 | 0 |
| 56 | MG | 1a | 1702 | 1/1 | 0.95 | 0.23 | 53,53,53,53 | 0 |
| 56 | MG | 2A | 3691 | 1/1 | 0.95 | 0.10 | 71,71,71,71 | 0 |
| 56 | MG | 1A | 3371 | 1/1 | 0.95 | 0.13 | 46,46,46,46 | 0 |
| 56 | MG | 2a | 3056 | 1/1 | 0.95 | 0.28 | 57,57,57,57 | 0 |
| 56 | MG | 1a | 1704 | 1/1 | 0.95 | 0.27 | 60,60,60,60 | 0 |
| 56 | MG | 2A | 3100 | 1/1 | 0.95 | 0.12 | 53,53,53,53 | 0 |
| 56 | MG | 2A | 3101 | 1/1 | 0.95 | 0.10 | 35,35,35,35 | 0 |
| 56 | MG | 2A | 3103 | 1/1 | 0.95 | 0.16 | 58,58,58,58 | 0 |
| 56 | MG | 2A | 3104 | 1/1 | 0.95 | 0.08 | 51,51,51,51 | 0 |
| 56 | MG | 1a | 1705 | 1/1 | 0.95 | 0.14 | 56,56,56,56 | 0 |
| 56 | MG | 1A | 3608 | 1/1 | 0.95 | 0.07 | 39,39,39,39 | 0 |
| 56 | MG | 2A | 3109 | 1/1 | 0.95 | 0.13 | 39,39,39,39 | 0 |
| 56 | MG | 1A | 3290 | 1/1 | 0.95 | 0.10 | 40,40,40,40 | 0 |
| 56 | MG | 1A | 3610 | 1/1 | 0.95 | 0.09 | 44,44,44,44 | 0 |
| 56 | MG | 1E | 307 | 1/1 | 0.95 | 0.13 | 57,57,57,57 | 0 |
| 56 | MG | 1A | 3377 | 1/1 | 0.95 | 0.07 | 47,47,47,47 | 0 |
| 56 | MG | 1a | 1711 | 1/1 | 0.95 | 0.08 | 39,39,39,39 | 0 |
| 56 | MG | 1A | 3612 | 1/1 | 0.95 | 0.12 | 51,51,51,51 | 0 |
| 56 | MG | 2A | 3398 | 1/1 | 0.95 | 0.18 | 58,58,58,58 | 0 |
| 56 | MG | 1A | 3056 | 1/1 | 0.95 | 0.21 | 45,45,45,45 | 0 |
| 56 | MG | 1A | 3616 | 1/1 | 0.95 | 0.09 | 19,19,19,19 | 0 |
| 56 | MG | 1E | 314 | 1/1 | 0.95 | 0.14 | 30,30,30,30 | 0 |
| 56 | MG | 1A | 3485 | 1/1 | 0.95 | 0.09 | 42,42,42,42 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 1A | 3950 | 1/1 | 0.95 | 0.08 | 55,55,55,55 | 0 |
| 56 | MG | 1a | 1719 | 1/1 | 0.95 | 0.09 | 41,41,41,41 | 0 |
| 56 | MG | 1A | 3058 | 1/1 | 0.95 | 0.06 | 32,32,32,32 | 0 |
| 56 | MG | 1A | 3213 | 1/1 | 0.95 | 0.09 | 44,44,44,44 | 0 |
| 56 | MG | 2A | 3132 | 1/1 | 0.95 | 0.06 | 36,36,36,36 | 0 |
| 56 | MG | 1F | 310 | 1/1 | 0.95 | 0.11 | 41,41,41,41 | 0 |
| 56 | MG | 2A | 3728 | 1/1 | 0.95 | 0.07 | 64,64,64,64 | 0 |
| 56 | MG | 1G | 202 | 1/1 | 0.95 | 0.15 | 51,51,51,51 | 0 |
| 56 | MG | 2A | 3411 | 1/1 | 0.95 | 0.06 | 46,46,46,46 | 0 |
| 56 | MG | 1A | 3956 | 1/1 | 0.95 | 0.13 | 45,45,45,45 | 0 |
| 56 | MG | 2A | 3141 | 1/1 | 0.95 | 0.23 | 39,39,39,39 | 0 |
| 56 | MG | 2a | 3091 | 1/1 | 0.95 | 0.17 | 62,62,62,62 | 0 |
| 56 | MG | 1A | 3488 | 1/1 | 0.95 | 0.07 | 33,33,33,33 | 0 |
| 56 | MG | 2A | 3145 | 1/1 | 0.95 | 0.23 | 66,66,66,66 | 0 |
| 56 | MG | 2A | 3147 | 1/1 | 0.95 | 0.22 | 31,31,31,31 | 0 |
| 56 | MG | 1A | 3959 | 1/1 | 0.95 | 0.09 | 46,46,46,46 | 0 |
| 56 | MG | 1N | 203 | 1/1 | 0.95 | 0.06 | 46,46,46,46 | 0 |
| 56 | MG | 1A | 3787 | 1/1 | 0.95 | 0.06 | 44,44,44,44 | 0 |
| 56 | MG | 1A | 3489 | 1/1 | 0.95 | 0.25 | 48,48,48,48 | 0 |
| 56 | MG | 1A | 3060 | 1/1 | 0.95 | 0.09 | 39,39,39,39 | 0 |
| 56 | MG | 1A | 3300 | 1/1 | 0.95 | 0.08 | 44,44,44,44 | 0 |
| 56 | MG | 1A | 3965 | 1/1 | 0.95 | 0.06 | 49,49,49,49 | 0 |
| 56 | MG | 2a | 3103 | 1/1 | 0.95 | 0.16 | 62,62,62,62 | 0 |
| 56 | MG | 1A | 3387 | 1/1 | 0.95 | 0.12 | 48,48,48,48 | 0 |
| 56 | MG | 2A | 3157 | 1/1 | 0.95 | 0.34 | 44,44,44,44 | 0 |
| 56 | MG | 2A | 3747 | 1/1 | 0.95 | 0.11 | 66,66,66,66 | 0 |
| 56 | MG | 1A | 3027 | 1/1 | 0.95 | 0.14 | 71,71,71,71 | 0 |
| 56 | MG | 1A | 3005 | 1/1 | 0.95 | 0.08 | 37,37,37,37 | 0 |
| 56 | MG | 1a | 1741 | 1/1 | 0.95 | 0.25 | 60,60,60,60 | 0 |
| 56 | MG | 1A | 3157 | 1/1 | 0.95 | 0.10 | 40,40,40,40 | 0 |
| 56 | MG | 2A | 3752 | 1/1 | 0.95 | 0.10 | 54,54,54,54 | 0 |
| 56 | MG | 1A | 3228 | 1/1 | 0.95 | 0.10 | 32,32,32,32 | 0 |
| 56 | MG | 1A | 3063 | 1/1 | 0.95 | 0.11 | 43,43,43,43 | 0 |
| 56 | MG | 1A | 3395 | 1/1 | 0.95 | 0.13 | 40,40,40,40 | 0 |
| 56 | MG | 1A | 3803 | 1/1 | 0.95 | 0.05 | 26,26,26,26 | 0 |
| 56 | MG | 1A | 3038 | 1/1 | 0.95 | 0.13 | 30,30,30,30 | 0 |
| 56 | MG | 1A | 3235 | 1/1 | 0.95 | 0.07 | 59,59,59,59 | 0 |
| 56 | MG | 2A | 3168 | 1/1 | 0.95 | 0.08 | 53,53,53,53 | 0 |
| 56 | MG | 1A | 3508 | 1/1 | 0.95 | 0.16 | 23,23,23,23 | 0 |
| 56 | MG | 1A | 3983 | 1/1 | 0.95 | 0.06 | 64,64,64,64 | 0 |
| 56 | MG | 1T | 202 | 1/1 | 0.95 | 0.10 | 45,45,45,45 | 0 |
| 56 | MG | 1T | 203 | 1/1 | 0.95 | 0.07 | 53,53,53,53 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 1A | 3811 | 1/1 | 0.95 | 0.10 | 49,49,49,49 | 0 |
| 56 | MG | 1A | 3313 | 1/1 | 0.95 | 0.09 | 39,39,39,39 | 0 |
| 56 | MG | 2a | 3125 | 1/1 | 0.95 | 0.10 | 64,64,64,64 | 0 |
| 56 | MG | 1U | 202 | 1/1 | 0.95 | 0.11 | 27,27,27,27 | 0 |
| 56 | MG | 2A | 3451 | 1/1 | 0.95 | 0.21 | 37,37,37,37 | 0 |
| 56 | MG | 1U | 206 | 1/1 | 0.95 | 0.07 | 33,33,33,33 | 0 |
| 56 | MG | 1A | 3652 | 1/1 | 0.95 | 0.09 | 31,31,31,31 | 0 |
| 56 | MG | 1U | 212 | 1/1 | 0.95 | 0.10 | 37,37,37,37 | 0 |
| 56 | MG | 1A | 3987 | 1/1 | 0.95 | 0.08 | 50,50,50,50 | 0 |
| 56 | MG | 2A | 3456 | 1/1 | 0.95 | 0.14 | 61,61,61,61 | 0 |
| 56 | MG | 2A | 3183 | 1/1 | 0.95 | 0.12 | 52,52,52,52 | 0 |
| 56 | MG | 2A | 3780 | 1/1 | 0.95 | 0.07 | 69,69,69,69 | 0 |
| 56 | MG | 2A | 3184 | 1/1 | 0.95 | 0.09 | 41,41,41,41 | 0 |
| 56 | MG | 2a | 3142 | 1/1 | 0.95 | 0.06 | 68,68,68,68 | 0 |
| 56 | MG | 1A | 3110 | 1/1 | 0.95 | 0.13 | 26,26,26,26 | 0 |
| 56 | MG | 1A | 3315 | 1/1 | 0.95 | 0.08 | 51,51,51,51 | 0 |
| 56 | MG | 1W | 201 | 1/1 | 0.95 | 0.18 | 49,49,49,49 | 0 |
| 56 | MG | 2a | 3148 | 1/1 | 0.95 | 0.07 | 63,63,63,63 | 0 |
| 56 | MG | 1A | 3655 | 1/1 | 0.95 | 0.07 | 58,58,58,58 | 0 |
| 56 | MG | 1X | 103 | 1/1 | 0.95 | 0.13 | 37,37,37,37 | 0 |
| 56 | MG | 2A | 3464 | 1/1 | 0.95 | 0.23 | 63,63,63,63 | 0 |
| 56 | MG | 1A | 3239 | 1/1 | 0.95 | 0.14 | 25,25,25,25 | 0 |
| 56 | MG | 1A | 3821 | 1/1 | 0.95 | 0.06 | 26,26,26,26 | 0 |
| 56 | MG | 2a | 3157 | 1/1 | 0.95 | 0.08 | 57,57,57,57 | 0 |
| 56 | MG | 1A | 3069 | 1/1 | 0.95 | 0.11 | 28,28,28,28 | 0 |
| 56 | MG | 2A | 3797 | 1/1 | 0.95 | 0.05 | 40,40,40,40 | 0 |
| 56 | MG | 1A | 3166 | 1/1 | 0.95 | 0.16 | 34,34,34,34 | 0 |
| 56 | MG | 1A | 3321 | 1/1 | 0.95 | 0.17 | 48,48,48,48 | 0 |
| 56 | MG | 1A | 3520 | 1/1 | 0.95 | 0.11 | 56,56,56,56 | 0 |
| 56 | MG | 1A | 3829 | 1/1 | 0.95 | 0.11 | 32,32,32,32 | 0 |
| 56 | MG | 10 | 103 | 1/1 | 0.95 | 0.07 | 32,32,32,32 | 0 |
| 56 | MG | 1A | 3831 | 1/1 | 0.95 | 0.08 | 37,37,37,37 | 0 |
| 56 | MG | 10 | 105 | 1/1 | 0.95 | 0.09 | 53,53,53,53 | 0 |
| 56 | MG | 1A | 3322 | 1/1 | 0.95 | 0.05 | 43,43,43,43 | 0 |
| 56 | MG | 2A | 3208 | 1/1 | 0.95 | 0.08 | 53,53,53,53 | 0 |
| 56 | MG | 1A | 3833 | 1/1 | 0.95 | 0.07 | 55,55,55,55 | 0 |
| 56 | MG | 2A | 3481 | 1/1 | 0.95 | 0.22 | 60,60,60,60 | 0 |
| 56 | MG | 2A | 3482 | 1/1 | 0.95 | 0.22 | 42,42,42,42 | 0 |
| 56 | MG | 1A | 3168 | 1/1 | 0.95 | 0.24 | 40,40,40,40 | 0 |
| 56 | MG | 1A | 3415 | 1/1 | 0.95 | 0.07 | 40,40,40,40 | 0 |
| 56 | MG | 1A | 3670 | 1/1 | 0.95 | 0.09 | 28,28,28,28 | 0 |
| 56 | MG | 1A | 3671 | 1/1 | 0.95 | 0.06 | 29,29,29,29 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 1a | 1806 | 1/1 | 0.95 | 0.09 | 59,59,59,59 | 0 |
| 56 | MG | 2A | 3488 | 1/1 | 0.95 | 0.08 | 56,56,56,56 | 0 |
| 56 | MG | 1A | 3246 | 1/1 | 0.95 | 0.16 | 50,50,50,50 | 0 |
| 56 | MG | 2A | 3218 | 1/1 | 0.95 | 0.23 | 35,35,35,35 | 0 |
| 56 | MG | 1A | 3326 | 1/1 | 0.95 | 0.06 | 48,48,48,48 | 0 |
| 56 | MG | 1A | 3841 | 1/1 | 0.95 | 0.09 | 39,39,39,39 | 0 |
| 56 | MG | 1a | 1817 | 1/1 | 0.95 | 0.07 | 58,58,58,58 | 0 |
| 56 | MG | 2A | 3224 | 1/1 | 0.95 | 0.13 | 49,49,49,49 | 0 |
| 56 | MG | 1A | 4014 | 1/1 | 0.95 | 0.06 | 46,46,46,46 | 0 |
| 56 | MG | 1a | 1819 | 1/1 | 0.95 | 0.09 | 68,68,68,68 | 0 |
| 56 | MG | 15 | 104 | 1/1 | 0.95 | 0.08 | 42,42,42,42 | 0 |
| 56 | MG | 2A | 3500 | 1/1 | 0.95 | 0.07 | 55,55,55,55 | 0 |
| 56 | MG | 1A | 3327 | 1/1 | 0.95 | 0.19 | 36,36,36,36 | 0 |
| 56 | MG | 2A | 3835 | 1/1 | 0.95 | 0.08 | 34,34,34,34 | 0 |
| 56 | MG | 1A | 3174 | 1/1 | 0.95 | 0.20 | 27,27,27,27 | 0 |
| 56 | MG | 16 | 103 | 1/1 | 0.95 | 0.07 | 51,51,51,51 | 0 |
| 56 | MG | 1A | 3679 | 1/1 | 0.95 | 0.07 | 34,34,34,34 | 0 |
| 56 | MG | 2A | 3506 | 1/1 | 0.95 | 0.08 | 36,36,36,36 | 0 |
| 56 | MG | 2a | 3207 | 1/1 | 0.95 | 0.09 | 62,62,62,62 | 0 |
| 56 | MG | 2A | 3842 | 1/1 | 0.95 | 0.07 | 42,42,42,42 | 0 |
| 56 | MG | 17 | 107 | 1/1 | 0.95 | 0.16 | 49,49,49,49 | 0 |
| 56 | MG | 2a | 3213 | 1/1 | 0.95 | 0.13 | 75,75,75,75 | 0 |
| 56 | MG | 2a | 3214 | 1/1 | 0.95 | 0.16 | 74,74,74,74 | 0 |
| 56 | MG | 2A | 3846 | 1/1 | 0.95 | 0.09 | 62,62,62,62 | 0 |
| 56 | MG | 1A | 3248 | 1/1 | 0.95 | 0.19 | 51,51,51,51 | 0 |
| 56 | MG | 2A | 3850 | 1/1 | 0.95 | 0.11 | 55,55,55,55 | 0 |
| 56 | MG | 2A | 3851 | 1/1 | 0.95 | 0.10 | 39,39,39,39 | 0 |
| 56 | MG | 2A | 3238 | 1/1 | 0.95 | 0.11 | 45,45,45,45 | 0 |
| 56 | MG | 18 | 102 | 1/1 | 0.95 | 0.19 | 41,41,41,41 | 0 |
| 56 | MG | 1A | 3681 | 1/1 | 0.95 | 0.10 | 47,47,47,47 | 0 |
| 56 | MG | 2a | 3222 | 1/1 | 0.95 | 0.19 | 55,55,55,55 | 0 |
| 56 | MG | 1A | 4021 | 1/1 | 0.95 | 0.06 | 32,32,32,32 | 0 |
| 56 | MG | 1A | 3249 | 1/1 | 0.95 | 0.19 | 42,42,42,42 | 0 |
| 56 | MG | 1A | 4024 | 1/1 | 0.95 | 0.11 | 70,70,70,70 | 0 |
| 56 | MG | 2A | 3244 | 1/1 | 0.95 | 0.10 | 43,43,43,43 | 0 |
| 56 | MG | 2A | 3519 | 1/1 | 0.95 | 0.09 | 33,33,33,33 | 0 |
| 56 | MG | 1f | 201 | 1/1 | 0.95 | 0.15 | 44,44,44,44 | 0 |
| 56 | MG | 2A | 3872 | 1/1 | 0.95 | 0.10 | 48,48,48,48 | 0 |
| 56 | MG | 2A | 3246 | 1/1 | 0.95 | 0.11 | 49,49,49,49 | 0 |
| 56 | MG | 19 | 101 | 1/1 | 0.95 | 0.06 | 34,34,34,34 | 0 |
| 56 | MG | 1h | 201 | 1/1 | 0.95 | 0.07 | 58,58,58,58 | 0 |
| 56 | MG | 2A | 3528 | 1/1 | 0.95 | 0.08 | 59,59,59,59 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 2A | 3249 | 1/1 | 0.95 | 0.08 | 55,55,55,55 | 0 |
| 56 | MG | 2A | 3879 | 1/1 | 0.95 | 0.16 | 47,47,47,47 | 0 |
| 56 | MG | 1m | 3002 | 1/1 | 0.95 | 0.09 | 56,56,56,56 | 0 |
| 56 | MG | 1n | 101 | 1/1 | 0.95 | 0.09 | 54,54,54,54 | 0 |
| 56 | MG | 1a | 1601 | 1/1 | 0.95 | 0.08 | 42,42,42,42 | 0 |
| 56 | MG | 2A | 3535 | 1/1 | 0.95 | 0.11 | 51,51,51,51 | 0 |
| 56 | MG | 1A | 3850 | 1/1 | 0.95 | 0.16 | 47,47,47,47 | 0 |
| 56 | MG | 1A | 3250 | 1/1 | 0.95 | 0.11 | 36,36,36,36 | 0 |
| 56 | MG | 1A | 3112 | 1/1 | 0.95 | 0.16 | 35,35,35,35 | 0 |
| 56 | MG | 1A | 3114 | 1/1 | 0.95 | 0.08 | 32,32,32,32 | 0 |
| 56 | MG | 1A | 3001 | 1/1 | 0.95 | 0.17 | 39,39,39,39 | 0 |
| 56 | MG | 2A | 3258 | 1/1 | 0.95 | 0.06 | 67,67,67,67 | 0 |
| 56 | MG | 1A | 4038 | 1/1 | 0.95 | 0.07 | 52,52,52,52 | 0 |
| 56 | MG | 1A | 3337 | 1/1 | 0.95 | 0.18 | 37,37,37,37 | 0 |
| 56 | MG | 1A | 3255 | 1/1 | 0.95 | 0.07 | 29,29,29,29 | 0 |
| 56 | MG | 2l | 201 | 1/1 | 0.95 | 0.09 | 55,55,55,55 | 0 |
| 56 | MG | 2l | 202 | 1/1 | 0.95 | 0.07 | 64,64,64,64 | 0 |
| 56 | MG | 2A | 3263 | 1/1 | 0.95 | 0.39 | 71,71,71,71 | 0 |
| 56 | MG | 1a | 1612 | 1/1 | 0.95 | 0.08 | 62,62,62,62 | 0 |
| 56 | MG | 1A | 3859 | 1/1 | 0.95 | 0.24 | 38,38,38,38 | 0 |
| 56 | MG | 2A | 3266 | 1/1 | 0.95 | 0.10 | 59,59,59,59 | 0 |
| 56 | MG | 1A | 3860 | 1/1 | 0.95 | 0.17 | 36,36,36,36 | 0 |
| 56 | MG | 1A | 3082 | 1/1 | 0.95 | 0.16 | 33,33,33,33 | 0 |
| 56 | MG | 2A | 3559 | 1/1 | 0.95 | 0.10 | 53,53,53,53 | 0 |
| 56 | MG | 1A | 3863 | 1/1 | 0.95 | 0.07 | 34,34,34,34 | 0 |
| 56 | MG | 2A | 3270 | 1/1 | 0.95 | 0.19 | 57,57,57,57 | 0 |
| 56 | MG | 1A | 3120 | 1/1 | 0.95 | 0.09 | 36,36,36,36 | 0 |
| 56 | MG | 1a | 1620 | 1/1 | 0.95 | 0.19 | 55,55,55,55 | 0 |
| 56 | MG | 1A | 3439 | 1/1 | 0.95 | 0.09 | 44,44,44,44 | 0 |
| 56 | MG | 1A | 3698 | 1/1 | 0.95 | 0.13 | 28,28,28,28 | 0 |
| 56 | MG | 1A | 4055 | 1/1 | 0.95 | 0.07 | 41,41,41,41 | 0 |
| 56 | MG | 2A | 3277 | 1/1 | 0.95 | 0.06 | 58,58,58,58 | 0 |
| 56 | MG | 2D | 303 | 1/1 | 0.95 | 0.18 | 42,42,42,42 | 0 |
| 56 | MG | 1A | 3040 | 1/1 | 0.95 | 0.05 | 30,30,30,30 | 0 |
| 56 | MG | 2y | 101 | 1/1 | 0.95 | 0.26 | 60,60,60,60 | 0 |
| 56 | MG | 1A | 3443 | 1/1 | 0.95 | 0.10 | 49,49,49,49 | 0 |
| 56 | MG | 1A | 3259 | 1/1 | 0.95 | 0.06 | 38,38,38,38 | 0 |
| 56 | MG | 1A | 3260 | 1/1 | 0.95 | 0.09 | 47,47,47,47 | 0 |
| 56 | MG | 1A | 3553 | 1/1 | 0.95 | 0.22 | 45,45,45,45 | 0 |
| 57 | CLM | 1A | 4102 | 20/20 | 0.95 | 0.09 | 18,29,44,60 | 0 |
| 57 | CLM | 2A | 3888 | 20/20 | 0.95 | 0.10 | 38,45,57,61 | 0 |
| 56 | MG | 1A | 3872 | 1/1 | 0.95 | 0.15 | 33,33,33,33 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 59 | ZN | 2n | 501 | 1/1 | 0.95 | 0.07 | 107,107,107,107 | 0 |
| 56 | MG | 1A | 3569 | 1/1 | 0.96 | 0.11 | 42,42,42,42 | 0 |
| 56 | MG | 1A | 3571 | 1/1 | 0.96 | 0.27 | 29,29,29,29 | 0 |
| 56 | MG | 1A | 3842 | 1/1 | 0.96 | 0.08 | 31,31,31,31 | 0 |
| 56 | MG | 1A | 3389 | 1/1 | 0.96 | 0.14 | 23,23,23,23 | 0 |
| 56 | MG | 1A | 3138 | 1/1 | 0.96 | 0.15 | 28,28,28,28 | 0 |
| 56 | MG | 1A | 3476 | 1/1 | 0.96 | 0.05 | 40,40,40,40 | 0 |
| 56 | MG | 1A | 3080 | 1/1 | 0.96 | 0.14 | 47,47,47,47 | 0 |
| 56 | MG | 1A | 3196 | 1/1 | 0.96 | 0.07 | 38,38,38,38 | 0 |
| 56 | MG | 1P | 208 | 1/1 | 0.96 | 0.17 | 42,42,42,42 | 0 |
| 56 | MG | 1A | 3393 | 1/1 | 0.96 | 0.07 | 43,43,43,43 | 0 |
| 56 | MG | 1Q | 201 | 1/1 | 0.96 | 0.29 | 42,42,42,42 | 0 |
| 56 | MG | 2A | 3082 | 1/1 | 0.96 | 0.06 | 43,43,43,43 | 0 |
| 56 | MG | 2A | 3336 | 1/1 | 0.96 | 0.14 | 62,62,62,62 | 0 |
| 56 | MG | 1A | 4003 | 1/1 | 0.96 | 0.08 | 42,42,42,42 | 0 |
| 56 | MG | 2A | 3084 | 1/1 | 0.96 | 0.06 | 46,46,46,46 | 0 |
| 56 | MG | 1a | 1713 | 1/1 | 0.96 | 0.07 | 50,50,50,50 | 0 |
| 56 | MG | 2A | 3340 | 1/1 | 0.96 | 0.09 | 53,53,53,53 | 0 |
| 56 | MG | 1A | 3849 | 1/1 | 0.96 | 0.07 | 52,52,52,52 | 0 |
| 56 | MG | 2A | 3625 | 1/1 | 0.96 | 0.12 | 57,57,57,57 | 0 |
| 56 | MG | 2A | 3626 | 1/1 | 0.96 | 0.10 | 33,33,33,33 | 0 |
| 56 | MG | 2A | 3342 | 1/1 | 0.96 | 0.17 | 55,55,55,55 | 0 |
| 56 | MG | 1Q | 206 | 1/1 | 0.96 | 0.06 | 51,51,51,51 | 0 |
| 56 | MG | 2A | 3344 | 1/1 | 0.96 | 0.12 | 48,48,48,48 | 0 |
| 56 | MG | 2A | 3345 | 1/1 | 0.96 | 0.07 | 39,39,39,39 | 0 |
| 56 | MG | 1A | 3197 | 1/1 | 0.96 | 0.22 | 38,38,38,38 | 0 |
| 56 | MG | 1R | 201 | 1/1 | 0.96 | 0.15 | 32,32,32,32 | 0 |
| 56 | MG | 1A | 3579 | 1/1 | 0.96 | 0.10 | 21,21,21,21 | 0 |
| 56 | MG | 1A | 3325 | 1/1 | 0.96 | 0.22 | 26,26,26,26 | 0 |
| 56 | MG | 2A | 3635 | 1/1 | 0.96 | 0.07 | 61,61,61,61 | 0 |
| 56 | MG | 1A | 3105 | 1/1 | 0.96 | 0.18 | 30,30,30,30 | 0 |
| 56 | MG | 1A | 3029 | 1/1 | 0.96 | 0.09 | 23,23,23,23 | 0 |
| 56 | MG | 25 | 102 | 1/1 | 0.96 | 0.27 | 50,50,50,50 | 0 |
| 56 | MG | 1A | 3856 | 1/1 | 0.96 | 0.05 | 16,16,16,16 | 0 |
| 56 | MG | 1A | 3583 | 1/1 | 0.96 | 0.07 | 44,44,44,44 | 0 |
| 56 | MG | 1a | 1725 | 1/1 | 0.96 | 0.12 | 42,42,42,42 | 0 |
| 56 | MG | 1A | 3108 | 1/1 | 0.96 | 0.13 | 36,36,36,36 | 0 |
| 56 | MG | 1A | 3149 | 1/1 | 0.96 | 0.15 | 29,29,29,29 | 0 |
| 56 | MG | 1A | 3109 | 1/1 | 0.96 | 0.27 | 31,31,31,31 | 0 |
| 56 | MG | 1A | 3588 | 1/1 | 0.96 | 0.33 | 36,36,36,36 | 0 |
| 56 | MG | 2A | 3102 | 1/1 | 0.96 | 0.10 | 59,59,59,59 | 0 |
| 56 | MG | 1U | 205 | 1/1 | 0.96 | 0.40 | 38,38,38,38 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 1A | 3059 | 1/1 | 0.96 | 0.16 | 47,47,47,47 | 0 |
| 56 | MG | 2A | 3105 | 1/1 | 0.96 | 0.10 | 57,57,57,57 | 0 |
| 56 | MG | 2a | 3004 | 1/1 | 0.96 | 0.24 | 51,51,51,51 | 0 |
| 56 | MG | 1A | 3715 | 1/1 | 0.96 | 0.09 | 48,48,48,48 | 0 |
| 56 | MG | 2A | 3366 | 1/1 | 0.96 | 0.19 | 60,60,60,60 | 0 |
| 56 | MG | 1A | 3590 | 1/1 | 0.96 | 0.10 | 26,26,26,26 | 0 |
| 56 | MG | 2A | 3655 | 1/1 | 0.96 | 0.15 | 56,56,56,56 | 0 |
| 56 | MG | 1A | 4023 | 1/1 | 0.96 | 0.05 | 30,30,30,30 | 0 |
| 56 | MG | 1A | 3030 | 1/1 | 0.96 | 0.25 | 32,32,32,32 | 0 |
| 56 | MG | 2A | 3111 | 1/1 | 0.96 | 0.11 | 59,59,59,59 | 0 |
| 56 | MG | 2A | 3660 | 1/1 | 0.96 | 0.06 | 33,33,33,33 | 0 |
| 56 | MG | 1A | 4027 | 1/1 | 0.96 | 0.18 | 65,65,65,65 | 0 |
| 56 | MG | 1a | 1738 | 1/1 | 0.96 | 0.07 | 57,57,57,57 | 0 |
| 56 | MG | 1A | 3720 | 1/1 | 0.96 | 0.15 | 44,44,44,44 | 0 |
| 56 | MG | 1a | 1740 | 1/1 | 0.96 | 0.15 | 43,43,43,43 | 0 |
| 56 | MG | 2A | 3667 | 1/1 | 0.96 | 0.13 | 57,57,57,57 | 0 |
| 56 | MG | 2A | 3375 | 1/1 | 0.96 | 0.09 | 64,64,64,64 | 0 |
| 56 | MG | 1W | 202 | 1/1 | 0.96 | 0.15 | 50,50,50,50 | 0 |
| 56 | MG | 1A | 3210 | 1/1 | 0.96 | 0.08 | 35,35,35,35 | 0 |
| 56 | MG | 2A | 3672 | 1/1 | 0.96 | 0.06 | 51,51,51,51 | 0 |
| 56 | MG | 1W | 205 | 1/1 | 0.96 | 0.05 | 39,39,39,39 | 0 |
| 56 | MG | 1A | 3405 | 1/1 | 0.96 | 0.07 | 52,52,52,52 | 0 |
| 56 | MG | 1A | 3334 | 1/1 | 0.96 | 0.18 | 43,43,43,43 | 0 |
| 56 | MG | 1a | 1749 | 1/1 | 0.96 | 0.10 | 33,33,33,33 | 0 |
| 56 | MG | 2A | 3677 | 1/1 | 0.96 | 0.05 | 51,51,51,51 | 0 |
| 56 | MG | 1a | 1750 | 1/1 | 0.96 | 0.05 | 39,39,39,39 | 0 |
| 56 | MG | 1A | 4035 | 1/1 | 0.96 | 0.06 | 64,64,64,64 | 0 |
| 56 | MG | 2A | 3126 | 1/1 | 0.96 | 0.11 | 44,44,44,44 | 0 |
| 56 | MG | 2A | 3385 | 1/1 | 0.96 | 0.17 | 53,53,53,53 | 0 |
| 56 | MG | 2A | 3129 | 1/1 | 0.96 | 0.09 | 54,54,54,54 | 0 |
| 56 | MG | 2A | 3388 | 1/1 | 0.96 | 0.09 | 62,62,62,62 | 0 |
| 56 | MG | 2A | 3130 | 1/1 | 0.96 | 0.09 | 54,54,54,54 | 0 |
| 56 | MG | 1A | 4036 | 1/1 | 0.96 | 0.09 | 41,41,41,41 | 0 |
| 56 | MG | 1Y | 203 | 1/1 | 0.96 | 0.13 | 47,47,47,47 | 0 |
| 56 | MG | 2A | 3134 | 1/1 | 0.96 | 0.05 | 39,39,39,39 | 0 |
| 56 | MG | 2A | 3689 | 1/1 | 0.96 | 0.06 | 59,59,59,59 | 0 |
| 56 | MG | 1A | 3211 | 1/1 | 0.96 | 0.18 | 34,34,34,34 | 0 |
| 56 | MG | 2A | 3136 | 1/1 | 0.96 | 0.10 | 38,38,38,38 | 0 |
| 56 | MG | 1A | 3598 | 1/1 | 0.96 | 0.11 | 35,35,35,35 | 0 |
| 56 | MG | 1a | 1756 | 1/1 | 0.96 | 0.11 | 54,54,54,54 | 0 |
| 56 | MG | 1A | 3412 | 1/1 | 0.96 | 0.07 | 38,38,38,38 | 0 |
| 56 | MG | 2A | 3143 | 1/1 | 0.96 | 0.12 | 47,47,47,47 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 1A | 4040 | 1/1 | 0.96 | 0.12 | 47,47,47,47 | 0 |
| 56 | MG | 1a | 1761 | 1/1 | 0.96 | 0.10 | 51,51,51,51 | 0 |
| 56 | MG | 2A | 3146 | 1/1 | 0.96 | 0.17 | 38,38,38,38 | 0 |
| 56 | MG | 1A | 3732 | 1/1 | 0.96 | 0.08 | 61,61,61,61 | 0 |
| 56 | MG | 1A | 3495 | 1/1 | 0.96 | 0.18 | 47,47,47,47 | 0 |
| 56 | MG | 1a | 1764 | 1/1 | 0.96 | 0.07 | 58,58,58,58 | 0 |
| 56 | MG | 2A | 3407 | 1/1 | 0.96 | 0.09 | 57,57,57,57 | 0 |
| 56 | MG | 1A | 3878 | 1/1 | 0.96 | 0.22 | 30,30,30,30 | 0 |
| 56 | MG | 10 | 106 | 1/1 | 0.96 | 0.06 | 49,49,49,49 | 0 |
| 56 | MG | 2a | 3055 | 1/1 | 0.96 | 0.07 | 60,60,60,60 | 0 |
| 56 | MG | 11 | 101 | 1/1 | 0.96 | 0.21 | 33,33,33,33 | 0 |
| 56 | MG | 1A | 3879 | 1/1 | 0.96 | 0.10 | 36,36,36,36 | 0 |
| 56 | MG | 1a | 1771 | 1/1 | 0.96 | 0.07 | 40,40,40,40 | 0 |
| 56 | MG | 2A | 3413 | 1/1 | 0.96 | 0.11 | 55,55,55,55 | 0 |
| 56 | MG | 1A | 3413 | 1/1 | 0.96 | 0.06 | 37,37,37,37 | 0 |
| 56 | MG | 2a | 3061 | 1/1 | 0.96 | 0.04 | 53,53,53,53 | 0 |
| 56 | MG | 1A | 3158 | 1/1 | 0.96 | 0.12 | 60,60,60,60 | 0 |
| 56 | MG | 1A | 3606 | 1/1 | 0.96 | 0.05 | 36,36,36,36 | 0 |
| 56 | MG | 1A | 3738 | 1/1 | 0.96 | 0.09 | 45,45,45,45 | 0 |
| 56 | MG | 2A | 3719 | 1/1 | 0.96 | 0.06 | 60,60,60,60 | 0 |
| 56 | MG | 1A | 3273 | 1/1 | 0.96 | 0.26 | 35,35,35,35 | 0 |
| 56 | MG | 13 | 101 | 1/1 | 0.96 | 0.09 | 26,26,26,26 | 0 |
| 56 | MG | 13 | 102 | 1/1 | 0.96 | 0.07 | 38,38,38,38 | 0 |
| 56 | MG | 1A | 3500 | 1/1 | 0.96 | 0.17 | 37,37,37,37 | 0 |
| 56 | MG | 1A | 3502 | 1/1 | 0.96 | 0.07 | 47,47,47,47 | 0 |
| 56 | MG | 2A | 3727 | 1/1 | 0.96 | 0.16 | 61,61,61,61 | 0 |
| 56 | MG | 15 | 101 | 1/1 | 0.96 | 0.18 | 31,31,31,31 | 0 |
| 56 | MG | 1A | 3743 | 1/1 | 0.96 | 0.07 | 22,22,22,22 | 0 |
| 56 | MG | 1A | 3744 | 1/1 | 0.96 | 0.07 | 50,50,50,50 | 0 |
| 56 | MG | 1A | 3745 | 1/1 | 0.96 | 0.05 | 14,14,14,14 | 0 |
| 56 | MG | 1A | 3043 | 1/1 | 0.96 | 0.13 | 33,33,33,33 | 0 |
| 56 | MG | 1A | 4062 | 1/1 | 0.96 | 0.06 | 32,32,32,32 | 0 |
| 56 | MG | 1a | 1791 | 1/1 | 0.96 | 0.06 | 64,64,64,64 | 0 |
| 56 | MG | 1A | 3113 | 1/1 | 0.96 | 0.10 | 37,37,37,37 | 0 |
| 56 | MG | 1a | 1794 | 1/1 | 0.96 | 0.07 | 60,60,60,60 | 0 |
| 56 | MG | 2A | 3436 | 1/1 | 0.96 | 0.06 | 41,41,41,41 | 0 |
| 56 | MG | 2A | 3174 | 1/1 | 0.96 | 0.25 | 56,56,56,56 | 0 |
| 56 | MG | 2A | 3740 | 1/1 | 0.96 | 0.05 | 67,67,67,67 | 0 |
| 56 | MG | 17 | 101 | 1/1 | 0.96 | 0.09 | 31,31,31,31 | 0 |
| 56 | MG | 17 | 102 | 1/1 | 0.96 | 0.07 | 32,32,32,32 | 0 |
| 56 | MG | 1A | 4066 | 1/1 | 0.96 | 0.05 | 24,24,24,24 | 0 |
| 56 | MG | 17 | 105 | 1/1 | 0.96 | 0.12 | 37,37,37,37 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 2A | 3180 | 1/1 | 0.96 | 0.19 | 47,47,47,47 | 0 |
| 56 | MG | 1A | 3024 | 1/1 | 0.96 | 0.08 | 43,43,43,43 | 0 |
| 56 | MG | 1A | 3749 | 1/1 | 0.96 | 0.05 | 30,30,30,30 | 0 |
| 56 | MG | 2A | 3445 | 1/1 | 0.96 | 0.32 | 60,60,60,60 | 0 |
| 56 | MG | 1A | 4069 | 1/1 | 0.96 | 0.05 | 20,20,20,20 | 0 |
| 56 | MG | 1A | 4070 | 1/1 | 0.96 | 0.05 | 52,52,52,52 | 0 |
| 56 | MG | 1a | 1808 | 1/1 | 0.96 | 0.06 | 50,50,50,50 | 0 |
| 56 | MG | 1A | 3750 | 1/1 | 0.96 | 0.07 | 34,34,34,34 | 0 |
| 56 | MG | 2a | 3099 | 1/1 | 0.96 | 0.09 | 52,52,52,52 | 0 |
| 56 | MG | 1a | 1810 | 1/1 | 0.96 | 0.06 | 59,59,59,59 | 0 |
| 56 | MG | 1A | 4072 | 1/1 | 0.96 | 0.07 | 48,48,48,48 | 0 |
| 56 | MG | 1a | 1815 | 1/1 | 0.96 | 0.11 | 66,66,66,66 | 0 |
| 56 | MG | 2A | 3193 | 1/1 | 0.96 | 0.31 | 63,63,63,63 | 0 |
| 56 | MG | 1A | 3751 | 1/1 | 0.96 | 0.10 | 42,42,42,42 | 0 |
| 56 | MG | 2A | 3195 | 1/1 | 0.96 | 0.05 | 44,44,44,44 | 0 |
| 56 | MG | 2A | 3760 | 1/1 | 0.96 | 0.13 | 54,54,54,54 | 0 |
| 56 | MG | 1A | 3219 | 1/1 | 0.96 | 0.11 | 32,32,32,32 | 0 |
| 56 | MG | 1A | 3507 | 1/1 | 0.96 | 0.15 | 42,42,42,42 | 0 |
| 56 | MG | 1a | 1821 | 1/1 | 0.96 | 0.05 | 53,53,53,53 | 0 |
| 56 | MG | 1A | 3903 | 1/1 | 0.96 | 0.10 | 45,45,45,45 | 0 |
| 56 | MG | 1A | 3617 | 1/1 | 0.96 | 0.05 | 36,36,36,36 | 0 |
| 56 | MG | 1A | 3619 | 1/1 | 0.96 | 0.11 | 41,41,41,41 | 0 |
| 56 | MG | 1A | 3620 | 1/1 | 0.96 | 0.08 | 52,52,52,52 | 0 |
| 56 | MG | 1A | 3343 | 1/1 | 0.96 | 0.14 | 47,47,47,47 | 0 |
| 56 | MG | 2A | 3769 | 1/1 | 0.96 | 0.10 | 39,39,39,39 | 0 |
| 56 | MG | 1A | 3423 | 1/1 | 0.96 | 0.14 | 42,42,42,42 | 0 |
| 56 | MG | 2A | 3465 | 1/1 | 0.96 | 0.13 | 48,48,48,48 | 0 |
| 56 | MG | 1a | 1608 | 1/1 | 0.96 | 0.17 | 45,45,45,45 | 0 |
| 56 | MG | 1A | 4085 | 1/1 | 0.96 | 0.08 | 17,17,17,17 | 0 |
| 56 | MG | 1a | 1610 | 1/1 | 0.96 | 0.06 | 23,23,23,23 | 0 |
| 56 | MG | 1A | 3511 | 1/1 | 0.96 | 0.06 | 36,36,36,36 | 0 |
| 56 | MG | 1A | 3282 | 1/1 | 0.96 | 0.26 | 38,38,38,38 | 0 |
| 56 | MG | 2A | 3471 | 1/1 | 0.96 | 0.06 | 32,32,32,32 | 0 |
| 56 | MG | 1A | 3912 | 1/1 | 0.96 | 0.16 | 31,31,31,31 | 0 |
| 56 | MG | 2A | 3783 | 1/1 | 0.96 | 0.08 | 58,58,58,58 | 0 |
| 56 | MG | 1a | 1614 | 1/1 | 0.96 | 0.11 | 58,58,58,58 | 0 |
| 56 | MG | 1a | 1615 | 1/1 | 0.96 | 0.06 | 43,43,43,43 | 0 |
| 56 | MG | 2A | 3787 | 1/1 | 0.96 | 0.06 | 72,72,72,72 | 0 |
| 56 | MG | 2a | 3131 | 1/1 | 0.96 | 0.35 | 60,60,60,60 | 0 |
| 56 | MG | 1A | 3003 | 1/1 | 0.96 | 0.04 | 19,19,19,19 | 0 |
| 56 | MG | 1m | 3001 | 1/1 | 0.96 | 0.09 | 54,54,54,54 | 0 |
| 56 | MG | 2A | 3790 | 1/1 | 0.96 | 0.07 | 61,61,61,61 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 1A | 3426 | 1/1 | 0.96 | 0.14 | 44,44,44,44 | 0 |
| 56 | MG | 1A | 3427 | 1/1 | 0.96 | 0.10 | 43,43,43,43 | 0 |
| 56 | MG | 2a | 3137 | 1/1 | 0.96 | 0.11 | 75,75,75,75 | 0 |
| 56 | MG | 1A | 4094 | 1/1 | 0.96 | 0.12 | 47,47,47,47 | 0 |
| 56 | MG | 2a | 3139 | 1/1 | 0.96 | 0.07 | 70,70,70,70 | 0 |
| 56 | MG | 2A | 3223 | 1/1 | 0.96 | 0.15 | 45,45,45,45 | 0 |
| 56 | MG | 1A | 3516 | 1/1 | 0.96 | 0.11 | 40,40,40,40 | 0 |
| 56 | MG | 2a | 3143 | 1/1 | 0.96 | 0.06 | 75,75,75,75 | 0 |
| 56 | MG | 1A | 3636 | 1/1 | 0.96 | 0.06 | 16,16,16,16 | 0 |
| 56 | MG | 1A | 3638 | 1/1 | 0.96 | 0.07 | 40,40,40,40 | 0 |
| 56 | MG | 1A | 3223 | 1/1 | 0.96 | 0.16 | 46,46,46,46 | 0 |
| 56 | MG | 2A | 3800 | 1/1 | 0.96 | 0.05 | 78,78,78,78 | 0 |
| 56 | MG | 2a | 3149 | 1/1 | 0.96 | 0.06 | 76,76,76,76 | 0 |
| 56 | MG | 1A | 3429 | 1/1 | 0.96 | 0.05 | 44,44,44,44 | 0 |
| 56 | MG | 1A | 4101 | 1/1 | 0.96 | 0.07 | 53,53,53,53 | 0 |
| 56 | MG | 1A | 3777 | 1/1 | 0.96 | 0.06 | 46,46,46,46 | 0 |
| 56 | MG | 1a | 1628 | 1/1 | 0.96 | 0.15 | 47,47,47,47 | 0 |
| 56 | MG | 1A | 3925 | 1/1 | 0.96 | 0.07 | 39,39,39,39 | 0 |
| 56 | MG | 1A | 3778 | 1/1 | 0.96 | 0.10 | 20,20,20,20 | 0 |
| 56 | MG | 2A | 3807 | 1/1 | 0.96 | 0.07 | 65,65,65,65 | 0 |
| 56 | MG | 1B | 204 | 1/1 | 0.96 | 0.18 | 42,42,42,42 | 0 |
| 56 | MG | 1B | 205 | 1/1 | 0.96 | 0.05 | 47,47,47,47 | 0 |
| 56 | MG | 1A | 3286 | 1/1 | 0.96 | 0.15 | 42,42,42,42 | 0 |
| 56 | MG | 1x | 102 | 1/1 | 0.96 | 0.16 | 46,46,46,46 | 0 |
| 56 | MG | 1x | 103 | 1/1 | 0.96 | 0.16 | 48,48,48,48 | 0 |
| 56 | MG | 2a | 3169 | 1/1 | 0.96 | 0.09 | 77,77,77,77 | 0 |
| 56 | MG | 2A | 3814 | 1/1 | 0.96 | 0.10 | 60,60,60,60 | 0 |
| 56 | MG | 1A | 3022 | 1/1 | 0.96 | 0.08 | 34,34,34,34 | 0 |
| 56 | MG | 1x | 105 | 1/1 | 0.96 | 0.04 | 49,49,49,49 | 0 |
| 56 | MG | 1a | 1636 | 1/1 | 0.96 | 0.10 | 49,49,49,49 | 0 |
| 56 | MG | 1A | 3434 | 1/1 | 0.96 | 0.13 | 40,40,40,40 | 0 |
| 56 | MG | 1A | 3227 | 1/1 | 0.96 | 0.13 | 37,37,37,37 | 0 |
| 56 | MG | 2A | 3820 | 1/1 | 0.96 | 0.08 | 73,73,73,73 | 0 |
| 56 | MG | 2A | 3504 | 1/1 | 0.96 | 0.16 | 49,49,49,49 | 0 |
| 56 | MG | 1B | 210 | 1/1 | 0.96 | 0.23 | 51,51,51,51 | 0 |
| 56 | MG | 1A | 3786 | 1/1 | 0.96 | 0.06 | 24,24,24,24 | 0 |
| 56 | MG | 1A | 3167 | 1/1 | 0.96 | 0.07 | 38,38,38,38 | 0 |
| 56 | MG | 1A | 3352 | 1/1 | 0.96 | 0.35 | 41,41,41,41 | 0 |
| 56 | MG | 1a | 1645 | 1/1 | 0.96 | 0.17 | 52,52,52,52 | 0 |
| 56 | MG | 1A | 3790 | 1/1 | 0.96 | 0.08 | 19,19,19,19 | 0 |
| 56 | MG | 1A | 3648 | 1/1 | 0.96 | 0.07 | 30,30,30,30 | 0 |
| 56 | MG | 1B | 218 | 1/1 | 0.96 | 0.08 | 39,39,39,39 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 2a | 3189 | 1/1 | 0.96 | 0.15 | 57,57,57,57 | 0 |
| 56 | MG | 1A | 3230 | 1/1 | 0.96 | 0.07 | 36,36,36,36 | 0 |
| 56 | MG | 2a | 3191 | 1/1 | 0.96 | 0.18 | 71,71,71,71 | 0 |
| 56 | MG | 1a | 1652 | 1/1 | 0.96 | 0.07 | 48,48,48,48 | 0 |
| 56 | MG | 1A | 3943 | 1/1 | 0.96 | 0.05 | 38,38,38,38 | 0 |
| 56 | MG | 1A | 3066 | 1/1 | 0.96 | 0.06 | 29,29,29,29 | 0 |
| 56 | MG | 2a | 3195 | 1/1 | 0.96 | 0.17 | 52,52,52,52 | 0 |
| 56 | MG | 2A | 3521 | 1/1 | 0.96 | 0.08 | 38,38,38,38 | 0 |
| 56 | MG | 2A | 3522 | 1/1 | 0.96 | 0.06 | 41,41,41,41 | 0 |
| 56 | MG | 2A | 3523 | 1/1 | 0.96 | 0.09 | 42,42,42,42 | 0 |
| 56 | MG | 1A | 3293 | 1/1 | 0.96 | 0.19 | 42,42,42,42 | 0 |
| 56 | MG | 1A | 3169 | 1/1 | 0.96 | 0.14 | 49,49,49,49 | 0 |
| 56 | MG | 1A | 3170 | 1/1 | 0.96 | 0.07 | 47,47,47,47 | 0 |
| 56 | MG | 1A | 3799 | 1/1 | 0.96 | 0.05 | 38,38,38,38 | 0 |
| 56 | MG | 2A | 3849 | 1/1 | 0.96 | 0.07 | 63,63,63,63 | 0 |
| 56 | MG | 1A | 3236 | 1/1 | 0.96 | 0.20 | 30,30,30,30 | 0 |
| 56 | MG | 2A | 3013 | 1/1 | 0.96 | 0.11 | 50,50,50,50 | 0 |
| 56 | MG | 2A | 3852 | 1/1 | 0.96 | 0.06 | 53,53,53,53 | 0 |
| 56 | MG | 1A | 3657 | 1/1 | 0.96 | 0.05 | 44,44,44,44 | 0 |
| 56 | MG | 1A | 3659 | 1/1 | 0.96 | 0.08 | 24,24,24,24 | 0 |
| 56 | MG | 1a | 1663 | 1/1 | 0.96 | 0.10 | 52,52,52,52 | 0 |
| 56 | MG | 1B | 231 | 1/1 | 0.96 | 0.08 | 39,39,39,39 | 0 |
| 56 | MG | 1A | 3237 | 1/1 | 0.96 | 0.14 | 30,30,30,30 | 0 |
| 56 | MG | 2A | 3861 | 1/1 | 0.96 | 0.06 | 62,62,62,62 | 0 |
| 56 | MG | 1A | 3960 | 1/1 | 0.96 | 0.11 | 50,50,50,50 | 0 |
| 56 | MG | 2A | 3866 | 1/1 | 0.96 | 0.13 | 38,38,38,38 | 0 |
| 56 | MG | 2A | 3273 | 1/1 | 0.96 | 0.10 | 49,49,49,49 | 0 |
| 56 | MG | 1A | 3172 | 1/1 | 0.96 | 0.05 | 36,36,36,36 | 0 |
| 56 | MG | 2A | 3023 | 1/1 | 0.96 | 0.22 | 51,51,51,51 | 0 |
| 56 | MG | 2A | 3870 | 1/1 | 0.96 | 0.10 | 42,42,42,42 | 0 |
| 56 | MG | 2A | 3871 | 1/1 | 0.96 | 0.07 | 39,39,39,39 | 0 |
| 56 | MG | 1A | 3067 | 1/1 | 0.96 | 0.04 | 32,32,32,32 | 0 |
| 56 | MG | 2A | 3544 | 1/1 | 0.96 | 0.07 | 35,35,35,35 | 0 |
| 56 | MG | 2A | 3545 | 1/1 | 0.96 | 0.12 | 35,35,35,35 | 0 |
| 56 | MG | 1A | 3049 | 1/1 | 0.96 | 0.20 | 39,39,39,39 | 0 |
| 56 | MG | 1A | 3451 | 1/1 | 0.96 | 0.17 | 42,42,42,42 | 0 |
| 56 | MG | 1A | 3543 | 1/1 | 0.96 | 0.20 | 34,34,34,34 | 0 |
| 56 | MG | 2A | 3028 | 1/1 | 0.96 | 0.24 | 48,48,48,48 | 0 |
| 56 | MG | 1D | 301 | 1/1 | 0.96 | 0.06 | 34,34,34,34 | 0 |
| 56 | MG | 1A | 3308 | 1/1 | 0.96 | 0.14 | 32,32,32,32 | 0 |
| 56 | MG | 2A | 3554 | 1/1 | 0.96 | 0.07 | 49,49,49,49 | 0 |
| 56 | MG | 2A | 3032 | 1/1 | 0.96 | 0.08 | 47,47,47,47 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 1A | 3097 | 1/1 | 0.96 | 0.14 | 35,35,35,35 | 0 |
| 56 | MG | 1A | 3368 | 1/1 | 0.96 | 0.06 | 37,37,37,37 | 0 |
| 56 | MG | 2A | 3036 | 1/1 | 0.96 | 0.05 | 28,28,28,28 | 0 |
| 56 | MG | 2A | 3560 | 1/1 | 0.96 | 0.10 | 38,38,38,38 | 0 |
| 56 | MG | 1D | 311 | 1/1 | 0.96 | 0.06 | 50,50,50,50 | 0 |
| 56 | MG | 1A | 3970 | 1/1 | 0.96 | 0.07 | 20,20,20,20 | 0 |
| 56 | MG | 1A | 3369 | 1/1 | 0.96 | 0.10 | 44,44,44,44 | 0 |
| 56 | MG | 1E | 302 | 1/1 | 0.96 | 0.16 | 47,47,47,47 | 0 |
| 56 | MG | 1A | 3818 | 1/1 | 0.96 | 0.07 | 42,42,42,42 | 0 |
| 56 | MG | 1a | 1681 | 1/1 | 0.96 | 0.08 | 56,56,56,56 | 0 |
| 56 | MG | 2A | 3044 | 1/1 | 0.96 | 0.12 | 59,59,59,59 | 0 |
| 56 | MG | 2A | 3296 | 1/1 | 0.96 | 0.10 | 50,50,50,50 | 0 |
| 56 | MG | 1a | 1682 | 1/1 | 0.96 | 0.20 | 40,40,40,40 | 0 |
| 56 | MG | 1A | 3673 | 1/1 | 0.96 | 0.09 | 17,17,17,17 | 0 |
| 56 | MG | 1A | 3129 | 1/1 | 0.96 | 0.17 | 47,47,47,47 | 0 |
| 56 | MG | 1A | 3978 | 1/1 | 0.96 | 0.09 | 36,36,36,36 | 0 |
| 56 | MG | 1A | 3550 | 1/1 | 0.96 | 0.18 | 40,40,40,40 | 0 |
| 56 | MG | 1A | 3311 | 1/1 | 0.96 | 0.15 | 40,40,40,40 | 0 |
| 56 | MG | 1A | 3552 | 1/1 | 0.96 | 0.14 | 27,27,27,27 | 0 |
| 56 | MG | 1A | 3072 | 1/1 | 0.96 | 0.22 | 31,31,31,31 | 0 |
| 56 | MG | 2A | 3579 | 1/1 | 0.96 | 0.07 | 45,45,45,45 | 0 |
| 56 | MG | 1A | 3375 | 1/1 | 0.96 | 0.14 | 42,42,42,42 | 0 |
| 56 | MG | 2A | 3055 | 1/1 | 0.96 | 0.21 | 53,53,53,53 | 0 |
| 56 | MG | 2D | 301 | 1/1 | 0.96 | 0.10 | 47,47,47,47 | 0 |
| 56 | MG | 2A | 3056 | 1/1 | 0.96 | 0.21 | 59,59,59,59 | 0 |
| 56 | MG | 2A | 3057 | 1/1 | 0.96 | 0.15 | 46,46,46,46 | 0 |
| 56 | MG | 1A | 3185 | 1/1 | 0.96 | 0.06 | 37,37,37,37 | 0 |
| 56 | MG | 1A | 3057 | 1/1 | 0.96 | 0.06 | 28,28,28,28 | 0 |
| 56 | MG | 1A | 3078 | 1/1 | 0.96 | 0.08 | 31,31,31,31 | 0 |
| 56 | MG | 2A | 3593 | 1/1 | 0.96 | 0.09 | 46,46,46,46 | 0 |
| 56 | MG | 2A | 3061 | 1/1 | 0.96 | 0.08 | 63,63,63,63 | 0 |
| 56 | MG | 1A | 3316 | 1/1 | 0.96 | 0.06 | 40,40,40,40 | 0 |
| 56 | MG | 1A | 3134 | 1/1 | 0.96 | 0.07 | 41,41,41,41 | 0 |
| 56 | MG | 1A | 3102 | 1/1 | 0.96 | 0.07 | 46,46,46,46 | 0 |
| 56 | MG | 1I | 201 | 1/1 | 0.96 | 0.07 | 61,61,61,61 | 0 |
| 56 | MG | 2F | 301 | 1/1 | 0.96 | 0.08 | 46,46,46,46 | 0 |
| 56 | MG | 1A | 3319 | 1/1 | 0.96 | 0.16 | 51,51,51,51 | 0 |
| 56 | MG | 2A | 3067 | 1/1 | 0.96 | 0.09 | 30,30,30,30 | 0 |
| 56 | MG | 1N | 202 | 1/1 | 0.96 | 0.07 | 42,42,42,42 | 0 |
| 56 | MG | 2F | 305 | 1/1 | 0.96 | 0.08 | 43,43,43,43 | 0 |
| 56 | MG | 1A | 3137 | 1/1 | 0.96 | 0.09 | 27,27,27,27 | 0 |
| 56 | MG | 2A | 3322 | 1/1 | 0.96 | 0.14 | 48,48,48,48 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 1A | 3242 | 1/1 | 0.97 | 0.15 | 22,22,22,22 | 0 |
| 56 | MG | 1A | 3025 | 1/1 | 0.97 | 0.06 | 30,30,30,30 | 0 |
| 56 | MG | 2a | 3016 | 1/1 | 0.97 | 0.06 | 52,52,52,52 | 0 |
| 56 | MG | 1A | 3244 | 1/1 | 0.97 | 0.10 | 42,42,42,42 | 0 |
| 56 | MG | 1A | 3077 | 1/1 | 0.97 | 0.11 | 35,35,35,35 | 0 |
| 56 | MG | 17 | 106 | 1/1 | 0.97 | 0.13 | 25,25,25,25 | 0 |
| 56 | MG | 1A | 3492 | 1/1 | 0.97 | 0.05 | 33,33,33,33 | 0 |
| 56 | MG | 17 | 108 | 1/1 | 0.97 | 0.06 | 45,45,45,45 | 0 |
| 56 | MG | 1A | 3820 | 1/1 | 0.97 | 0.04 | 18,18,18,18 | 0 |
| 56 | MG | 1A | 3421 | 1/1 | 0.97 | 0.14 | 32,32,32,32 | 0 |
| 56 | MG | 2A | 3494 | 1/1 | 0.97 | 0.06 | 67,67,67,67 | 0 |
| 56 | MG | 2A | 3080 | 1/1 | 0.97 | 0.15 | 56,56,56,56 | 0 |
| 56 | MG | 1A | 3299 | 1/1 | 0.97 | 0.05 | 30,30,30,30 | 0 |
| 56 | MG | 2A | 3288 | 1/1 | 0.97 | 0.08 | 36,36,36,36 | 0 |
| 56 | MG | 1A | 3692 | 1/1 | 0.97 | 0.08 | 55,55,55,55 | 0 |
| 56 | MG | 2A | 3290 | 1/1 | 0.97 | 0.08 | 36,36,36,36 | 0 |
| 56 | MG | 1A | 3824 | 1/1 | 0.97 | 0.05 | 30,30,30,30 | 0 |
| 56 | MG | 1A | 3094 | 1/1 | 0.97 | 0.07 | 20,20,20,20 | 0 |
| 56 | MG | 1A | 3695 | 1/1 | 0.97 | 0.03 | 25,25,25,25 | 0 |
| 56 | MG | 1A | 3828 | 1/1 | 0.97 | 0.10 | 45,45,45,45 | 0 |
| 56 | MG | 1a | 1770 | 1/1 | 0.97 | 0.05 | 49,49,49,49 | 0 |
| 56 | MG | 1A | 3301 | 1/1 | 0.97 | 0.05 | 24,24,24,24 | 0 |
| 56 | MG | 1B | 220 | 1/1 | 0.97 | 0.05 | 32,32,32,32 | 0 |
| 56 | MG | 1a | 1773 | 1/1 | 0.97 | 0.09 | 54,54,54,54 | 0 |
| 56 | MG | 1A | 3135 | 1/1 | 0.97 | 0.09 | 23,23,23,23 | 0 |
| 56 | MG | 1A | 3206 | 1/1 | 0.97 | 0.10 | 42,42,42,42 | 0 |
| 56 | MG | 1A | 3045 | 1/1 | 0.97 | 0.04 | 28,28,28,28 | 0 |
| 56 | MG | 1A | 3037 | 1/1 | 0.97 | 0.09 | 32,32,32,32 | 0 |
| 56 | MG | 1a | 1778 | 1/1 | 0.97 | 0.09 | 55,55,55,55 | 0 |
| 56 | MG | 1A | 3362 | 1/1 | 0.97 | 0.06 | 35,35,35,35 | 0 |
| 56 | MG | 1A | 3430 | 1/1 | 0.97 | 0.06 | 47,47,47,47 | 0 |
| 56 | MG | 1a | 1781 | 1/1 | 0.97 | 0.10 | 75,75,75,75 | 0 |
| 56 | MG | 2A | 3520 | 1/1 | 0.97 | 0.09 | 49,49,49,49 | 0 |
| 56 | MG | 1A | 3013 | 1/1 | 0.97 | 0.12 | 26,26,26,26 | 0 |
| 56 | MG | 1a | 1783 | 1/1 | 0.97 | 0.10 | 57,57,57,57 | 0 |
| 56 | MG | 1B | 228 | 1/1 | 0.97 | 0.05 | 42,42,42,42 | 0 |
| 56 | MG | 1A | 3432 | 1/1 | 0.97 | 0.19 | 36,36,36,36 | 0 |
| 56 | MG | 1A | 3593 | 1/1 | 0.97 | 0.25 | 27,27,27,27 | 0 |
| 56 | MG | 1A | 3252 | 1/1 | 0.97 | 0.12 | 37,37,37,37 | 0 |
| 56 | MG | 1A | 3595 | 1/1 | 0.97 | 0.07 | 34,34,34,34 | 0 |
| 56 | MG | 1A | 3171 | 1/1 | 0.97 | 0.08 | 44,44,44,44 | 0 |
| 56 | MG | 1A | 3509 | 1/1 | 0.97 | 0.12 | 31,31,31,31 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 2A | 3530 | 1/1 | 0.97 | 0.10 | 49,49,49,49 | 0 |
| 56 | MG | 2A | 3774 | 1/1 | 0.97 | 0.09 | 64,64,64,64 | 0 |
| 56 | MG | 1A | 3006 | 1/1 | 0.97 | 0.14 | 47,47,47,47 | 0 |
| 56 | MG | 1A | 3599 | 1/1 | 0.97 | 0.12 | 42,42,42,42 | 0 |
| 56 | MG | 2A | 3778 | 1/1 | 0.97 | 0.10 | 58,58,58,58 | 0 |
| 56 | MG | 1A | 3173 | 1/1 | 0.97 | 0.17 | 34,34,34,34 | 0 |
| 56 | MG | 1A | 3017 | 1/1 | 0.97 | 0.18 | 50,50,50,50 | 0 |
| 56 | MG | 1A | 3179 | 1/1 | 0.97 | 0.05 | 29,29,29,29 | 0 |
| 56 | MG | 2A | 3537 | 1/1 | 0.97 | 0.06 | 56,56,56,56 | 0 |
| 56 | MG | 1D | 302 | 1/1 | 0.97 | 0.08 | 36,36,36,36 | 0 |
| 56 | MG | 2A | 3539 | 1/1 | 0.97 | 0.06 | 48,48,48,48 | 0 |
| 56 | MG | 1a | 1624 | 1/1 | 0.97 | 0.13 | 62,62,62,62 | 0 |
| 56 | MG | 1D | 303 | 1/1 | 0.97 | 0.08 | 17,17,17,17 | 0 |
| 56 | MG | 1a | 1801 | 1/1 | 0.97 | 0.07 | 64,64,64,64 | 0 |
| 56 | MG | 1a | 1802 | 1/1 | 0.97 | 0.09 | 63,63,63,63 | 0 |
| 56 | MG | 1D | 304 | 1/1 | 0.97 | 0.05 | 35,35,35,35 | 0 |
| 56 | MG | 2a | 3073 | 1/1 | 0.97 | 0.11 | 50,50,50,50 | 0 |
| 56 | MG | 2A | 3328 | 1/1 | 0.97 | 0.07 | 41,41,41,41 | 0 |
| 56 | MG | 1D | 305 | 1/1 | 0.97 | 0.16 | 29,29,29,29 | 0 |
| 56 | MG | 1A | 3603 | 1/1 | 0.97 | 0.09 | 39,39,39,39 | 0 |
| 56 | MG | 2A | 3548 | 1/1 | 0.97 | 0.13 | 35,35,35,35 | 0 |
| 56 | MG | 1A | 3994 | 1/1 | 0.97 | 0.05 | 70,70,70,70 | 0 |
| 56 | MG | 2a | 3079 | 1/1 | 0.97 | 0.15 | 56,56,56,56 | 0 |
| 56 | MG | 2A | 3125 | 1/1 | 0.97 | 0.05 | 58,58,58,58 | 0 |
| 56 | MG | 1D | 309 | 1/1 | 0.97 | 0.17 | 20,20,20,20 | 0 |
| 56 | MG | 2A | 3127 | 1/1 | 0.97 | 0.16 | 65,65,65,65 | 0 |
| 56 | MG | 2A | 3553 | 1/1 | 0.97 | 0.11 | 49,49,49,49 | 0 |
| 56 | MG | 2A | 3128 | 1/1 | 0.97 | 0.04 | 42,42,42,42 | 0 |
| 56 | MG | 1a | 1631 | 1/1 | 0.97 | 0.05 | 33,33,33,33 | 0 |
| 56 | MG | 1A | 3851 | 1/1 | 0.97 | 0.06 | 11,11,11,11 | 0 |
| 56 | MG | 2a | 3087 | 1/1 | 0.97 | 0.13 | 59,59,59,59 | 0 |
| 56 | MG | 1a | 1813 | 1/1 | 0.97 | 0.06 | 53,53,53,53 | 0 |
| 56 | MG | 2A | 3558 | 1/1 | 0.97 | 0.08 | 52,52,52,52 | 0 |
| 56 | MG | 1A | 3604 | 1/1 | 0.97 | 0.08 | 27,27,27,27 | 0 |
| 56 | MG | 2A | 3133 | 1/1 | 0.97 | 0.07 | 55,55,55,55 | 0 |
| 56 | MG | 2A | 3561 | 1/1 | 0.97 | 0.07 | 36,36,36,36 | 0 |
| 56 | MG | 1a | 1816 | 1/1 | 0.97 | 0.09 | 53,53,53,53 | 0 |
| 56 | MG | 1A | 3215 | 1/1 | 0.97 | 0.08 | 39,39,39,39 | 0 |
| 56 | MG | 1A | 3146 | 1/1 | 0.97 | 0.18 | 25,25,25,25 | 0 |
| 56 | MG | 2A | 3813 | 1/1 | 0.97 | 0.07 | 53,53,53,53 | 0 |
| 56 | MG | 1E | 301 | 1/1 | 0.97 | 0.28 | 28,28,28,28 | 0 |
| 56 | MG | 1A | 3723 | 1/1 | 0.97 | 0.07 | 40,40,40,40 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 1a | 1822 | 1/1 | 0.97 | 0.06 | 69,69,69,69 | 0 |
| 56 | MG | 2A | 3142 | 1/1 | 0.97 | 0.10 | 43,43,43,43 | 0 |
| 56 | MG | 1a | 1824 | 1/1 | 0.97 | 0.05 | 60,60,60,60 | 0 |
| 56 | MG | 1A | 3441 | 1/1 | 0.97 | 0.07 | 41,41,41,41 | 0 |
| 56 | MG | 1E | 305 | 1/1 | 0.97 | 0.08 | 32,32,32,32 | 0 |
| 56 | MG | 1a | 1828 | 1/1 | 0.97 | 0.17 | 42,42,42,42 | 0 |
| 56 | MG | 2A | 3822 | 1/1 | 0.97 | 0.06 | 61,61,61,61 | 0 |
| 56 | MG | 1E | 306 | 1/1 | 0.97 | 0.13 | 26,26,26,26 | 0 |
| 56 | MG | 1A | 3442 | 1/1 | 0.97 | 0.08 | 36,36,36,36 | 0 |
| 56 | MG | 1A | 3218 | 1/1 | 0.97 | 0.13 | 34,34,34,34 | 0 |
| 56 | MG | 2A | 3355 | 1/1 | 0.97 | 0.07 | 51,51,51,51 | 0 |
| 56 | MG | 2A | 3577 | 1/1 | 0.97 | 0.15 | 57,57,57,57 | 0 |
| 56 | MG | 1A | 4004 | 1/1 | 0.97 | 0.05 | 51,51,51,51 | 0 |
| 56 | MG | 1A | 3181 | 1/1 | 0.97 | 0.08 | 39,39,39,39 | 0 |
| 56 | MG | 1E | 312 | 1/1 | 0.97 | 0.12 | 39,39,39,39 | 0 |
| 56 | MG | 1a | 1649 | 1/1 | 0.97 | 0.14 | 44,44,44,44 | 0 |
| 56 | MG | 1A | 3521 | 1/1 | 0.97 | 0.05 | 47,47,47,47 | 0 |
| 56 | MG | 1A | 3445 | 1/1 | 0.97 | 0.10 | 36,36,36,36 | 0 |
| 56 | MG | 2A | 3362 | 1/1 | 0.97 | 0.10 | 43,43,43,43 | 0 |
| 56 | MG | 1E | 315 | 1/1 | 0.97 | 0.05 | 40,40,40,40 | 0 |
| 56 | MG | 1a | 1653 | 1/1 | 0.97 | 0.14 | 56,56,56,56 | 0 |
| 56 | MG | 2A | 3840 | 1/1 | 0.97 | 0.05 | 51,51,51,51 | 0 |
| 56 | MG | 1F | 302 | 1/1 | 0.97 | 0.08 | 30,30,30,30 | 0 |
| 56 | MG | 1A | 3376 | 1/1 | 0.97 | 0.10 | 44,44,44,44 | 0 |
| 56 | MG | 1l | 201 | 1/1 | 0.97 | 0.08 | 56,56,56,56 | 0 |
| 56 | MG | 1l | 202 | 1/1 | 0.97 | 0.09 | 41,41,41,41 | 0 |
| 56 | MG | 2A | 3847 | 1/1 | 0.97 | 0.06 | 47,47,47,47 | 0 |
| 56 | MG | 1A | 3614 | 1/1 | 0.97 | 0.12 | 35,35,35,35 | 0 |
| 56 | MG | 1F | 306 | 1/1 | 0.97 | 0.10 | 23,23,23,23 | 0 |
| 56 | MG | 2a | 3128 | 1/1 | 0.97 | 0.12 | 44,44,44,44 | 0 |
| 56 | MG | 1A | 3220 | 1/1 | 0.97 | 0.12 | 49,49,49,49 | 0 |
| 56 | MG | 1A | 3736 | 1/1 | 0.97 | 0.06 | 38,38,38,38 | 0 |
| 56 | MG | 1A | 3525 | 1/1 | 0.97 | 0.13 | 31,31,31,31 | 0 |
| 56 | MG | 1G | 201 | 1/1 | 0.97 | 0.10 | 43,43,43,43 | 0 |
| 56 | MG | 1A | 3087 | 1/1 | 0.97 | 0.14 | 35,35,35,35 | 0 |
| 56 | MG | 2A | 3857 | 1/1 | 0.97 | 0.06 | 66,66,66,66 | 0 |
| 56 | MG | 1A | 3527 | 1/1 | 0.97 | 0.13 | 32,32,32,32 | 0 |
| 56 | MG | 2A | 3607 | 1/1 | 0.97 | 0.08 | 57,57,57,57 | 0 |
| 56 | MG | 1A | 3264 | 1/1 | 0.97 | 0.05 | 36,36,36,36 | 0 |
| 56 | MG | 1A | 3622 | 1/1 | 0.97 | 0.05 | 22,22,22,22 | 0 |
| 56 | MG | 2A | 3862 | 1/1 | 0.97 | 0.05 | 57,57,57,57 | 0 |
| 56 | MG | 2A | 3863 | 1/1 | 0.97 | 0.06 | 28,28,28,28 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 1A | 3529 | 1/1 | 0.97 | 0.19 | 28,28,28,28 | 0 |
| 56 | MG | 2A | 3865 | 1/1 | 0.97 | 0.04 | 51,51,51,51 | 0 |
| 56 | MG | 1A | 3119 | 1/1 | 0.97 | 0.10 | 23,23,23,23 | 0 |
| 56 | MG | 1A | 3874 | 1/1 | 0.97 | 0.14 | 27,27,27,27 | 0 |
| 56 | MG | 1w | 108 | 1/1 | 0.97 | 0.06 | 74,74,74,74 | 0 |
| 56 | MG | 1A | 3625 | 1/1 | 0.97 | 0.11 | 53,53,53,53 | 0 |
| 56 | MG | 1A | 3266 | 1/1 | 0.97 | 0.15 | 40,40,40,40 | 0 |
| 56 | MG | 1N | 206 | 1/1 | 0.97 | 0.08 | 37,37,37,37 | 0 |
| 56 | MG | 2a | 3152 | 1/1 | 0.97 | 0.06 | 70,70,70,70 | 0 |
| 56 | MG | 2A | 3386 | 1/1 | 0.97 | 0.39 | 55,55,55,55 | 0 |
| 56 | MG | 1A | 4025 | 1/1 | 0.97 | 0.09 | 40,40,40,40 | 0 |
| 56 | MG | 1O | 204 | 1/1 | 0.97 | 0.08 | 46,46,46,46 | 0 |
| 56 | MG | 2a | 3156 | 1/1 | 0.97 | 0.06 | 72,72,72,72 | 0 |
| 56 | MG | 2A | 3389 | 1/1 | 0.97 | 0.15 | 36,36,36,36 | 0 |
| 56 | MG | 1A | 3452 | 1/1 | 0.97 | 0.08 | 38,38,38,38 | 0 |
| 56 | MG | 2A | 3877 | 1/1 | 0.97 | 0.07 | 49,49,49,49 | 0 |
| 56 | MG | 1P | 201 | 1/1 | 0.97 | 0.14 | 25,25,25,25 | 0 |
| 56 | MG | 1A | 3629 | 1/1 | 0.97 | 0.04 | 29,29,29,29 | 0 |
| 56 | MG | 2A | 3393 | 1/1 | 0.97 | 0.17 | 40,40,40,40 | 0 |
| 56 | MG | 1x | 106 | 1/1 | 0.97 | 0.17 | 52,52,52,52 | 0 |
| 56 | MG | 1A | 3630 | 1/1 | 0.97 | 0.06 | 29,29,29,29 | 0 |
| 56 | MG | 1A | 3631 | 1/1 | 0.97 | 0.04 | 14,14,14,14 | 0 |
| 56 | MG | 2a | 3171 | 1/1 | 0.97 | 0.09 | 64,64,64,64 | 0 |
| 56 | MG | 1A | 3453 | 1/1 | 0.97 | 0.20 | 31,31,31,31 | 0 |
| 56 | MG | 2A | 3192 | 1/1 | 0.97 | 0.12 | 60,60,60,60 | 0 |
| 56 | MG | 1A | 4034 | 1/1 | 0.97 | 0.09 | 61,61,61,61 | 0 |
| 56 | MG | 1A | 3753 | 1/1 | 0.97 | 0.06 | 34,34,34,34 | 0 |
| 56 | MG | 1A | 3755 | 1/1 | 0.97 | 0.05 | 46,46,46,46 | 0 |
| 56 | MG | 1Q | 202 | 1/1 | 0.97 | 0.19 | 34,34,34,34 | 0 |
| 56 | MG | 2A | 3197 | 1/1 | 0.97 | 0.15 | 55,55,55,55 | 0 |
| 56 | MG | 1A | 3267 | 1/1 | 0.97 | 0.14 | 40,40,40,40 | 0 |
| 56 | MG | 1x | 116 | 1/1 | 0.97 | 0.12 | 65,65,65,65 | 0 |
| 56 | MG | 1A | 3455 | 1/1 | 0.97 | 0.11 | 28,28,28,28 | 0 |
| 56 | MG | 1A | 3758 | 1/1 | 0.97 | 0.06 | 40,40,40,40 | 0 |
| 56 | MG | 1A | 3384 | 1/1 | 0.97 | 0.08 | 41,41,41,41 | 0 |
| 56 | MG | 2a | 3184 | 1/1 | 0.97 | 0.15 | 57,57,57,57 | 0 |
| 56 | MG | 1A | 3637 | 1/1 | 0.97 | 0.09 | 48,48,48,48 | 0 |
| 56 | MG | 1R | 202 | 1/1 | 0.97 | 0.21 | 36,36,36,36 | 0 |
| 56 | MG | 1A | 3385 | 1/1 | 0.97 | 0.05 | 27,27,27,27 | 0 |
| 56 | MG | 1A | 4046 | 1/1 | 0.97 | 0.06 | 44,44,44,44 | 0 |
| 56 | MG | 1A | 3068 | 1/1 | 0.97 | 0.09 | 48,48,48,48 | 0 |
| 56 | MG | 2A | 3209 | 1/1 | 0.97 | 0.13 | 43,43,43,43 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 2A | 3647 | 1/1 | 0.97 | 0.32 | 64,64,64,64 | 0 |
| 56 | MG | 1A | 3269 | 1/1 | 0.97 | 0.05 | 29,29,29,29 | 0 |
| 56 | MG | 2A | 3211 | 1/1 | 0.97 | 0.07 | 45,45,45,45 | 0 |
| 56 | MG | 1A | 3540 | 1/1 | 0.97 | 0.06 | 45,45,45,45 | 0 |
| 56 | MG | 2A | 3010 | 1/1 | 0.97 | 0.16 | 46,46,46,46 | 0 |
| 56 | MG | 1A | 3225 | 1/1 | 0.97 | 0.06 | 39,39,39,39 | 0 |
| 56 | MG | 1A | 3542 | 1/1 | 0.97 | 0.11 | 37,37,37,37 | 0 |
| 56 | MG | 1A | 3226 | 1/1 | 0.97 | 0.11 | 43,43,43,43 | 0 |
| 56 | MG | 1A | 3645 | 1/1 | 0.97 | 0.10 | 20,20,20,20 | 0 |
| 56 | MG | 2A | 3423 | 1/1 | 0.97 | 0.13 | 35,35,35,35 | 0 |
| 56 | MG | 1A | 3902 | 1/1 | 0.97 | 0.10 | 43,43,43,43 | 0 |
| 56 | MG | 2A | 3659 | 1/1 | 0.97 | 0.11 | 58,58,58,58 | 0 |
| 56 | MG | 1A | 3272 | 1/1 | 0.97 | 0.13 | 22,22,22,22 | 0 |
| 56 | MG | 2a | 3205 | 1/1 | 0.97 | 0.07 | 60,60,60,60 | 0 |
| 56 | MG | 2A | 3220 | 1/1 | 0.97 | 0.07 | 52,52,52,52 | 0 |
| 56 | MG | 1A | 3150 | 1/1 | 0.97 | 0.08 | 31,31,31,31 | 0 |
| 56 | MG | 1A | 3275 | 1/1 | 0.97 | 0.17 | 31,31,31,31 | 0 |
| 56 | MG | 1U | 210 | 1/1 | 0.97 | 0.19 | 25,25,25,25 | 0 |
| 56 | MG | 2A | 3666 | 1/1 | 0.97 | 0.06 | 44,44,44,44 | 0 |
| 56 | MG | 2A | 3430 | 1/1 | 0.97 | 0.15 | 31,31,31,31 | 0 |
| 56 | MG | 1A | 3186 | 1/1 | 0.97 | 0.12 | 37,37,37,37 | 0 |
| 56 | MG | 2A | 3669 | 1/1 | 0.97 | 0.10 | 59,59,59,59 | 0 |
| 56 | MG | 1V | 201 | 1/1 | 0.97 | 0.25 | 30,30,30,30 | 0 |
| 56 | MG | 2F | 306 | 1/1 | 0.97 | 0.17 | 51,51,51,51 | 0 |
| 56 | MG | 1A | 3229 | 1/1 | 0.97 | 0.18 | 32,32,32,32 | 0 |
| 56 | MG | 2N | 201 | 1/1 | 0.97 | 0.05 | 35,35,35,35 | 0 |
| 56 | MG | 2A | 3434 | 1/1 | 0.97 | 0.24 | 46,46,46,46 | 0 |
| 56 | MG | 1V | 204 | 1/1 | 0.97 | 0.17 | 32,32,32,32 | 0 |
| 56 | MG | 1A | 3009 | 1/1 | 0.97 | 0.05 | 17,17,17,17 | 0 |
| 56 | MG | 1V | 206 | 1/1 | 0.97 | 0.06 | 29,29,29,29 | 0 |
| 56 | MG | 2A | 3231 | 1/1 | 0.97 | 0.20 | 50,50,50,50 | 0 |
| 56 | MG | 2a | 3226 | 1/1 | 0.97 | 0.12 | 50,50,50,50 | 0 |
| 56 | MG | 2A | 3232 | 1/1 | 0.97 | 0.07 | 60,60,60,60 | 0 |
| 56 | MG | 2A | 3233 | 1/1 | 0.97 | 0.07 | 33,33,33,33 | 0 |
| 56 | MG | 1A | 4063 | 1/1 | 0.97 | 0.07 | 46,46,46,46 | 0 |
| 56 | MG | 1A | 3335 | 1/1 | 0.97 | 0.07 | 36,36,36,36 | 0 |
| 56 | MG | 1A | 3231 | 1/1 | 0.97 | 0.16 | 33,33,33,33 | 0 |
| 56 | MG | 2A | 3031 | 1/1 | 0.97 | 0.05 | 48,48,48,48 | 0 |
| 56 | MG | 1A | 3281 | 1/1 | 0.97 | 0.21 | 31,31,31,31 | 0 |
| 56 | MG | 1A | 3782 | 1/1 | 0.97 | 0.07 | 48,48,48,48 | 0 |
| 56 | MG | 2T | 203 | 1/1 | 0.97 | 0.12 | 50,50,50,50 | 0 |
| 56 | MG | 2A | 3685 | 1/1 | 0.97 | 0.06 | 60,60,60,60 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 1A | 3656 | 1/1 | 0.97 | 0.07 | 34,34,34,34 | 0 |
| 56 | MG | 2A | 3035 | 1/1 | 0.97 | 0.08 | 36,36,36,36 | 0 |
| 56 | MG | 1A | 3554 | 1/1 | 0.97 | 0.26 | 41,41,41,41 | 0 |
| 56 | MG | 1A | 3658 | 1/1 | 0.97 | 0.08 | 42,42,42,42 | 0 |
| 56 | MG | 1A | 3555 | 1/1 | 0.97 | 0.05 | 23,23,23,23 | 0 |
| 56 | MG | 1A | 3788 | 1/1 | 0.97 | 0.05 | 35,35,35,35 | 0 |
| 56 | MG | 2A | 3692 | 1/1 | 0.97 | 0.06 | 66,66,66,66 | 0 |
| 56 | MG | 1A | 3154 | 1/1 | 0.97 | 0.15 | 39,39,39,39 | 0 |
| 56 | MG | 1A | 3922 | 1/1 | 0.97 | 0.04 | 70,70,70,70 | 0 |
| 56 | MG | 2A | 3042 | 1/1 | 0.97 | 0.08 | 44,44,44,44 | 0 |
| 56 | MG | 1A | 3122 | 1/1 | 0.97 | 0.11 | 37,37,37,37 | 0 |
| 56 | MG | 1A | 3156 | 1/1 | 0.97 | 0.23 | 39,39,39,39 | 0 |
| 56 | MG | 1A | 3792 | 1/1 | 0.97 | 0.06 | 45,45,45,45 | 0 |
| 56 | MG | 1A | 3285 | 1/1 | 0.97 | 0.25 | 26,26,26,26 | 0 |
| 56 | MG | 1A | 4082 | 1/1 | 0.97 | 0.07 | 35,35,35,35 | 0 |
| 56 | MG | 1A | 3560 | 1/1 | 0.97 | 0.07 | 51,51,51,51 | 0 |
| 56 | MG | 1A | 3104 | 1/1 | 0.97 | 0.04 | 25,25,25,25 | 0 |
| 56 | MG | 23 | 103 | 1/1 | 0.97 | 0.06 | 55,55,55,55 | 0 |
| 56 | MG | 1A | 3562 | 1/1 | 0.97 | 0.06 | 43,43,43,43 | 0 |
| 56 | MG | 2A | 3705 | 1/1 | 0.97 | 0.15 | 51,51,51,51 | 0 |
| 56 | MG | 1A | 3406 | 1/1 | 0.97 | 0.13 | 43,43,43,43 | 0 |
| 56 | MG | 1A | 3407 | 1/1 | 0.97 | 0.07 | 36,36,36,36 | 0 |
| 56 | MG | 1A | 3287 | 1/1 | 0.97 | 0.06 | 43,43,43,43 | 0 |
| 56 | MG | 1A | 3672 | 1/1 | 0.97 | 0.04 | 35,35,35,35 | 0 |
| 56 | MG | 1A | 3410 | 1/1 | 0.97 | 0.06 | 39,39,39,39 | 0 |
| 56 | MG | 1A | 3940 | 1/1 | 0.97 | 0.04 | 28,28,28,28 | 0 |
| 56 | MG | 1A | 3567 | 1/1 | 0.97 | 0.12 | 29,29,29,29 | 0 |
| 56 | MG | 1A | 3804 | 1/1 | 0.97 | 0.06 | 22,22,22,22 | 0 |
| 56 | MG | 2A | 3716 | 1/1 | 0.97 | 0.05 | 51,51,51,51 | 0 |
| 56 | MG | 1A | 3568 | 1/1 | 0.97 | 0.14 | 30,30,30,30 | 0 |
| 56 | MG | 1A | 3090 | 1/1 | 0.97 | 0.09 | 30,30,30,30 | 0 |
| 56 | MG | 1A | 3159 | 1/1 | 0.97 | 0.17 | 30,30,30,30 | 0 |
| 56 | MG | 2A | 3720 | 1/1 | 0.97 | 0.06 | 48,48,48,48 | 0 |
| 56 | MG | 1A | 3106 | 1/1 | 0.97 | 0.06 | 26,26,26,26 | 0 |
| 56 | MG | 1a | 1745 | 1/1 | 0.97 | 0.06 | 54,54,54,54 | 0 |
| 56 | MG | 1A | 3812 | 1/1 | 0.97 | 0.05 | 54,54,54,54 | 0 |
| 56 | MG | 1a | 1747 | 1/1 | 0.97 | 0.06 | 52,52,52,52 | 0 |
| 56 | MG | 1A | 3951 | 1/1 | 0.97 | 0.05 | 42,42,42,42 | 0 |
| 56 | MG | 16 | 101 | 1/1 | 0.97 | 0.06 | 41,41,41,41 | 0 |
| 59 | ZN | 14 | 102 | 1/1 | 0.97 | 0.04 | 87,87,87,87 | 0 |
| 56 | MG | 1A | 3347 | 1/1 | 0.97 | 0.20 | 41,41,41,41 | 0 |
| 56 | MG | 1A | 3033 | 1/1 | 0.97 | 0.30 | 24,24,24,24 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 60 | SF4 | 1d | 302 | 8/8 | 0.97 | 0.06 | 68,78,85,86 | 0 |
| 60 | SF4 | 2d | 302 | 8/8 | 0.97 | 0.05 | 59,73,81,82 | 0 |
| 56 | MG | 1B | 216 | 1/1 | 0.98 | 0.05 | 47,47,47,47 | 0 |
| 56 | MG | 2A | 3534 | 1/1 | 0.98 | 0.05 | 41,41,41,41 | 0 |
| 56 | MG | 1B | 217 | 1/1 | 0.98 | 0.13 | 47,47,47,47 | 0 |
| 56 | MG | 1A | 3729 | 1/1 | 0.98 | 0.04 | 32,32,32,32 | 0 |
| 56 | MG | 1A | 3731 | 1/1 | 0.98 | 0.05 | 24,24,24,24 | 0 |
| 56 | MG | 2A | 3707 | 1/1 | 0.98 | 0.07 | 36,36,36,36 | 0 |
| 56 | MG | 2A | 3229 | 1/1 | 0.98 | 0.16 | 33,33,33,33 | 0 |
| 56 | MG | 1A | 3419 | 1/1 | 0.98 | 0.10 | 32,32,32,32 | 0 |
| 56 | MG | 1W | 203 | 1/1 | 0.98 | 0.06 | 31,31,31,31 | 0 |
| 56 | MG | 1a | 1814 | 1/1 | 0.98 | 0.05 | 67,67,67,67 | 0 |
| 56 | MG | 1A | 3153 | 1/1 | 0.98 | 0.07 | 26,26,26,26 | 0 |
| 56 | MG | 1A | 3081 | 1/1 | 0.98 | 0.08 | 27,27,27,27 | 0 |
| 56 | MG | 1X | 101 | 1/1 | 0.98 | 0.06 | 32,32,32,32 | 0 |
| 56 | MG | 1X | 102 | 1/1 | 0.98 | 0.10 | 35,35,35,35 | 0 |
| 56 | MG | 1A | 4013 | 1/1 | 0.98 | 0.06 | 62,62,62,62 | 0 |
| 56 | MG | 1A | 3015 | 1/1 | 0.98 | 0.05 | 39,39,39,39 | 0 |
| 56 | MG | 1A | 3023 | 1/1 | 0.98 | 0.03 | 15,15,15,15 | 0 |
| 56 | MG | 1a | 1823 | 1/1 | 0.98 | 0.04 | 59,59,59,59 | 0 |
| 56 | MG | 1A | 3035 | 1/1 | 0.98 | 0.03 | 39,39,39,39 | 0 |
| 56 | MG | 1a | 1825 | 1/1 | 0.98 | 0.14 | 43,43,43,43 | 0 |
| 56 | MG | 1A | 3280 | 1/1 | 0.98 | 0.06 | 21,21,21,21 | 0 |
| 56 | MG | 2A | 3092 | 1/1 | 0.98 | 0.15 | 48,48,48,48 | 0 |
| 56 | MG | 1A | 3373 | 1/1 | 0.98 | 0.12 | 43,43,43,43 | 0 |
| 56 | MG | 1A | 3125 | 1/1 | 0.98 | 0.18 | 34,34,34,34 | 0 |
| 56 | MG | 1Z | 303 | 1/1 | 0.98 | 0.07 | 42,42,42,42 | 0 |
| 56 | MG | 1A | 3241 | 1/1 | 0.98 | 0.23 | 30,30,30,30 | 0 |
| 56 | MG | 1A | 3126 | 1/1 | 0.98 | 0.16 | 34,34,34,34 | 0 |
| 56 | MG | 2D | 305 | 1/1 | 0.98 | 0.05 | 33,33,33,33 | 0 |
| 56 | MG | 1A | 3827 | 1/1 | 0.98 | 0.06 | 39,39,39,39 | 0 |
| 56 | MG | 1A | 3200 | 1/1 | 0.98 | 0.05 | 33,33,33,33 | 0 |
| 56 | MG | 2A | 3733 | 1/1 | 0.98 | 0.05 | 51,51,51,51 | 0 |
| 56 | MG | 1A | 3160 | 1/1 | 0.98 | 0.21 | 26,26,26,26 | 0 |
| 56 | MG | 1A | 3669 | 1/1 | 0.98 | 0.05 | 19,19,19,19 | 0 |
| 56 | MG | 1A | 3127 | 1/1 | 0.98 | 0.07 | 42,42,42,42 | 0 |
| 56 | MG | 1A | 3204 | 1/1 | 0.98 | 0.04 | 29,29,29,29 | 0 |
| 56 | MG | 1B | 238 | 1/1 | 0.98 | 0.06 | 37,37,37,37 | 0 |
| 56 | MG | 1A | 3128 | 1/1 | 0.98 | 0.15 | 36,36,36,36 | 0 |
| 56 | MG | 2A | 3106 | 1/1 | 0.98 | 0.07 | 36,36,36,36 | 0 |
| 56 | MG | 2a | 3130 | 1/1 | 0.98 | 0.05 | 68,68,68,68 | 0 |
| 56 | MG | 1A | 3383 | 1/1 | 0.98 | 0.17 | 31,31,31,31 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 2A | 3260 | 1/1 | 0.98 | 0.06 | 57,57,57,57 | 0 |
| 56 | MG | 1A | 3927 | 1/1 | 0.98 | 0.06 | 55,55,55,55 | 0 |
| 56 | MG | 1A | 3549 | 1/1 | 0.98 | 0.12 | 30,30,30,30 | 0 |
| 56 | MG | 1A | 3752 | 1/1 | 0.98 | 0.04 | 37,37,37,37 | 0 |
| 56 | MG | 1A | 3085 | 1/1 | 0.98 | 0.07 | 23,23,23,23 | 0 |
| 56 | MG | 1A | 3086 | 1/1 | 0.98 | 0.15 | 28,28,28,28 | 0 |
| 56 | MG | 1D | 307 | 1/1 | 0.98 | 0.10 | 44,44,44,44 | 0 |
| 56 | MG | 1A | 3386 | 1/1 | 0.98 | 0.07 | 30,30,30,30 | 0 |
| 56 | MG | 1A | 3010 | 1/1 | 0.98 | 0.07 | 36,36,36,36 | 0 |
| 56 | MG | 2a | 3141 | 1/1 | 0.98 | 0.06 | 68,68,68,68 | 0 |
| 56 | MG | 1A | 3132 | 1/1 | 0.98 | 0.06 | 33,33,33,33 | 0 |
| 56 | MG | 1A | 3936 | 1/1 | 0.98 | 0.06 | 14,14,14,14 | 0 |
| 56 | MG | 2A | 3580 | 1/1 | 0.98 | 0.09 | 45,45,45,45 | 0 |
| 56 | MG | 1A | 4044 | 1/1 | 0.98 | 0.04 | 43,43,43,43 | 0 |
| 56 | MG | 2a | 3146 | 1/1 | 0.98 | 0.07 | 68,68,68,68 | 0 |
| 56 | MG | 1A | 3011 | 1/1 | 0.98 | 0.10 | 31,31,31,31 | 0 |
| 56 | MG | 2A | 3756 | 1/1 | 0.98 | 0.14 | 55,55,55,55 | 0 |
| 56 | MG | 1A | 3938 | 1/1 | 0.98 | 0.04 | 54,54,54,54 | 0 |
| 56 | MG | 1A | 3615 | 1/1 | 0.98 | 0.05 | 33,33,33,33 | 0 |
| 56 | MG | 1A | 4050 | 1/1 | 0.98 | 0.09 | 46,46,46,46 | 0 |
| 56 | MG | 2A | 3588 | 1/1 | 0.98 | 0.07 | 37,37,37,37 | 0 |
| 56 | MG | 2A | 3589 | 1/1 | 0.98 | 0.05 | 44,44,44,44 | 0 |
| 56 | MG | 1A | 3761 | 1/1 | 0.98 | 0.06 | 36,36,36,36 | 0 |
| 56 | MG | 2A | 3591 | 1/1 | 0.98 | 0.07 | 46,46,46,46 | 0 |
| 56 | MG | 1A | 3683 | 1/1 | 0.98 | 0.10 | 20,20,20,20 | 0 |
| 56 | MG | 1A | 3294 | 1/1 | 0.98 | 0.06 | 41,41,41,41 | 0 |
| 56 | MG | 2a | 3158 | 1/1 | 0.98 | 0.10 | 54,54,54,54 | 0 |
| 56 | MG | 1A | 3764 | 1/1 | 0.98 | 0.05 | 14,14,14,14 | 0 |
| 56 | MG | 2a | 3161 | 1/1 | 0.98 | 0.04 | 67,67,67,67 | 0 |
| 56 | MG | 1A | 3295 | 1/1 | 0.98 | 0.04 | 22,22,22,22 | 0 |
| 56 | MG | 1A | 3012 | 1/1 | 0.98 | 0.06 | 28,28,28,28 | 0 |
| 56 | MG | 1E | 311 | 1/1 | 0.98 | 0.06 | 52,52,52,52 | 0 |
| 56 | MG | 1A | 3949 | 1/1 | 0.98 | 0.07 | 54,54,54,54 | 0 |
| 56 | MG | 2a | 3166 | 1/1 | 0.98 | 0.04 | 67,67,67,67 | 0 |
| 56 | MG | 2A | 3435 | 1/1 | 0.98 | 0.07 | 28,28,28,28 | 0 |
| 56 | MG | 2a | 3168 | 1/1 | 0.98 | 0.06 | 51,51,51,51 | 0 |
| 56 | MG | 1A | 3688 | 1/1 | 0.98 | 0.07 | 33,33,33,33 | 0 |
| 56 | MG | 1a | 1723 | 1/1 | 0.98 | 0.23 | 46,46,46,46 | 0 |
| 56 | MG | 1A | 3007 | 1/1 | 0.98 | 0.05 | 26,26,26,26 | 0 |
| 56 | MG | 2A | 3603 | 1/1 | 0.98 | 0.04 | 60,60,60,60 | 0 |
| 56 | MG | 2A | 3604 | 1/1 | 0.98 | 0.10 | 44,44,44,44 | 0 |
| 56 | MG | 1A | 3298 | 1/1 | 0.98 | 0.06 | 36,36,36,36 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 18 | 106 | 1/1 | 0.98 | 0.05 | 26,26,26,26 | 0 |
| 56 | MG | 1a | 1727 | 1/1 | 0.98 | 0.13 | 36,36,36,36 | 0 |
| 56 | MG | 1F | 301 | 1/1 | 0.98 | 0.04 | 27,27,27,27 | 0 |
| 56 | MG | 2A | 3782 | 1/1 | 0.98 | 0.06 | 55,55,55,55 | 0 |
| 56 | MG | 1A | 3028 | 1/1 | 0.98 | 0.13 | 21,21,21,21 | 0 |
| 56 | MG | 1F | 303 | 1/1 | 0.98 | 0.09 | 28,28,28,28 | 0 |
| 56 | MG | 1A | 3396 | 1/1 | 0.98 | 0.17 | 26,26,26,26 | 0 |
| 56 | MG | 2A | 3786 | 1/1 | 0.98 | 0.08 | 51,51,51,51 | 0 |
| 56 | MG | 1A | 3957 | 1/1 | 0.98 | 0.09 | 50,50,50,50 | 0 |
| 56 | MG | 1A | 3071 | 1/1 | 0.98 | 0.09 | 29,29,29,29 | 0 |
| 56 | MG | 1F | 307 | 1/1 | 0.98 | 0.13 | 30,30,30,30 | 0 |
| 56 | MG | 1A | 4065 | 1/1 | 0.98 | 0.08 | 36,36,36,36 | 0 |
| 56 | MG | 2a | 3187 | 1/1 | 0.98 | 0.06 | 70,70,70,70 | 0 |
| 56 | MG | 1A | 3773 | 1/1 | 0.98 | 0.04 | 46,46,46,46 | 0 |
| 56 | MG | 1A | 3694 | 1/1 | 0.98 | 0.08 | 41,41,41,41 | 0 |
| 56 | MG | 1A | 3042 | 1/1 | 0.98 | 0.18 | 22,22,22,22 | 0 |
| 56 | MG | 2A | 3794 | 1/1 | 0.98 | 0.04 | 65,65,65,65 | 0 |
| 56 | MG | 1A | 3139 | 1/1 | 0.98 | 0.11 | 36,36,36,36 | 0 |
| 56 | MG | 1A | 3862 | 1/1 | 0.98 | 0.11 | 36,36,36,36 | 0 |
| 56 | MG | 2A | 3153 | 1/1 | 0.98 | 0.06 | 41,41,41,41 | 0 |
| 56 | MG | 1A | 3175 | 1/1 | 0.98 | 0.17 | 30,30,30,30 | 0 |
| 56 | MG | 1a | 1742 | 1/1 | 0.98 | 0.06 | 55,55,55,55 | 0 |
| 56 | MG | 1A | 3628 | 1/1 | 0.98 | 0.04 | 51,51,51,51 | 0 |
| 56 | MG | 2A | 3307 | 1/1 | 0.98 | 0.05 | 54,54,54,54 | 0 |
| 56 | MG | 2A | 3009 | 1/1 | 0.98 | 0.05 | 38,38,38,38 | 0 |
| 56 | MG | 1A | 3176 | 1/1 | 0.98 | 0.10 | 27,27,27,27 | 0 |
| 56 | MG | 1A | 3177 | 1/1 | 0.98 | 0.12 | 25,25,25,25 | 0 |
| 56 | MG | 1A | 3178 | 1/1 | 0.98 | 0.05 | 17,17,17,17 | 0 |
| 56 | MG | 1A | 3702 | 1/1 | 0.98 | 0.03 | 8,8,8,8 | 0 |
| 56 | MG | 1A | 4077 | 1/1 | 0.98 | 0.06 | 27,27,27,27 | 0 |
| 56 | MG | 1A | 3570 | 1/1 | 0.98 | 0.12 | 29,29,29,29 | 0 |
| 56 | MG | 1A | 3785 | 1/1 | 0.98 | 0.06 | 37,37,37,37 | 0 |
| 56 | MG | 2A | 3017 | 1/1 | 0.98 | 0.04 | 36,36,36,36 | 0 |
| 56 | MG | 1O | 202 | 1/1 | 0.98 | 0.15 | 47,47,47,47 | 0 |
| 56 | MG | 1O | 203 | 1/1 | 0.98 | 0.09 | 40,40,40,40 | 0 |
| 56 | MG | 2a | 3210 | 1/1 | 0.98 | 0.09 | 57,57,57,57 | 0 |
| 56 | MG | 2a | 3211 | 1/1 | 0.98 | 0.07 | 50,50,50,50 | 0 |
| 56 | MG | 2a | 3212 | 1/1 | 0.98 | 0.10 | 59,59,59,59 | 0 |
| 56 | MG | 1A | 3633 | 1/1 | 0.98 | 0.05 | 28,28,28,28 | 0 |
| 56 | MG | 1A | 3975 | 1/1 | 0.98 | 0.06 | 50,50,50,50 | 0 |
| 56 | MG | 1A | 3014 | 1/1 | 0.98 | 0.06 | 22,22,22,22 | 0 |
| 56 | MG | 1A | 3977 | 1/1 | 0.98 | 0.13 | 59,59,59,59 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 1a | 1758 | 1/1 | 0.98 | 0.05 | 32,32,32,32 | 0 |
| 56 | MG | 1P | 203 | 1/1 | 0.98 | 0.10 | 25,25,25,25 | 0 |
| 56 | MG | 2A | 3477 | 1/1 | 0.98 | 0.12 | 23,23,23,23 | 0 |
| 56 | MG | 1P | 204 | 1/1 | 0.98 | 0.18 | 23,23,23,23 | 0 |
| 56 | MG | 1A | 3457 | 1/1 | 0.98 | 0.05 | 25,25,25,25 | 0 |
| 56 | MG | 1A | 3354 | 1/1 | 0.98 | 0.06 | 34,34,34,34 | 0 |
| 56 | MG | 2A | 3177 | 1/1 | 0.98 | 0.14 | 35,35,35,35 | 0 |
| 56 | MG | 1A | 3875 | 1/1 | 0.98 | 0.25 | 35,35,35,35 | 0 |
| 56 | MG | 2A | 3825 | 1/1 | 0.98 | 0.03 | 43,43,43,43 | 0 |
| 56 | MG | 1A | 3355 | 1/1 | 0.98 | 0.26 | 25,25,25,25 | 0 |
| 56 | MG | 2A | 3651 | 1/1 | 0.98 | 0.07 | 44,44,44,44 | 0 |
| 56 | MG | 1A | 3517 | 1/1 | 0.98 | 0.06 | 44,44,44,44 | 0 |
| 56 | MG | 1A | 4091 | 1/1 | 0.98 | 0.05 | 31,31,31,31 | 0 |
| 56 | MG | 1A | 3142 | 1/1 | 0.98 | 0.05 | 14,14,14,14 | 0 |
| 56 | MG | 1Q | 203 | 1/1 | 0.98 | 0.09 | 24,24,24,24 | 0 |
| 56 | MG | 1a | 1637 | 1/1 | 0.98 | 0.13 | 54,54,54,54 | 0 |
| 56 | MG | 2A | 3185 | 1/1 | 0.98 | 0.12 | 47,47,47,47 | 0 |
| 56 | MG | 1A | 3075 | 1/1 | 0.98 | 0.04 | 21,21,21,21 | 0 |
| 56 | MG | 1A | 3409 | 1/1 | 0.98 | 0.12 | 41,41,41,41 | 0 |
| 56 | MG | 2A | 3837 | 1/1 | 0.98 | 0.09 | 66,66,66,66 | 0 |
| 56 | MG | 2A | 3188 | 1/1 | 0.98 | 0.06 | 43,43,43,43 | 0 |
| 56 | MG | 1A | 3795 | 1/1 | 0.98 | 0.06 | 19,19,19,19 | 0 |
| 56 | MG | 1Q | 207 | 1/1 | 0.98 | 0.05 | 44,44,44,44 | 0 |
| 56 | MG | 2A | 3663 | 1/1 | 0.98 | 0.05 | 54,54,54,54 | 0 |
| 56 | MG | 1A | 3145 | 1/1 | 0.98 | 0.18 | 21,21,21,21 | 0 |
| 56 | MG | 2A | 3496 | 1/1 | 0.98 | 0.05 | 55,55,55,55 | 0 |
| 56 | MG | 1A | 4097 | 1/1 | 0.98 | 0.06 | 35,35,35,35 | 0 |
| 56 | MG | 1a | 1644 | 1/1 | 0.98 | 0.09 | 39,39,39,39 | 0 |
| 56 | MG | 1A | 3115 | 1/1 | 0.98 | 0.04 | 32,32,32,32 | 0 |
| 56 | MG | 2A | 3045 | 1/1 | 0.98 | 0.20 | 53,53,53,53 | 0 |
| 56 | MG | 1A | 3021 | 1/1 | 0.98 | 0.04 | 21,21,21,21 | 0 |
| 56 | MG | 1A | 3716 | 1/1 | 0.98 | 0.06 | 31,31,31,31 | 0 |
| 56 | MG | 1a | 1648 | 1/1 | 0.98 | 0.05 | 48,48,48,48 | 0 |
| 56 | MG | 2A | 3199 | 1/1 | 0.98 | 0.18 | 50,50,50,50 | 0 |
| 56 | MG | 1A | 3886 | 1/1 | 0.98 | 0.04 | 23,23,23,23 | 0 |
| 56 | MG | 2A | 3856 | 1/1 | 0.98 | 0.05 | 58,58,58,58 | 0 |
| 56 | MG | 1A | 3466 | 1/1 | 0.98 | 0.07 | 36,36,36,36 | 0 |
| 56 | MG | 2A | 3507 | 1/1 | 0.98 | 0.10 | 44,44,44,44 | 0 |
| 56 | MG | 1A | 3031 | 1/1 | 0.98 | 0.16 | 31,31,31,31 | 0 |
| 56 | MG | 2A | 3510 | 1/1 | 0.98 | 0.06 | 41,41,41,41 | 0 |
| 56 | MG | 1A | 3118 | 1/1 | 0.98 | 0.14 | 22,22,22,22 | 0 |
| 56 | MG | 1A | 3995 | 1/1 | 0.98 | 0.05 | 61,61,61,61 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 1A | 3890 | 1/1 | 0.98 | 0.03 | 33,33,33,33 | 0 |
| 56 | MG | 1A | 3721 | 1/1 | 0.98 | 0.07 | 27,27,27,27 | 0 |
| 56 | MG | 1A | 3469 | 1/1 | 0.98 | 0.05 | 33,33,33,33 | 0 |
| 56 | MG | 1U | 203 | 1/1 | 0.98 | 0.26 | 28,28,28,28 | 0 |
| 56 | MG | 1A | 3806 | 1/1 | 0.98 | 0.05 | 26,26,26,26 | 0 |
| 56 | MG | 1a | 1792 | 1/1 | 0.98 | 0.06 | 60,60,60,60 | 0 |
| 56 | MG | 1A | 3649 | 1/1 | 0.98 | 0.04 | 29,29,29,29 | 0 |
| 56 | MG | 1U | 207 | 1/1 | 0.98 | 0.14 | 29,29,29,29 | 0 |
| 56 | MG | 1U | 208 | 1/1 | 0.98 | 0.19 | 30,30,30,30 | 0 |
| 56 | MG | 1a | 1796 | 1/1 | 0.98 | 0.06 | 59,59,59,59 | 0 |
| 56 | MG | 1A | 3586 | 1/1 | 0.98 | 0.17 | 31,31,31,31 | 0 |
| 56 | MG | 1A | 3032 | 1/1 | 0.98 | 0.12 | 26,26,26,26 | 0 |
| 56 | MG | 1U | 211 | 1/1 | 0.98 | 0.11 | 28,28,28,28 | 0 |
| 56 | MG | 1A | 3810 | 1/1 | 0.98 | 0.06 | 25,25,25,25 | 0 |
| 56 | MG | 1A | 3099 | 1/1 | 0.98 | 0.10 | 16,16,16,16 | 0 |
| 56 | MG | 1A | 3152 | 1/1 | 0.98 | 0.03 | 29,29,29,29 | 0 |
| 56 | MG | 1V | 203 | 1/1 | 0.98 | 0.18 | 26,26,26,26 | 0 |
| 56 | MG | 1a | 1804 | 1/1 | 0.98 | 0.05 | 53,53,53,53 | 0 |
| 59 | ZN | 2Y | 501 | 1/1 | 0.98 | 0.04 | 81,81,81,81 | 0 |
| 56 | MG | 1a | 1805 | 1/1 | 0.98 | 0.08 | 55,55,55,55 | 0 |
| 56 | MG | 2A | 3882 | 1/1 | 0.98 | 0.06 | 42,42,42,42 | 0 |
| 56 | MG | 2A | 3700 | 1/1 | 0.98 | 0.04 | 58,58,58,58 | 0 |
| 56 | MG | 1A | 3274 | 1/1 | 0.98 | 0.11 | 38,38,38,38 | 0 |
| 56 | MG | 2A | 3776 | 1/1 | 0.99 | 0.04 | 56,56,56,56 | 0 |
| 56 | MG | 2A | 3854 | 1/1 | 0.99 | 0.06 | 35,35,35,35 | 0 |
| 56 | MG | 1A | 3305 | 1/1 | 0.99 | 0.18 | 34,34,34,34 | 0 |
| 56 | MG | 1A | 3233 | 1/1 | 0.99 | 0.03 | 30,30,30,30 | 0 |
| 56 | MG | 2A | 3019 | 1/1 | 0.99 | 0.04 | 30,30,30,30 | 0 |
| 56 | MG | 1A | 3307 | 1/1 | 0.99 | 0.08 | 26,26,26,26 | 0 |
| 56 | MG | 1A | 3974 | 1/1 | 0.99 | 0.04 | 54,54,54,54 | 0 |
| 56 | MG | 1A | 4020 | 1/1 | 0.99 | 0.04 | 33,33,33,33 | 0 |
| 56 | MG | 1A | 3216 | 1/1 | 0.99 | 0.15 | 32,32,32,32 | 0 |
| 56 | MG | 1A | 3201 | 1/1 | 0.99 | 0.03 | 22,22,22,22 | 0 |
| 56 | MG | 1A | 3496 | 1/1 | 0.99 | 0.06 | 25,25,25,25 | 0 |
| 56 | MG | 1A | 3187 | 1/1 | 0.99 | 0.05 | 31,31,31,31 | 0 |
| 56 | MG | 1A | 3830 | 1/1 | 0.99 | 0.19 | 48,48,48,48 | 0 |
| 56 | MG | 1A | 4026 | 1/1 | 0.99 | 0.04 | 35,35,35,35 | 0 |
| 56 | MG | 2A | 3642 | 1/1 | 0.99 | 0.04 | 41,41,41,41 | 0 |
| 56 | MG | 1A | 3144 | 1/1 | 0.99 | 0.10 | 42,42,42,42 | 0 |
| 56 | MG | 1A | 4080 | 1/1 | 0.99 | 0.04 | 39,39,39,39 | 0 |
| 56 | MG | 1A | 3740 | 1/1 | 0.99 | 0.04 | 49,49,49,49 | 0 |
| 56 | MG | 1A | 4029 | 1/1 | 0.99 | 0.05 | 50,50,50,50 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 1A | 3899 | 1/1 | 0.99 | 0.04 | 38,38,38,38 | 0 |
| 56 | MG | 1A | 4031 | 1/1 | 0.99 | 0.07 | 60,60,60,60 | 0 |
| 56 | MG | 2A | 3508 | 1/1 | 0.99 | 0.05 | 64,64,64,64 | 0 |
| 56 | MG | 1X | 105 | 1/1 | 0.99 | 0.06 | 29,29,29,29 | 0 |
| 56 | MG | 1A | 3939 | 1/1 | 0.99 | 0.08 | 21,21,21,21 | 0 |
| 56 | MG | 2A | 3725 | 1/1 | 0.99 | 0.06 | 34,34,34,34 | 0 |
| 56 | MG | 1A | 4086 | 1/1 | 0.99 | 0.08 | 28,28,28,28 | 0 |
| 56 | MG | 1A | 3900 | 1/1 | 0.99 | 0.03 | 20,20,20,20 | 0 |
| 56 | MG | 2A | 3582 | 1/1 | 0.99 | 0.06 | 39,39,39,39 | 0 |
| 56 | MG | 1A | 3079 | 1/1 | 0.99 | 0.15 | 26,26,26,26 | 0 |
| 56 | MG | 2A | 3584 | 1/1 | 0.99 | 0.05 | 59,59,59,59 | 0 |
| 56 | MG | 1A | 3687 | 1/1 | 0.99 | 0.08 | 27,27,27,27 | 0 |
| 56 | MG | 1A | 3190 | 1/1 | 0.99 | 0.15 | 25,25,25,25 | 0 |
| 56 | MG | 1A | 3944 | 1/1 | 0.99 | 0.05 | 44,44,44,44 | 0 |
| 56 | MG | 1A | 3501 | 1/1 | 0.99 | 0.07 | 28,28,28,28 | 0 |
| 56 | MG | 1A | 3946 | 1/1 | 0.99 | 0.03 | 40,40,40,40 | 0 |
| 56 | MG | 1A | 3805 | 1/1 | 0.99 | 0.03 | 35,35,35,35 | 0 |
| 56 | MG | 1w | 111 | 1/1 | 0.99 | 0.06 | 69,69,69,69 | 0 |
| 56 | MG | 1A | 4041 | 1/1 | 0.99 | 0.02 | 42,42,42,42 | 0 |
| 56 | MG | 1A | 3374 | 1/1 | 0.99 | 0.03 | 30,30,30,30 | 0 |
| 56 | MG | 2a | 3159 | 1/1 | 0.99 | 0.03 | 56,56,56,56 | 0 |
| 56 | MG | 1A | 3839 | 1/1 | 0.99 | 0.07 | 43,43,43,43 | 0 |
| 56 | MG | 1A | 3908 | 1/1 | 0.99 | 0.04 | 32,32,32,32 | 0 |
| 56 | MG | 1A | 4045 | 1/1 | 0.99 | 0.03 | 17,17,17,17 | 0 |
| 56 | MG | 1A | 3222 | 1/1 | 0.99 | 0.16 | 29,29,29,29 | 0 |
| 56 | MG | 1A | 3952 | 1/1 | 0.99 | 0.04 | 39,39,39,39 | 0 |
| 56 | MG | 2A | 3119 | 1/1 | 0.99 | 0.11 | 36,36,36,36 | 0 |
| 56 | MG | 1A | 4048 | 1/1 | 0.99 | 0.05 | 34,34,34,34 | 0 |
| 56 | MG | 1E | 304 | 1/1 | 0.99 | 0.11 | 34,34,34,34 | 0 |
| 56 | MG | 1A | 3953 | 1/1 | 0.99 | 0.03 | 50,50,50,50 | 0 |
| 56 | MG | 1A | 3666 | 1/1 | 0.99 | 0.05 | 35,35,35,35 | 0 |
| 56 | MG | 1A | 3719 | 1/1 | 0.99 | 0.09 | 47,47,47,47 | 0 |
| 56 | MG | 1A | 3779 | 1/1 | 0.99 | 0.03 | 18,18,18,18 | 0 |
| 56 | MG | 1a | 1811 | 1/1 | 0.99 | 0.05 | 38,38,38,38 | 0 |
| 56 | MG | 1x | 114 | 1/1 | 0.99 | 0.05 | 51,51,51,51 | 0 |
| 56 | MG | 1A | 3008 | 1/1 | 0.99 | 0.08 | 26,26,26,26 | 0 |
| 56 | MG | 2A | 3829 | 1/1 | 0.99 | 0.04 | 45,45,45,45 | 0 |
| 56 | MG | 1A | 3914 | 1/1 | 0.99 | 0.04 | 19,19,19,19 | 0 |
| 56 | MG | 1A | 3073 | 1/1 | 0.99 | 0.07 | 14,14,14,14 | 0 |
| 56 | MG | 1A | 3064 | 1/1 | 0.99 | 0.06 | 32,32,32,32 | 0 |
| 56 | MG | 1A | 3036 | 1/1 | 0.99 | 0.05 | 15,15,15,15 | 0 |
| 56 | MG | 1A | 3076 | 1/1 | 0.99 | 0.10 | 20,20,20,20 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 1a | 1757 | 1/1 | 0.99 | 0.04 | 35,35,35,35 | 0 |
| 56 | MG | 1A | 3161 | 1/1 | 0.99 | 0.12 | 22,22,22,22 | 0 |
| 56 | MG | 2a | 3022 | 1/1 | 0.99 | 0.11 | 43,43,43,43 | 0 |
| 56 | MG | 1a | 1820 | 1/1 | 0.99 | 0.03 | 68,68,68,68 | 0 |
| 56 | MG | 2A | 3137 | 1/1 | 0.99 | 0.14 | 40,40,40,40 | 0 |
| 56 | MG | 1A | 3141 | 1/1 | 0.99 | 0.10 | 26,26,26,26 | 0 |
| 56 | MG | 2A | 3139 | 1/1 | 0.99 | 0.12 | 34,34,34,34 | 0 |
| 56 | MG | 1U | 204 | 1/1 | 0.99 | 0.04 | 22,22,22,22 | 0 |
| 56 | MG | 2E | 303 | 1/1 | 0.99 | 0.11 | 36,36,36,36 | 0 |
| 56 | MG | 1A | 3070 | 1/1 | 0.99 | 0.06 | 12,12,12,12 | 0 |
| 56 | MG | 2A | 3843 | 1/1 | 0.99 | 0.11 | 35,35,35,35 | 0 |
| 56 | MG | 2y | 105 | 1/1 | 0.99 | 0.03 | 76,76,76,76 | 0 |
| 56 | MG | 17 | 103 | 1/1 | 0.99 | 0.03 | 22,22,22,22 | 0 |
| 56 | MG | 2A | 3845 | 1/1 | 0.99 | 0.04 | 44,44,44,44 | 0 |
| 56 | MG | 1A | 4010 | 1/1 | 0.99 | 0.06 | 28,28,28,28 | 0 |
| 58 | K | 1A | 4103 | 1/1 | 0.99 | 0.02 | 21,21,21,21 | 0 |
| 58 | K | 2A | 3889 | 1/1 | 0.99 | 0.02 | 36,36,36,36 | 0 |
| 59 | ZN | 1Y | 204 | 1/1 | 0.99 | 0.02 | 53,53,53,53 | 0 |
| 56 | MG | 1A | 3199 | 1/1 | 0.99 | 0.14 | 20,20,20,20 | 0 |
| 59 | ZN | 16 | 104 | 1/1 | 0.99 | 0.04 | 37,37,37,37 | 0 |
| 59 | ZN | 1n | 102 | 1/1 | 0.99 | 0.03 | 66,66,66,66 | 0 |
| 56 | MG | 1A | 3967 | 1/1 | 0.99 | 0.04 | 46,46,46,46 | 0 |
| 56 | MG | 1A | 3047 | 1/1 | 0.99 | 0.07 | 23,23,23,23 | 0 |
| 59 | ZN | 25 | 106 | 1/1 | 0.99 | 0.04 | 57,57,57,57 | 0 |
| 59 | ZN | 26 | 501 | 1/1 | 0.99 | 0.06 | 64,64,64,64 | 0 |
| 59 | ZN | 29 | 501 | 1/1 | 0.99 | 0.04 | 72,72,72,72 | 0 |
| 56 | MG | 1A | 3730 | 1/1 | 0.99 | 0.04 | 19,19,19,19 | 0 |
| 56 | MG | 1A | 3677 | 1/1 | 0.99 | 0.04 | 23,23,23,23 | 0 |
| 56 | MG | 1a | 1769 | 1/1 | 0.99 | 0.11 | 52,52,52,52 | 0 |
| 56 | MG | 1A | 3618 | 1/1 | 1.00 | 0.06 | 26,26,26,26 | 0 |
| 56 | MG | 1A | 3935 | 1/1 | 1.00 | 0.02 | 40,40,40,40 | 0 |
| 59 | ZN | 15 | 106 | 1/1 | 1.00 | 0.03 | 38,38,38,38 | 0 |
| 56 | MG | 2A | 3708 | 1/1 | 1.00 | 0.04 | 31,31,31,31 | 0 |
| 59 | ZN | 19 | 102 | 1/1 | 1.00 | 0.04 | 40,40,40,40 | 0 |
| 56 | MG | 1A | 3754 | 1/1 | 1.00 | 0.04 | 18,18,18,18 | 0 |
| 56 | MG | 1A | 3915 | 1/1 | 1.00 | 0.02 | 26,26,26,26 | 0 |

## 6.5 Other polymers (i)

There are no such residues in this entry.