# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 12:20 PM UTC

| | | |
|---|---|---|
| PDB ID | : | 6XQD / pdb_00006xqd |
| Title | : | Crystal structure of the Thermus thermophilus 70S ribosome in complex with sarecycline, UUC-mRNA, and deacylated P-site tRNA at 2.80A resolution |
| Authors | : | Batool, Z.; Lomakin, I.B.; Bunick, C.G.; Polikanov, Y.S. |
| Deposited on | : | 2020-07-09 |
| Resolution | : | 2.80 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.

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

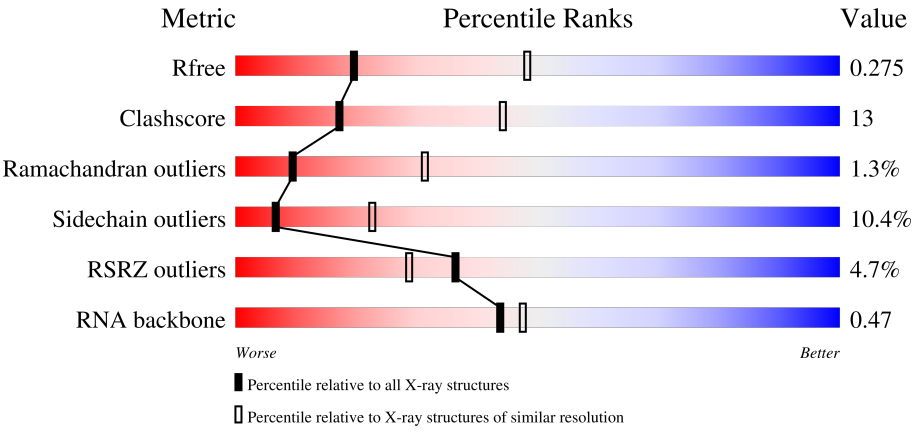
| | | |
|---|---|---|
| MolProbity | : | 4-5-2 with Phenix2.0 |
| Mogul | : | 2022.3.0, CSD as543be (2022) |
| Xtriage (Phenix) | : | 2.0 |
| EDS | : | 3.0 |
| Buster-report | : | wwPDB partial adaption of 1.1.7 (2018) |
| Percentile statistics | : | 20250101.v01 (using entries in the PDB archive January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

# 1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.80 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 | 3866 (2.80-2.80) |
| Clashscore | 190562 | 4276 (2.80-2.80) |
| Ramachandran outliers | 187476 | 4196 (2.80-2.80) |
| Sidechain outliers | 187428 | 4198 (2.80-2.80) |
| RSRZ outliers | 180081 | 3869 (2.80-2.80) |
| RNA backbone | 3983 | 1114 (3.00-2.60) |

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 | 2% 50% 40% 9% |
| 1 | 2A | 2915 | 3% 45% 42% 9% |
| 2 | 1B | 121 | % 60% 33% 6% |
| 2 | 2B | 121 | 5% 39% 47% 13% |

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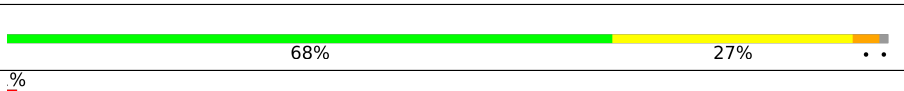
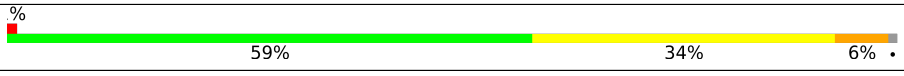
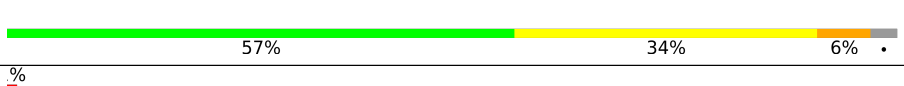
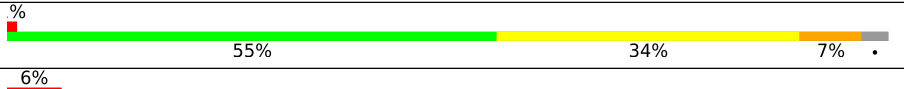
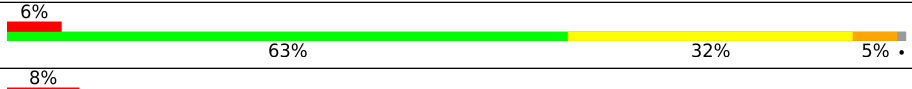
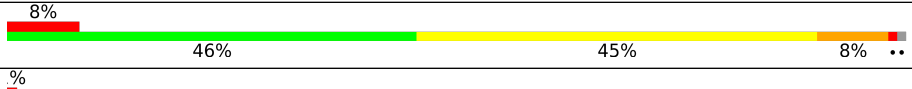
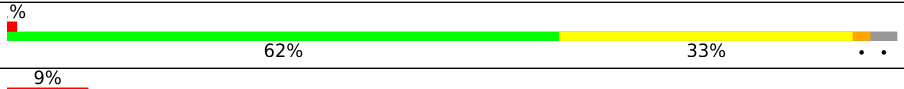
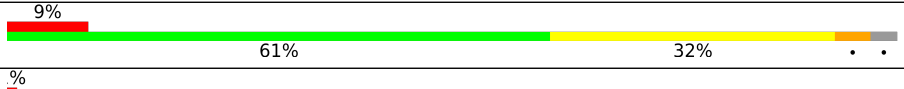
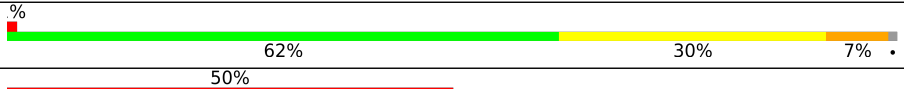
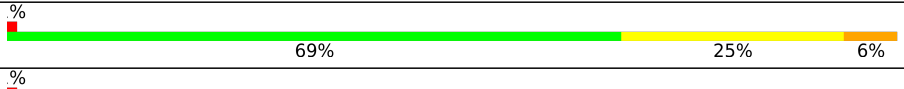
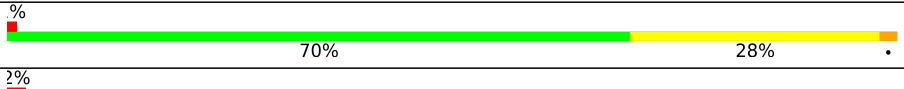
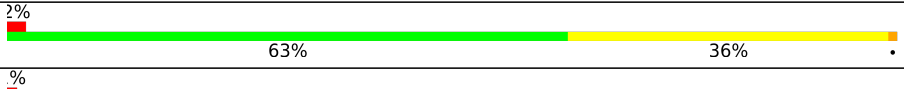
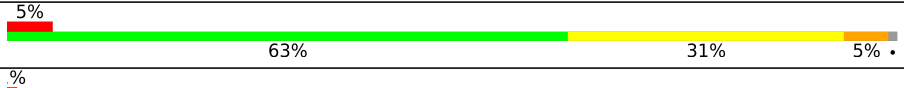
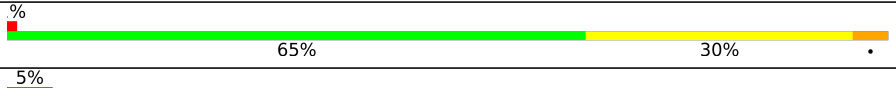
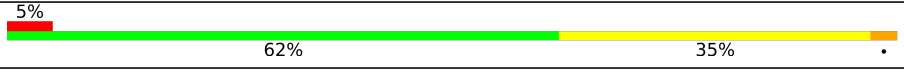
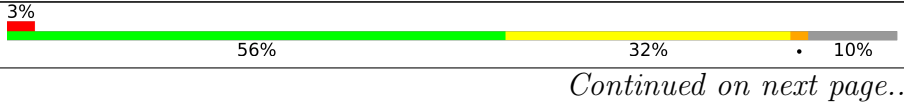
| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 3 | 1D | 276 | |
| 3 | 2D | 276 | |
| 4 | 1E | 206 |   |
| 4 | 2E | 206 |   |
| 5 | 1F | 210 |   |
| 5 | 2F | 210 |   |
| 6 | 1G | 182 |   |
| 6 | 2G | 182 |   |
| 7 | 1H | 180 |   |
| 7 | 2H | 180 |   |
| 8 | 1I | 148 |   |
| 8 | 2I | 148 | |
| 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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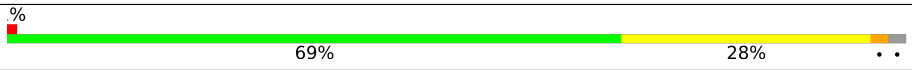
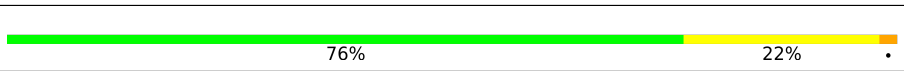
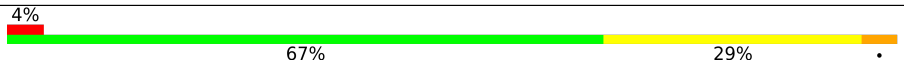
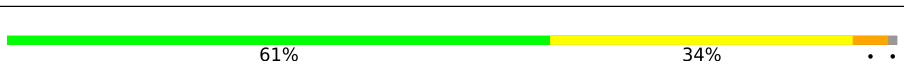
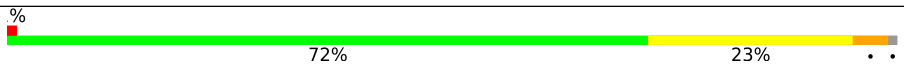
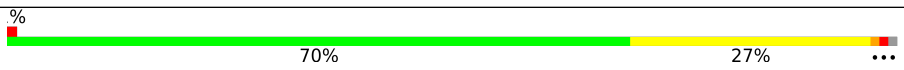
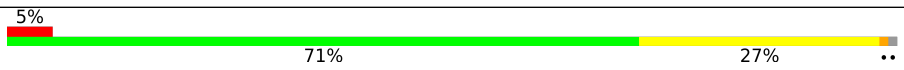
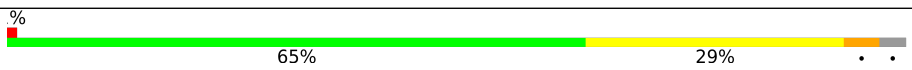
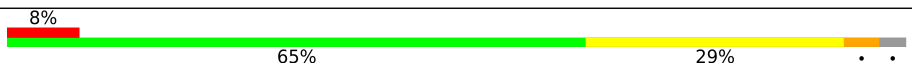
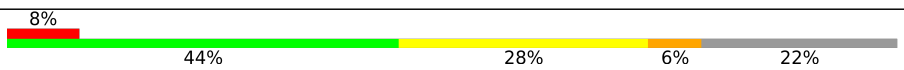
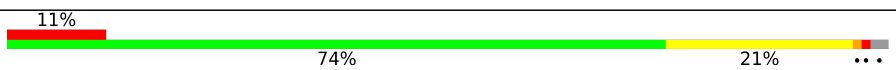
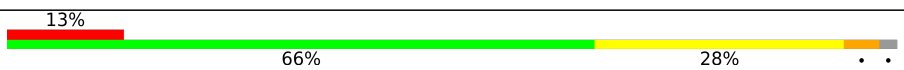
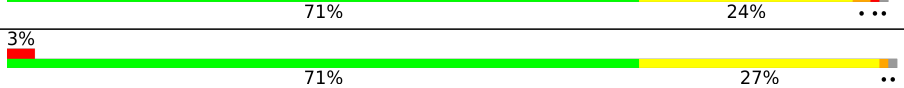
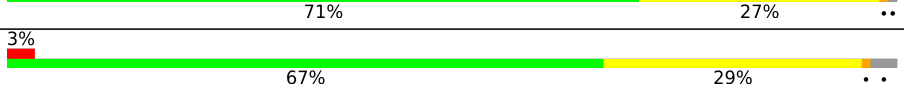
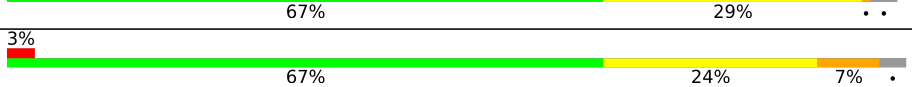
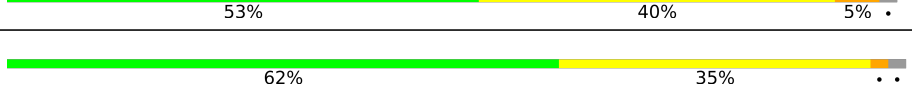
| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 15 | 2T | 146 | |
| 16 | 1U | 118 | |
| 16 | 2U | 118 |   |
| 17 | 1V | 101 |   |
| 17 | 2V | 101 |   |
| 18 | 1W | 113 |   |
| 18 | 2W | 113 |   |
| 19 | 1X | 96 |   |
| 19 | 2X | 96 |   |
| 20 | 1Y | 110 |   |
| 20 | 2Y | 110 |   |
| 21 | 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 |   |
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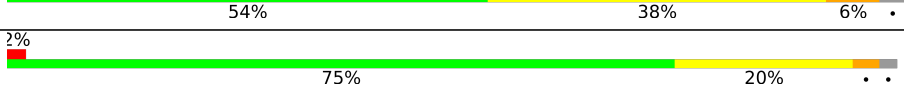
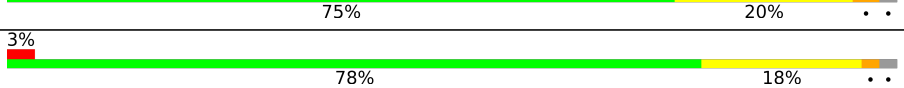
| 26 | 24 | 71 | |
| 27 | 15 | 60 |   |
| 27 | 25 | 60 |   |

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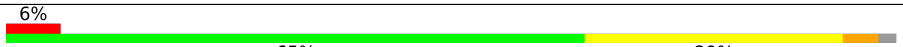
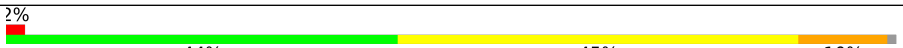
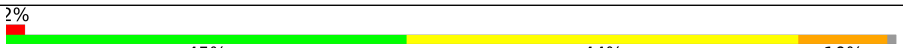
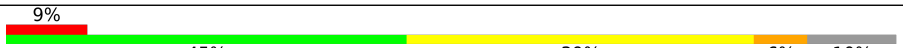
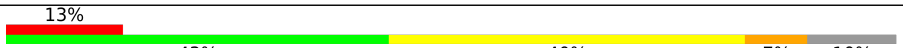
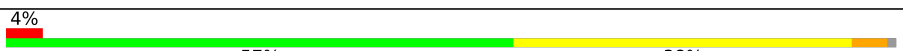
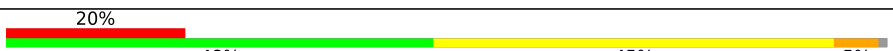
| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 28 | 16 | 54 | |
| 28 | 26 | 54 | |
| 29 | 17 | 49 | |
| 29 | 27 | 49 |   |
| 30 | 18 | 65 | |
| 30 | 28 | 65 | |
| 31 | 19 | 37 | |
| 31 | 29 | 37 | |
| 32 | 1a | 1521 |   |
| 32 | 2a | 1521 |   |
| 33 | 1b | 256 |   |
| 33 | 2b | 256 |   |
| 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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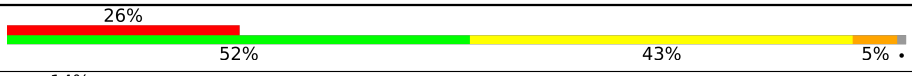
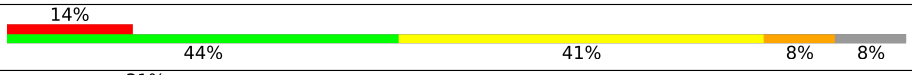
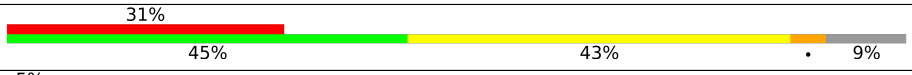
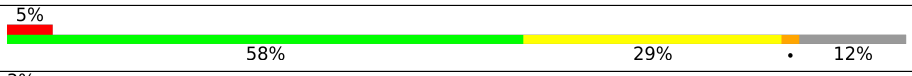
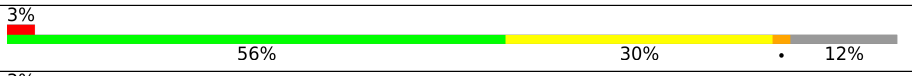
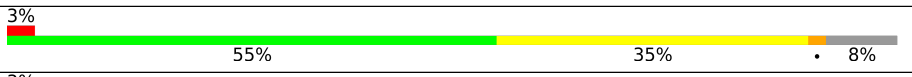
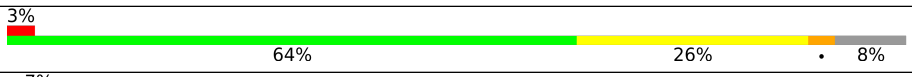
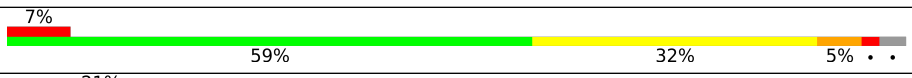
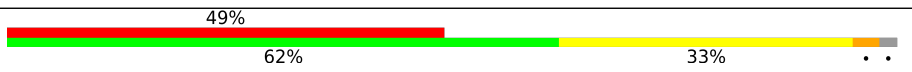
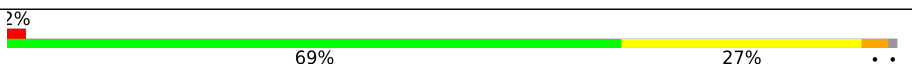
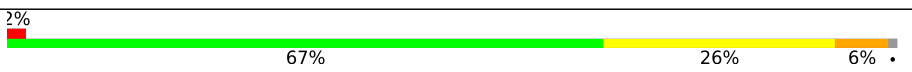
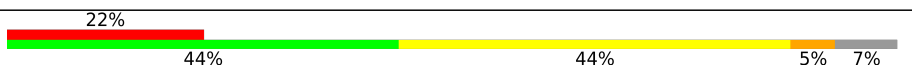
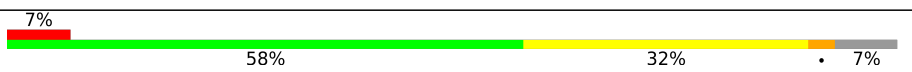
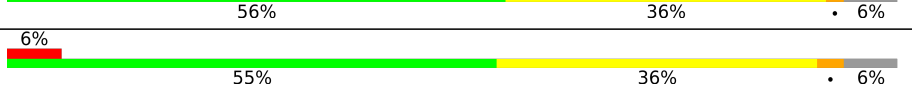
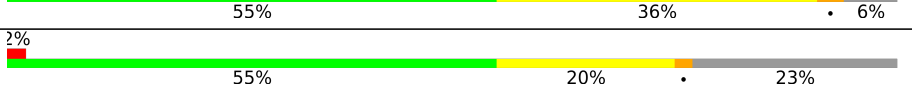
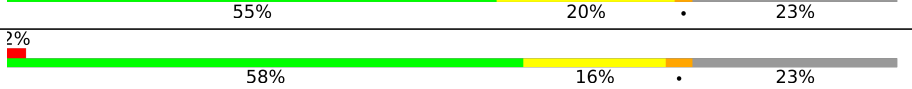
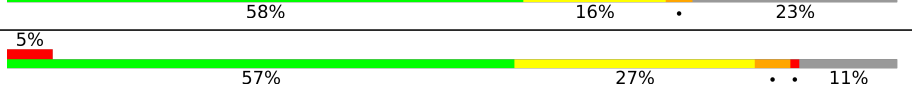
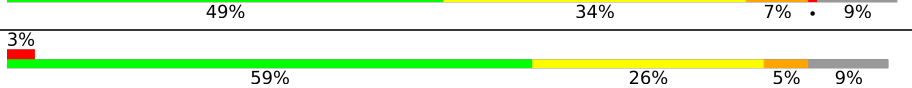
| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 40 | 2i | 128 |   |
| 41 | 1j | 105 |   |
| 41 | 2j | 105 |   |
| 42 | 1k | 129 |   |
| 42 | 2k | 129 |   |
| 43 | 1l | 132 |   |
| 43 | 2l | 132 |   |
| 44 | 1m | 126 |   |
| 44 | 2m | 126 | |
| 45 | 1n | 61 | |
| 45 | 2n | 61 |   |
| 46 | 1o | 89 |   |
| 46 | 2o | 89 |   |
| 47 | 1p | 88 |   |
| 47 | 2p | 88 |   |
| 48 | 1q | 105 | |
| 48 | 2q | 105 |   |
| 49 | 1r | 88 |   |
| 49 | 2r | 88 |   |
| 50 | 1s | 93 |   |
| 50 | 2s | 93 | |
| 51 | 1t | 106 | |
| 51 | 2t | 106 |   |
| 52 | 1u | 27 | |
| 52 | 2u | 27 | |

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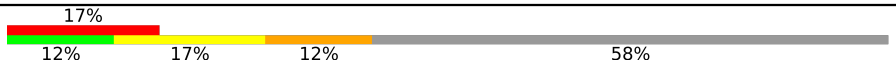
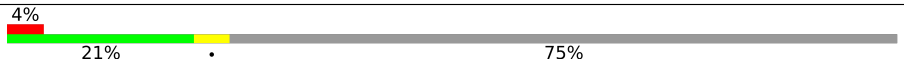
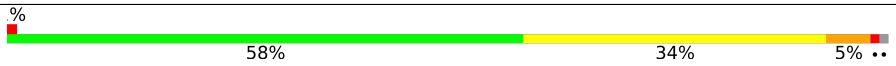
| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 53 | 1v | 24 |   |
| 53 | 2v | 24 |   |
| 54 | 1x | 77 |   |
| 54 | 2x | 77 | |

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

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|---|---|---|---|---|---|---|---|
| 55 | MG | 1A | 3541 | - | - | - | X |
| 55 | MG | 1B | 229 | - | - | - | X |
| 55 | MG | 1U | 207 | - | - | - | X |
| 55 | MG | 1a | 1662 | - | - | - | X |
| 55 | MG | 2A | 3484 | - | - | - | X |
| 55 | MG | 2a | 3092 | - | - | - | X |
| 55 | MG | 2i | 201 | - | - | - | X |
| 58 | SF4 | 1d | 501 | - | - | X | - |

# 2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 292670 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 44 | 1m | 122 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 951 | 587 | 197 | 165 | 2 | | | |
| 44 | 2m | 121 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 943 | 581 | 196 | 164 | 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 | 10 | Total 213 | C 96 | N 39 | O 68 | P 10 | 0 | 0 | 0 |
| 53 | 2v | 6 | Total 113 | C 49 | N 22 | O 36 | P 6 | 0 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 54 | 1x | 76 | Total 1625 | C 725 | N 294 | O 529 | P 76 | S 1 | 0 | 0 | 0 |
| 54 | 2x | 76 | Total 1625 | C 725 | N 294 | O 529 | P 76 | S 1 | 0 | 0 | 0 |

- Molecule 55 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|
| 55 | 1A | 1117 | Total 1117 | Mg 1117 | 0 | 0 |
| 55 | 1B | 35 | Total 35 | Mg 35 | 0 | 0 |
| 55 | 1D | 13 | Total 13 | Mg 13 | 0 | 0 |
| 55 | 1E | 11 | Total 11 | Mg 11 | 0 | 0 |
| 55 | 1F | 11 | Total 11 | Mg 11 | 0 | 0 |
| 55 | 1G | 4 | Total 4 | Mg 4 | 0 | 0 |
| 55 | 1N | 4 | Total 4 | Mg 4 | 0 | 0 |
| 55 | 1O | 4 | Total 4 | Mg 4 | 0 | 0 |
| 55 | 1P | 3 | Total 3 | Mg 3 | 0 | 0 |
| 55 | 1Q | 7 | Total 7 | Mg 7 | 0 | 0 |
| 55 | 1R | 2 | Total 2 | Mg 2 | 0 | 0 |
| 55 | 1S | 1 | Total 1 | Mg 1 | 0 | 0 |
| 55 | 1T | 3 | Total 3 | Mg 3 | 0 | 0 |
| 55 | 1U | 7 | Total 7 | Mg 7 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 55 | 1V | 4 | Total Mg<br>4 4 | 0 | 0 |
| 55 | 1W | 5 | Total Mg<br>5 5 | 0 | 0 |
| 55 | 1X | 6 | Total Mg<br>6 6 | 0 | 0 |
| 55 | 1Y | 4 | Total Mg<br>4 4 | 0 | 0 |
| 55 | 1Z | 2 | Total Mg<br>2 2 | 0 | 0 |
| 55 | 10 | 5 | Total Mg<br>5 5 | 0 | 0 |
| 55 | 11 | 4 | Total Mg<br>4 4 | 0 | 0 |
| 55 | 12 | 2 | Total Mg<br>2 2 | 0 | 0 |
| 55 | 13 | 3 | Total Mg<br>3 3 | 0 | 0 |
| 55 | 15 | 5 | Total Mg<br>5 5 | 0 | 0 |
| 55 | 16 | 1 | Total Mg<br>1 1 | 0 | 0 |
| 55 | 17 | 4 | Total Mg<br>4 4 | 0 | 0 |
| 55 | 18 | 6 | Total Mg<br>6 6 | 0 | 0 |
| 55 | 19 | 1 | Total Mg<br>1 1 | 0 | 0 |
| 55 | 1a | 234 | Total Mg<br>234 234 | 0 | 0 |
| 55 | 1b | 1 | Total Mg<br>1 1 | 0 | 0 |
| 55 | 1e | 2 | Total Mg<br>2 2 | 0 | 0 |
| 55 | 1f | 2 | Total Mg<br>2 2 | 0 | 0 |
| 55 | 1l | 4 | Total Mg<br>4 4 | 0 | 0 |
| 55 | 1n | 2 | Total Mg<br>2 2 | 0 | 0 |
| 55 | 1t | 1 | Total Mg<br>1 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 55 | 1v | 2 | Total Mg<br>2 2 | 0 | 0 |
| 55 | 1x | 13 | Total Mg<br>13 13 | 0 | 0 |
| 55 | 2A | 862 | Total Mg<br>862 862 | 0 | 0 |
| 55 | 2B | 19 | Total Mg<br>19 19 | 0 | 0 |
| 55 | 2D | 3 | Total Mg<br>3 3 | 0 | 0 |
| 55 | 2E | 9 | Total Mg<br>9 9 | 0 | 0 |
| 55 | 2F | 6 | Total Mg<br>6 6 | 0 | 0 |
| 55 | 2G | 1 | Total Mg<br>1 1 | 0 | 0 |
| 55 | 2N | 2 | Total Mg<br>2 2 | 0 | 0 |
| 55 | 2O | 2 | Total Mg<br>2 2 | 0 | 0 |
| 55 | 2P | 2 | Total Mg<br>2 2 | 0 | 0 |
| 55 | 2Q | 4 | Total Mg<br>4 4 | 0 | 0 |
| 55 | 2R | 2 | Total Mg<br>2 2 | 0 | 0 |
| 55 | 2T | 3 | Total Mg<br>3 3 | 0 | 0 |
| 55 | 2U | 2 | Total Mg<br>2 2 | 0 | 0 |
| 55 | 2V | 3 | Total Mg<br>3 3 | 0 | 0 |
| 55 | 2W | 2 | Total Mg<br>2 2 | 0 | 0 |
| 55 | 2X | 2 | Total Mg<br>2 2 | 0 | 0 |
| 55 | 2Z | 1 | Total Mg<br>1 1 | 0 | 0 |
| 55 | 20 | 1 | Total Mg<br>1 1 | 0 | 0 |
| 55 | 23 | 1 | Total Mg<br>1 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 55 | 25 | 2 | Total Mg<br>2 2 | 0 | 0 |
| 55 | 26 | 1 | Total Mg<br>1 1 | 0 | 0 |
| 55 | 27 | 1 | Total Mg<br>1 1 | 0 | 0 |
| 55 | 28 | 3 | Total Mg<br>3 3 | 0 | 0 |
| 55 | 2a | 209 | Total Mg<br>209 209 | 0 | 0 |
| 55 | 2d | 2 | Total Mg<br>2 2 | 0 | 0 |
| 55 | 2e | 1 | Total Mg<br>1 1 | 0 | 0 |
| 55 | 2f | 2 | Total Mg<br>2 2 | 0 | 0 |
| 55 | 2g | 1 | Total Mg<br>1 1 | 0 | 0 |
| 55 | 2i | 1 | Total Mg<br>1 1 | 0 | 0 |
| 55 | 2j | 2 | Total Mg<br>2 2 | 0 | 0 |
| 55 | 2l | 3 | Total Mg<br>3 3 | 0 | 0 |
| 55 | 2p | 1 | Total Mg<br>1 1 | 0 | 0 |
| 55 | 2q | 1 | Total Mg<br>1 1 | 0 | 0 |
| 55 | 2r | 1 | Total Mg<br>1 1 | 0 | 0 |
| 55 | 2t | 1 | Total Mg<br>1 1 | 0 | 0 |
| 55 | 2x | 5 | Total Mg<br>5 5 | 0 | 0 |

- Molecule 56 is ZINC ION (CCD ID: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 56 | 1Y | 1 | Total Zn<br>1 1 | 0 | 0 |
| 56 | 14 | 1 | Total Zn<br>1 1 | 0 | 0 |

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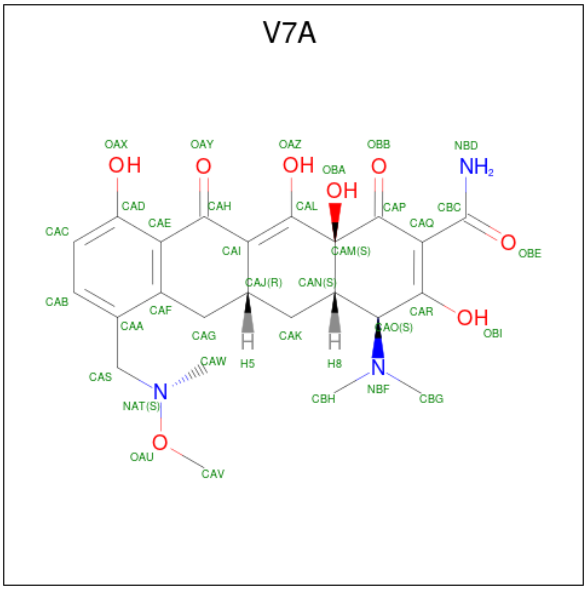
| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 56 | 15 | 1 | Total Zn<br>1 1 | 0 | 0 |
| 56 | 16 | 1 | Total Zn<br>1 1 | 0 | 0 |
| 56 | 19 | 1 | Total Zn<br>1 1 | 0 | 0 |
| 56 | 1n | 1 | Total Zn<br>1 1 | 0 | 0 |
| 56 | 2Y | 1 | Total Zn<br>1 1 | 0 | 0 |
| 56 | 24 | 1 | Total Zn<br>1 1 | 0 | 0 |
| 56 | 25 | 1 | Total Zn<br>1 1 | 0 | 0 |
| 56 | 26 | 1 | Total Zn<br>1 1 | 0 | 0 |
| 56 | 29 | 1 | Total Zn<br>1 1 | 0 | 0 |
| 56 | 2n | 1 | Total Zn<br>1 1 | 0 | 0 |

- Molecule 57 is Sarecycline (CCD ID: V7A) (formula: $C_{24}H_{29}N_3O_8$).




| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 57 | 1a | 1 | Total C N O<br>35 24 3 8 | 0 | 0 |

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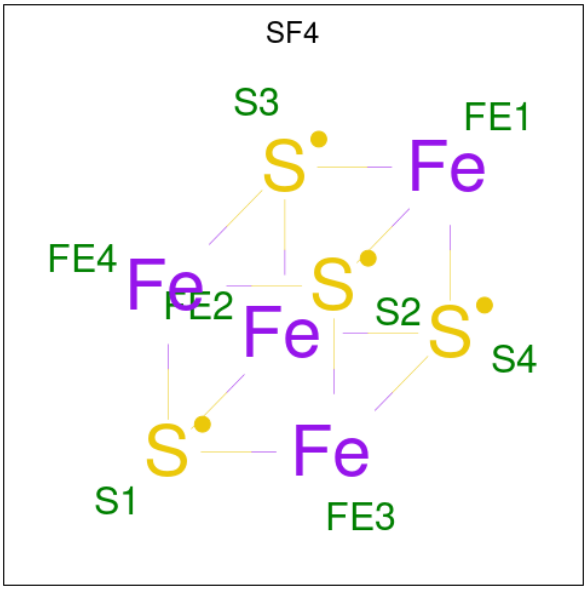
| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 57 | 2a | 1 | Total C N O<br>35 24 3 8 | 0 | 0 |

- Molecule 58 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: $Fe_4S_4$).




| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 58 | 1d | 1 | Total Fe S<br>8 4 4 | 0 | 0 |
| 58 | 2d | 1 | Total Fe S<br>8 4 4 | 0 | 0 |

- Molecule 59 is water.

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 59 | 1A | 1716 | Total O<br>1716 1716 | 0 | 0 |
| 59 | 1B | 47 | Total O<br>47 47 | 0 | 0 |
| 59 | 1D | 21 | Total O<br>21 21 | 0 | 0 |
| 59 | 1E | 25 | Total O<br>25 25 | 0 | 0 |
| 59 | 1F | 13 | Total O<br>13 13 | 0 | 0 |
| 59 | 1G | 2 | Total O<br>2 2 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 59 | 1H | 2 | Total O<br>2 2 | 0 | 0 |
| 59 | 1I | 2 | Total O<br>2 2 | 0 | 0 |
| 59 | 1N | 3 | Total O<br>3 3 | 0 | 0 |
| 59 | 1O | 7 | Total O<br>7 7 | 0 | 0 |
| 59 | 1P | 17 | Total O<br>17 17 | 0 | 0 |
| 59 | 1Q | 6 | Total O<br>6 6 | 0 | 0 |
| 59 | 1R | 9 | Total O<br>9 9 | 0 | 0 |
| 59 | 1S | 1 | Total O<br>1 1 | 0 | 0 |
| 59 | 1T | 8 | Total O<br>8 8 | 0 | 0 |
| 59 | 1U | 13 | Total O<br>13 13 | 0 | 0 |
| 59 | 1V | 9 | Total O<br>9 9 | 0 | 0 |
| 59 | 1W | 8 | Total O<br>8 8 | 0 | 0 |
| 59 | 1X | 6 | Total O<br>6 6 | 0 | 0 |
| 59 | 1Y | 2 | Total O<br>2 2 | 0 | 0 |
| 59 | 10 | 8 | Total O<br>8 8 | 0 | 0 |
| 59 | 11 | 7 | Total O<br>7 7 | 0 | 0 |
| 59 | 12 | 1 | Total O<br>1 1 | 0 | 0 |
| 59 | 13 | 4 | Total O<br>4 4 | 0 | 0 |
| 59 | 15 | 7 | Total O<br>7 7 | 0 | 0 |
| 59 | 16 | 2 | Total O<br>2 2 | 0 | 0 |
| 59 | 17 | 6 | Total O<br>6 6 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 59 | 18 | 9 | Total O<br>9 9 | 0 | 0 |
| 59 | 1a | 294 | Total O<br>294 294 | 0 | 0 |
| 59 | 1b | 1 | Total O<br>1 1 | 0 | 0 |
| 59 | 1d | 3 | Total O<br>3 3 | 0 | 0 |
| 59 | 1e | 1 | Total O<br>1 1 | 0 | 0 |
| 59 | 1i | 1 | Total O<br>1 1 | 0 | 0 |
| 59 | 1j | 1 | Total O<br>1 1 | 0 | 0 |
| 59 | 1l | 4 | Total O<br>4 4 | 0 | 0 |
| 59 | 1m | 1 | Total O<br>1 1 | 0 | 0 |
| 59 | 1o | 1 | Total O<br>1 1 | 0 | 0 |
| 59 | 1q | 2 | Total O<br>2 2 | 0 | 0 |
| 59 | 1v | 4 | Total O<br>4 4 | 0 | 0 |
| 59 | 1x | 17 | Total O<br>17 17 | 0 | 0 |
| 59 | 2A | 867 | Total O<br>867 867 | 0 | 0 |
| 59 | 2B | 14 | Total O<br>14 14 | 0 | 0 |
| 59 | 2D | 16 | Total O<br>16 16 | 0 | 0 |
| 59 | 2E | 8 | Total O<br>8 8 | 0 | 0 |
| 59 | 2F | 13 | Total O<br>13 13 | 0 | 0 |
| 59 | 2I | 1 | Total O<br>1 1 | 0 | 0 |
| 59 | 2N | 1 | Total O<br>1 1 | 0 | 0 |
| 59 | 2O | 1 | Total O<br>1 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 59 | 2P | 4 | Total O<br>4 4 | 0 | 0 |
| 59 | 2Q | 2 | Total O<br>2 2 | 0 | 0 |
| 59 | 2R | 2 | Total O<br>2 2 | 0 | 0 |
| 59 | 2T | 4 | Total O<br>4 4 | 0 | 0 |
| 59 | 2U | 3 | Total O<br>3 3 | 0 | 0 |
| 59 | 2W | 5 | Total O<br>5 5 | 0 | 0 |
| 59 | 2X | 2 | Total O<br>2 2 | 0 | 0 |
| 59 | 2Z | 1 | Total O<br>1 1 | 0 | 0 |
| 59 | 20 | 3 | Total O<br>3 3 | 0 | 0 |
| 59 | 21 | 8 | Total O<br>8 8 | 0 | 0 |
| 59 | 22 | 1 | Total O<br>1 1 | 0 | 0 |
| 59 | 25 | 1 | Total O<br>1 1 | 0 | 0 |
| 59 | 27 | 1 | Total O<br>1 1 | 0 | 0 |
| 59 | 28 | 3 | Total O<br>3 3 | 0 | 0 |
| 59 | 29 | 1 | Total O<br>1 1 | 0 | 0 |
| 59 | 2a | 146 | Total O<br>146 146 | 0 | 0 |
| 59 | 2g | 1 | Total O<br>1 1 | 0 | 0 |
| 59 | 2j | 2 | Total O<br>2 2 | 0 | 0 |
| 59 | 2l | 4 | Total O<br>4 4 | 0 | 0 |
| 59 | 2p | 1 | Total O<br>1 1 | 0 | 0 |
| 59 | 2r | 1 | Total O<br>1 1 | 0 | 0 |

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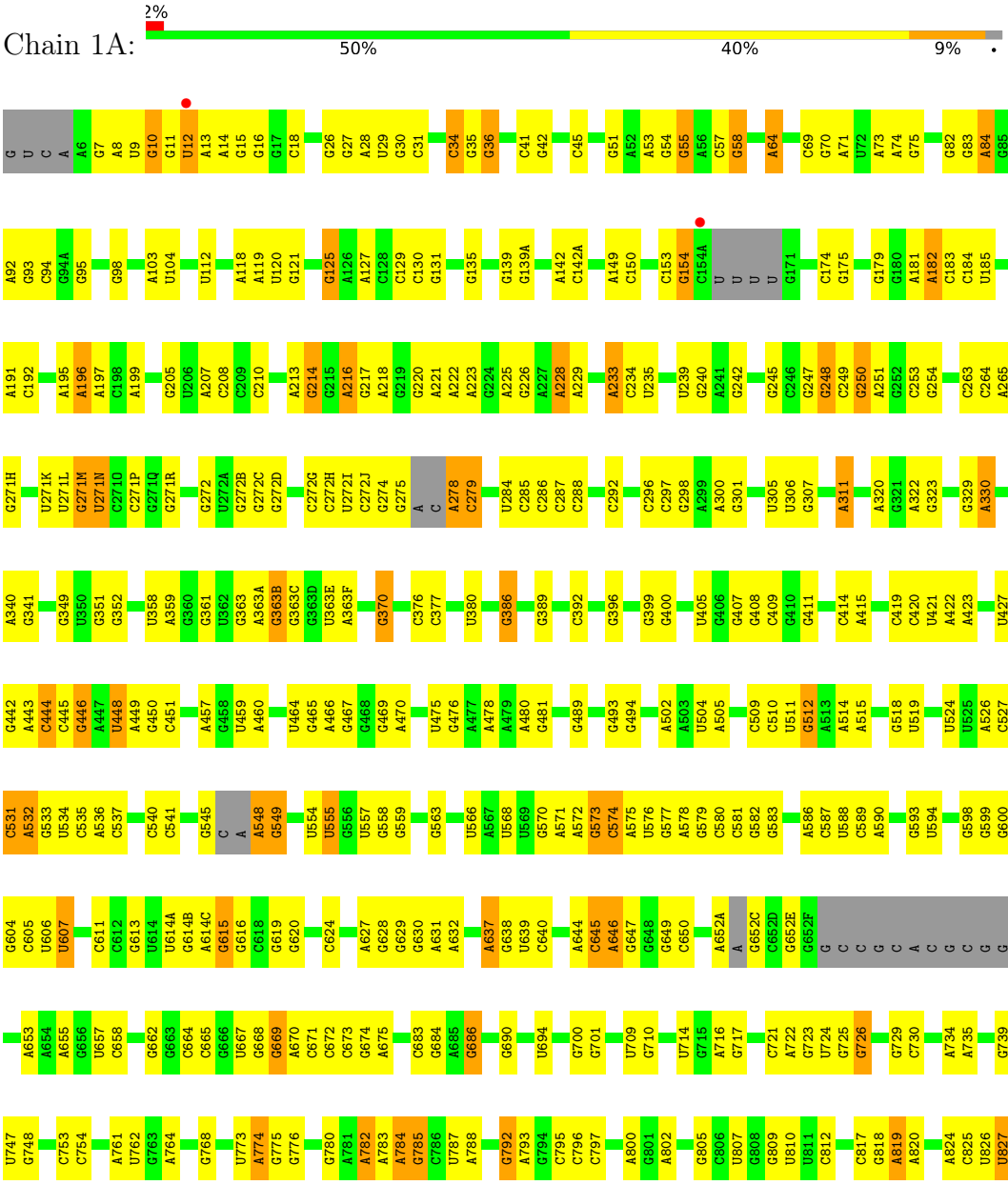
| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 59 | 2t | 1 | Total O<br>1 1 | 0 | 0 |
| 59 | 2v | 1 | Total O<br>1 1 | 0 | 0 |
| 59 | 2x | 6 | Total O<br>6 6 | 0 | 0 |

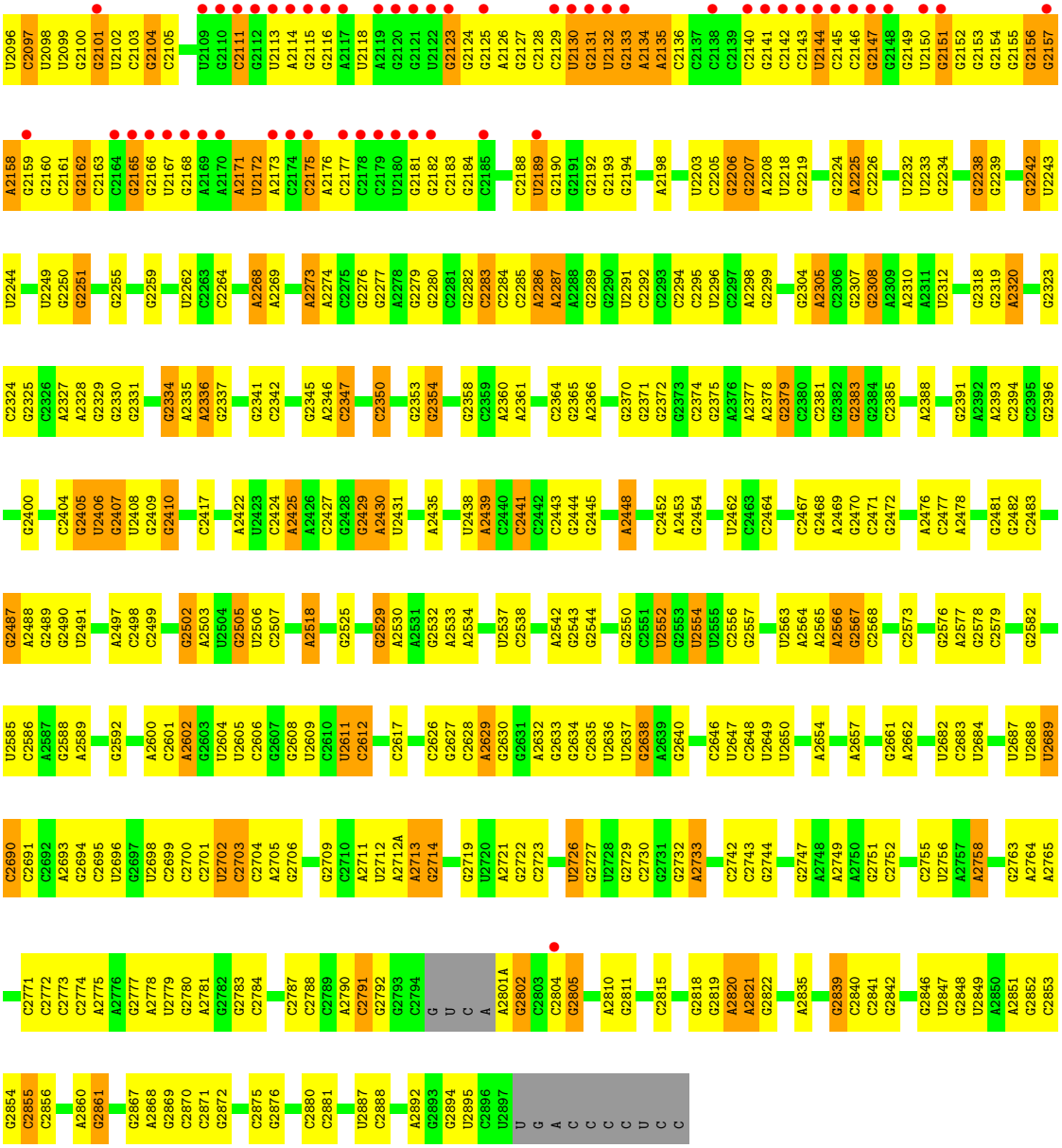
# 3 Residue-property plots (i)

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

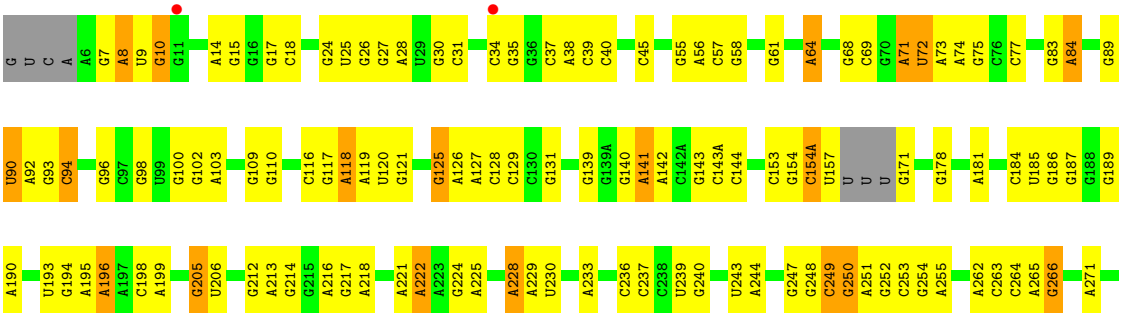
Chain 1A:

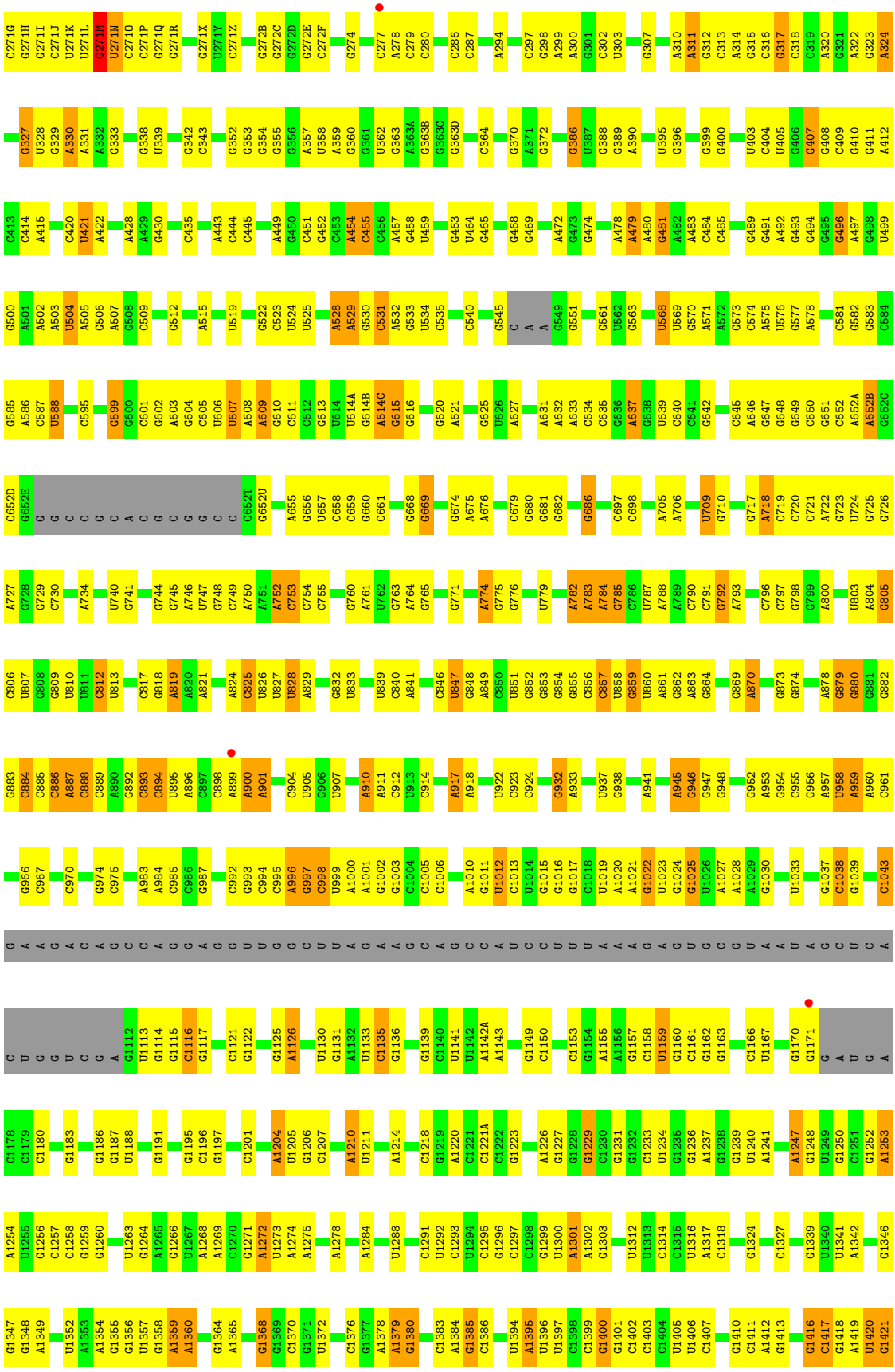


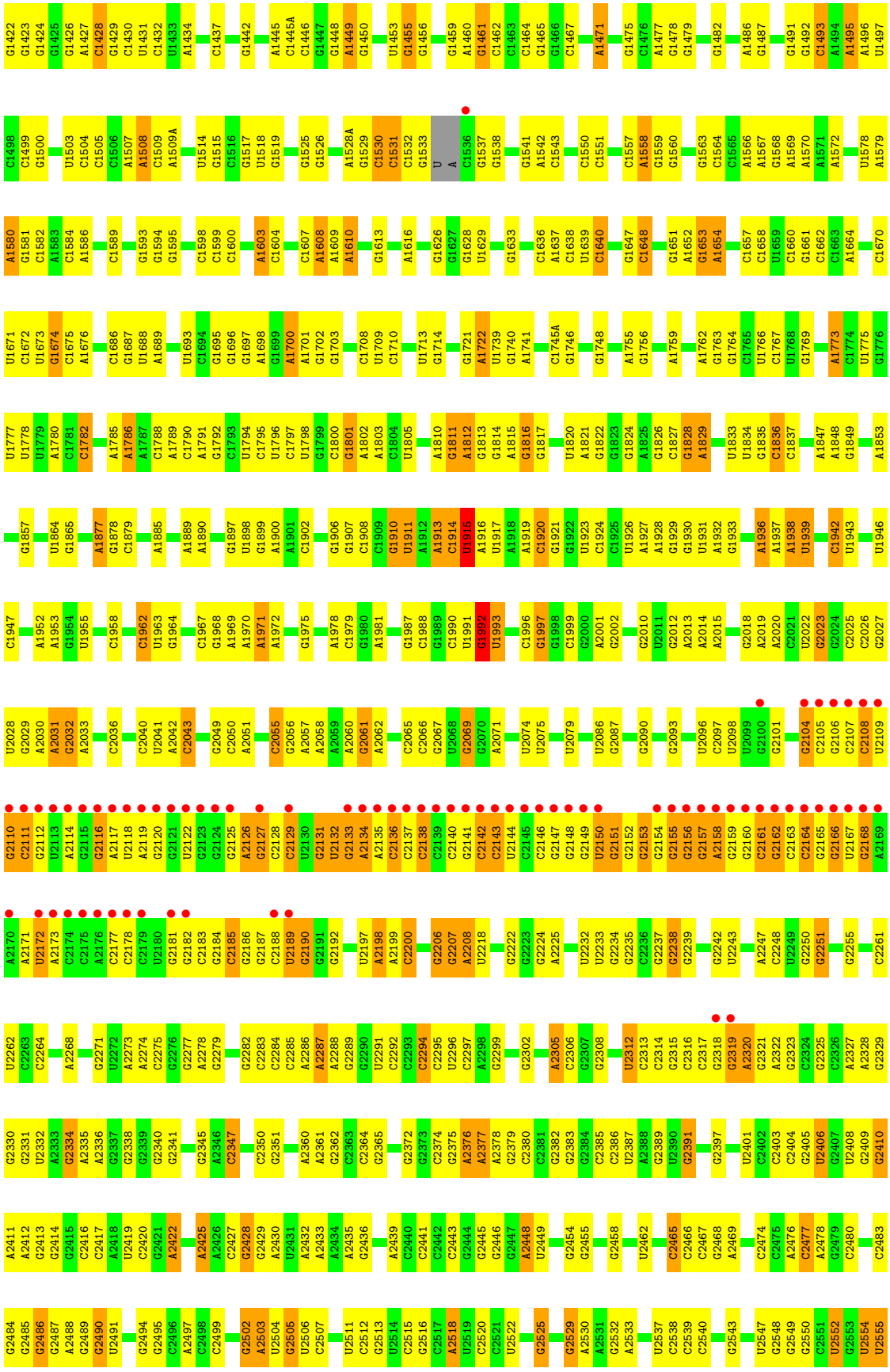


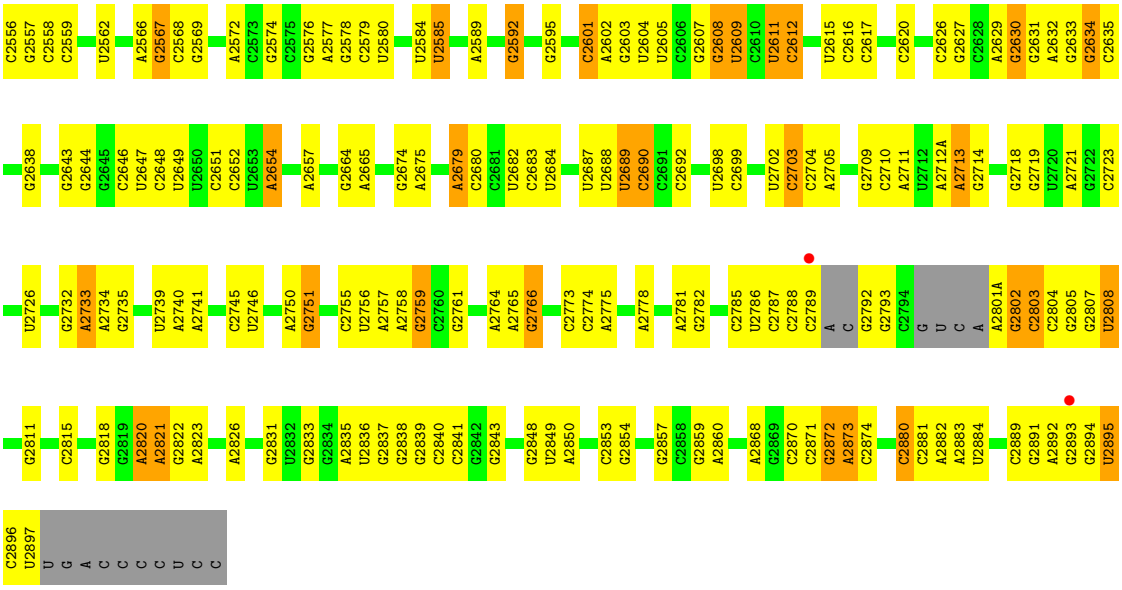
• Molecule 1: 23S Ribosomal RNA

Chain 2A:



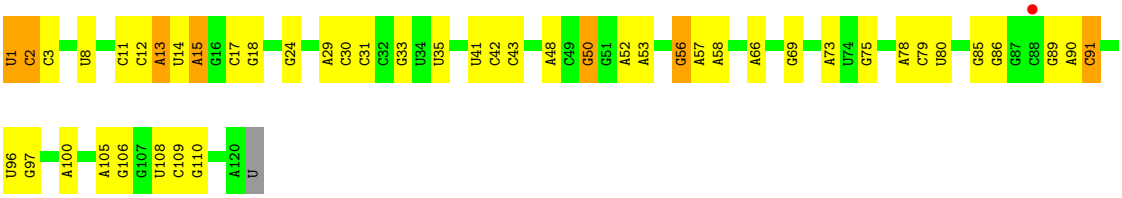






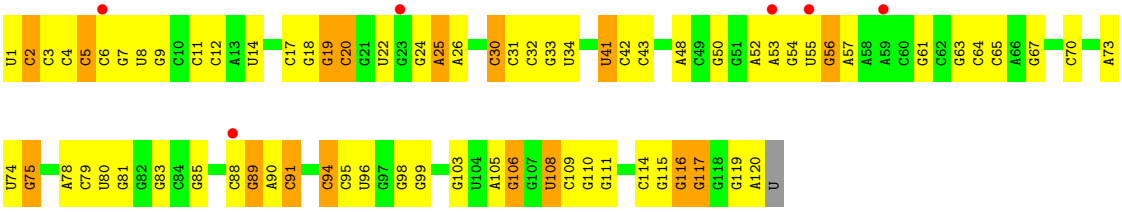
• Molecule 2: 5S Ribosomal RNA

Chain 1B:



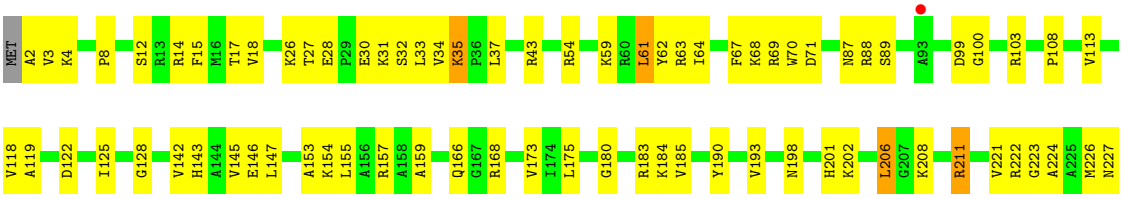
• Molecule 2: 5S Ribosomal RNA

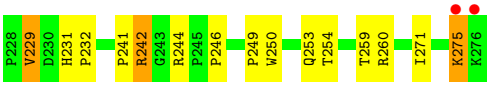
Chain 2B:



• Molecule 3: 50S ribosomal protein L2

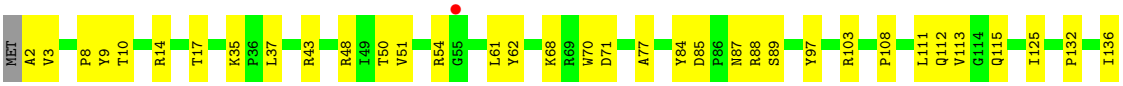
Chain 1D:

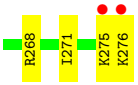





• Molecule 3: 50S ribosomal protein L2

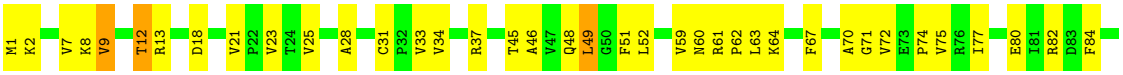
Chain 2D:

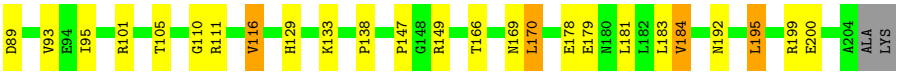





• Molecule 4: 50S ribosomal protein L3

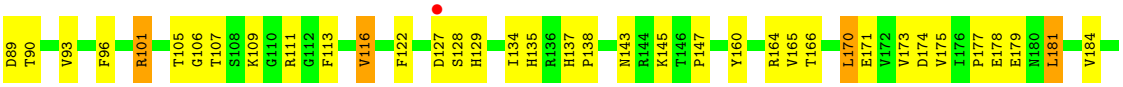
Chain 1E:

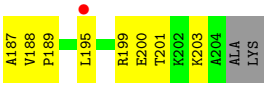



• Molecule 4: 50S ribosomal protein L3

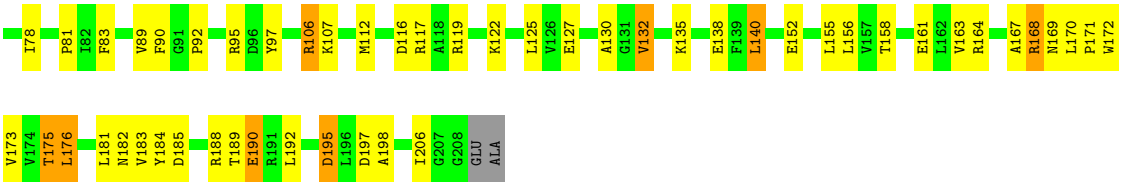
Chain 2E:



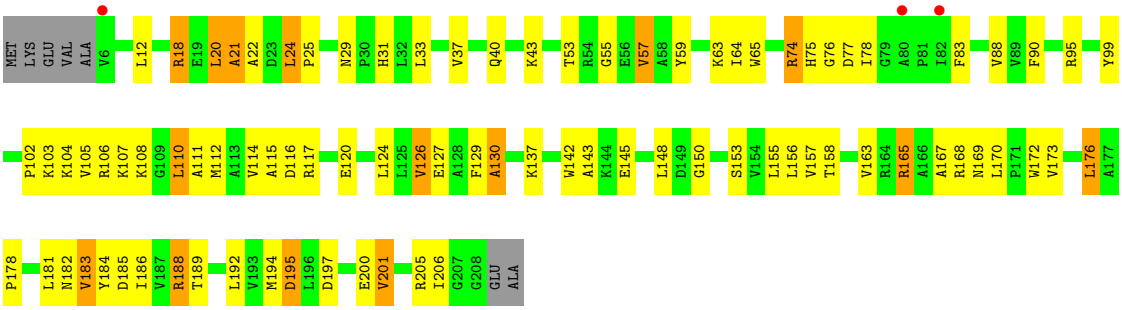

• Molecule 5: 50S ribosomal protein L4

Chain 1F:



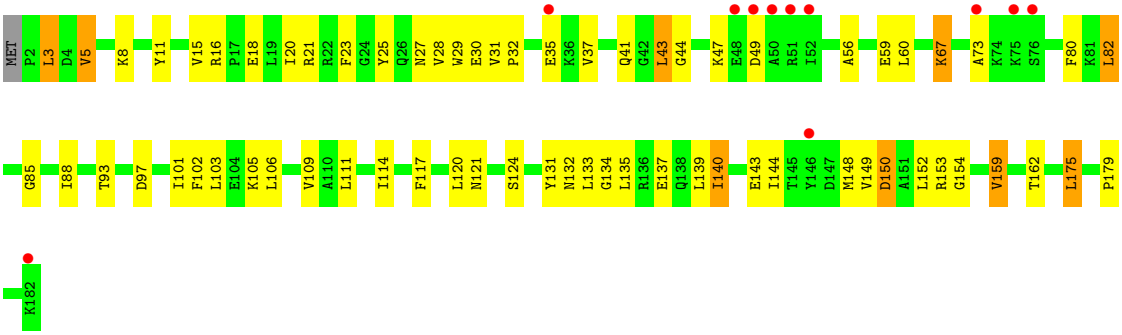
• Molecule 5: 50S ribosomal protein L4

Chain 2F:



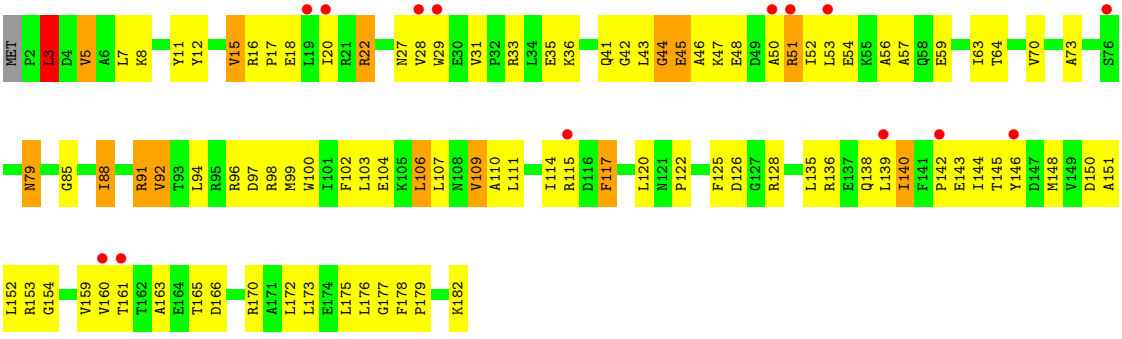
• Molecule 6: 50S ribosomal protein L5

Chain 1G:



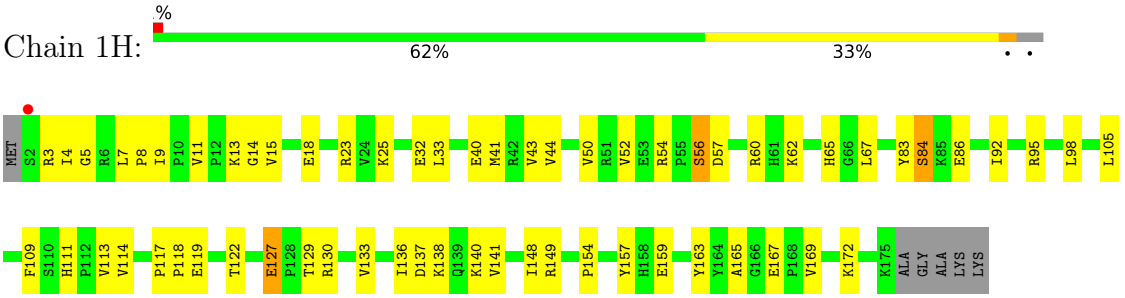
• Molecule 6: 50S ribosomal protein L5

Chain 2G:



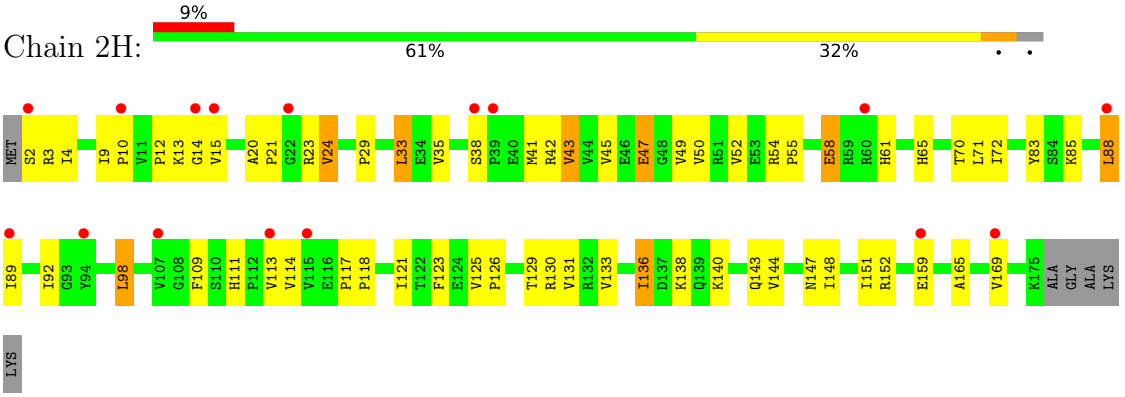
• Molecule 7: 50S ribosomal protein L6

Chain 1H:



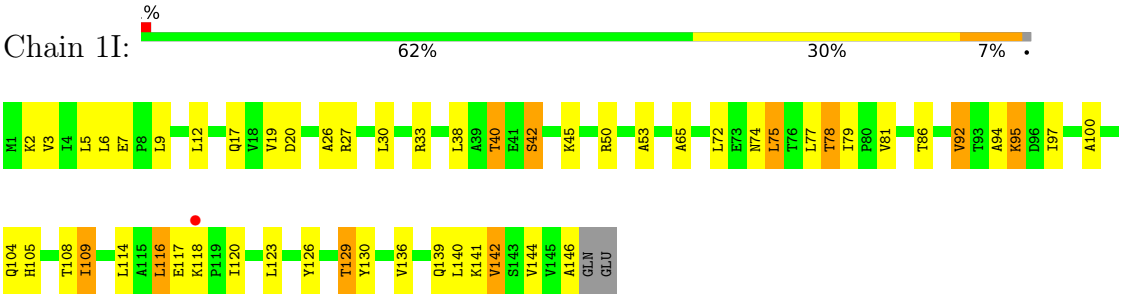

• Molecule 7: 50S ribosomal protein L6

Chain 2H:



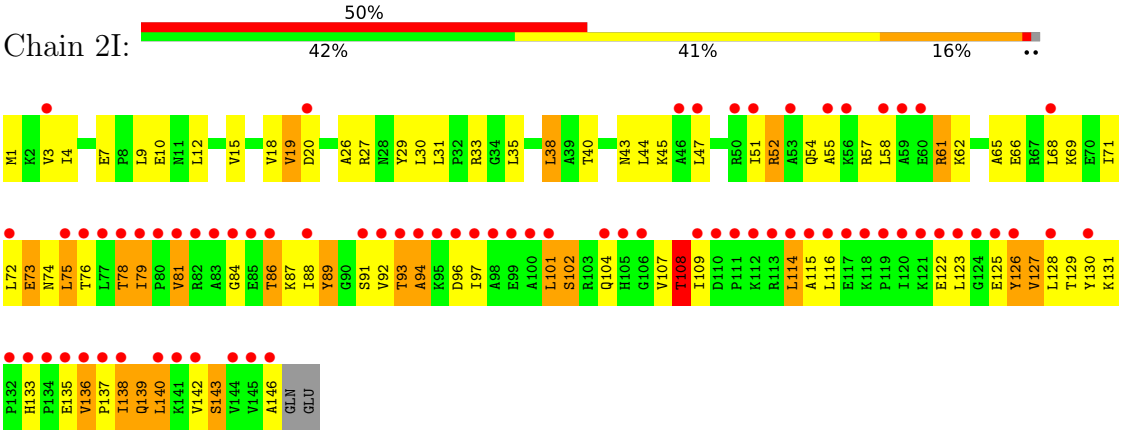

• Molecule 8: 50S ribosomal protein L9

Chain 1I:



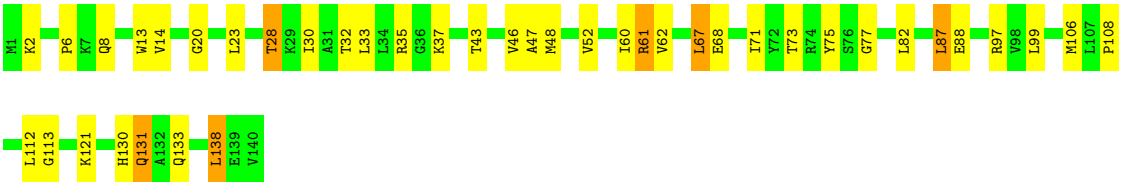

• Molecule 8: 50S ribosomal protein L9

Chain 2I:

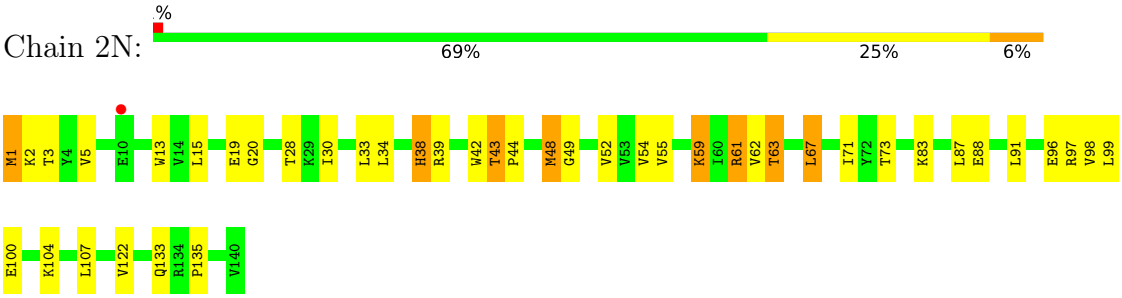



• Molecule 9: 50S ribosomal protein L13

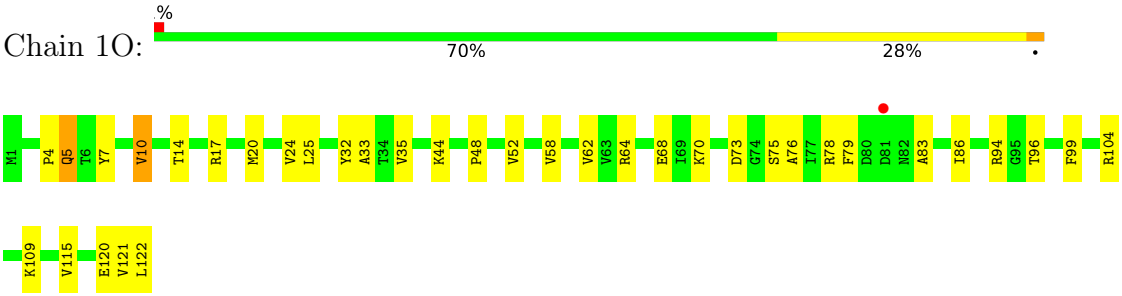
Chain 1N:



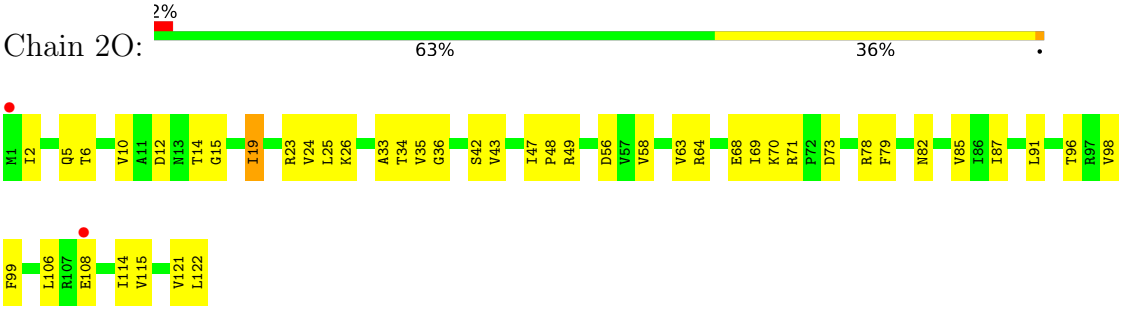

• Molecule 9: 50S ribosomal protein L13



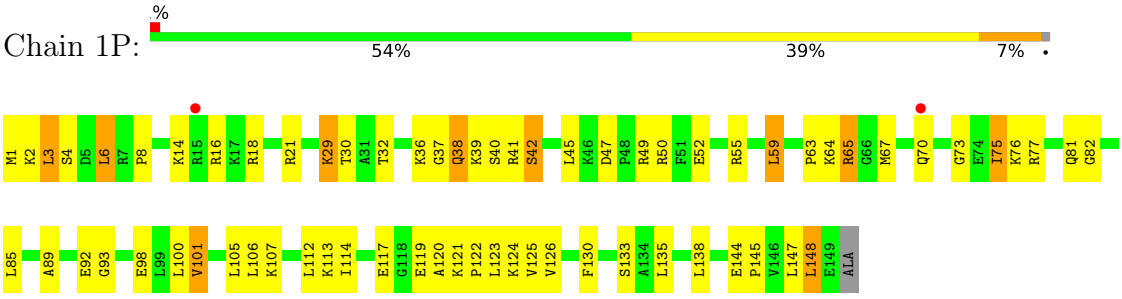

• Molecule 10: 50S ribosomal protein L14




• Molecule 10: 50S ribosomal protein L14

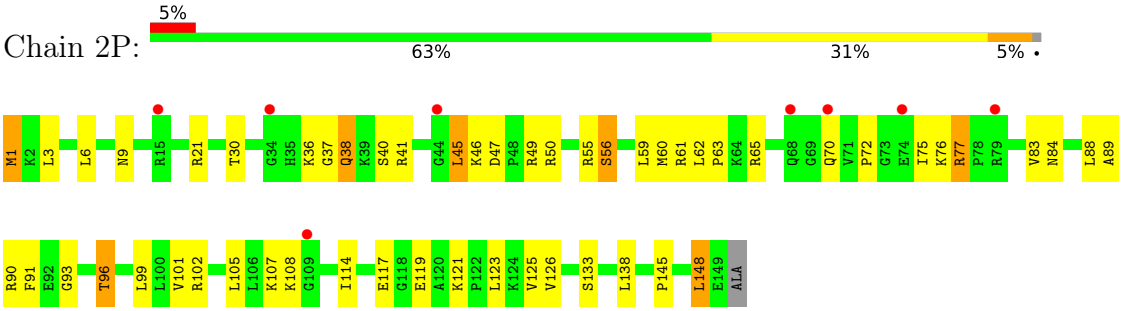



• Molecule 11: 50S ribosomal protein L15



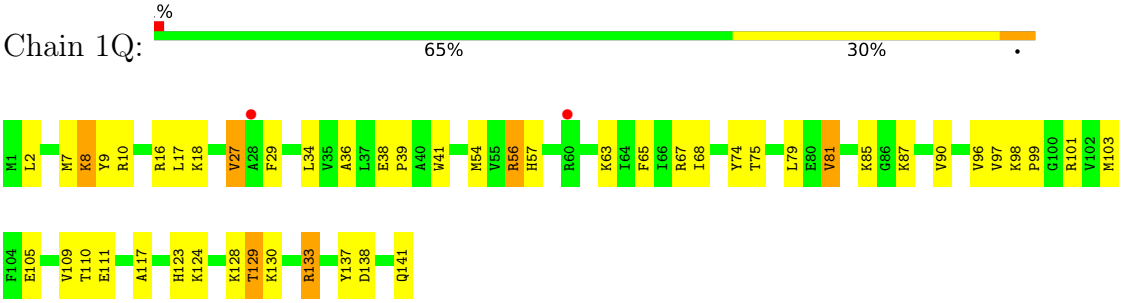

• Molecule 11: 50S ribosomal protein L15

Chain 2P:



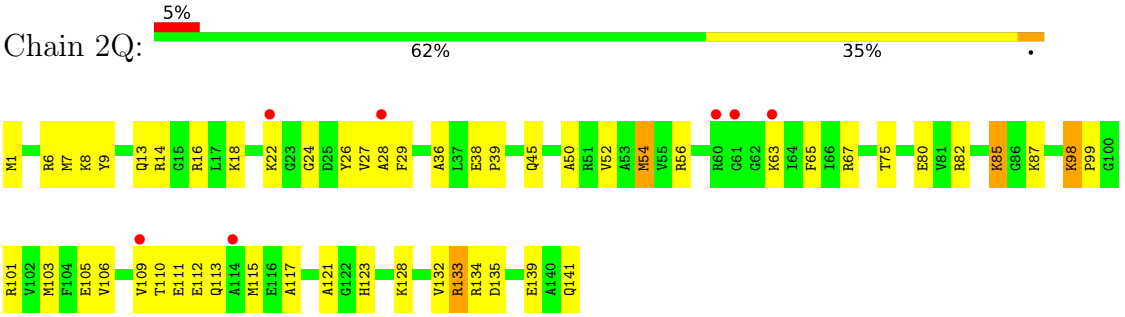

• Molecule 12: 50S ribosomal protein L16

Chain 1Q:



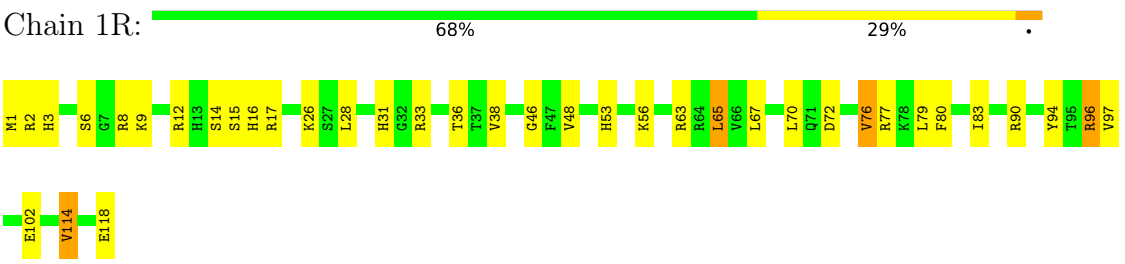

• Molecule 12: 50S ribosomal protein L16

Chain 2Q:



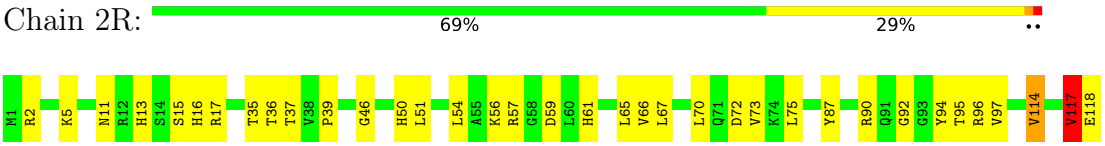

• Molecule 13: 50S ribosomal protein L17

Chain 1R:



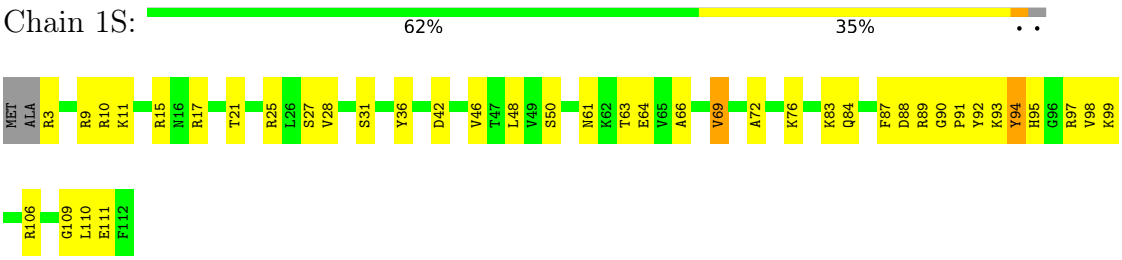

• Molecule 13: 50S ribosomal protein L17

Chain 2R:



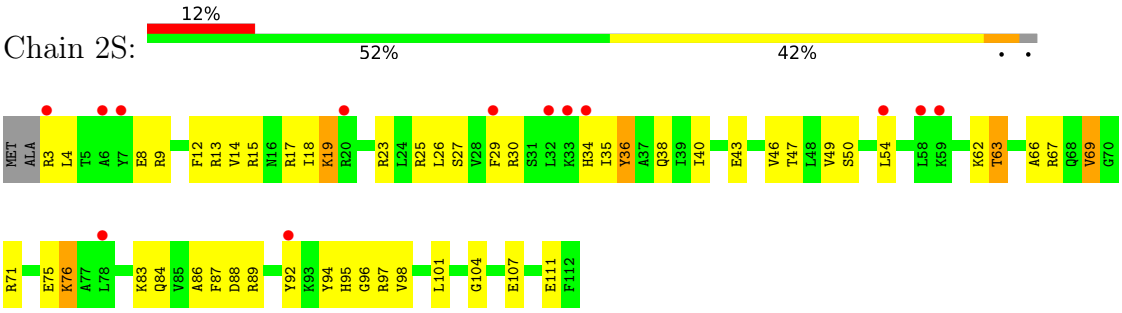

• Molecule 14: 50S ribosomal protein L18

Chain 1S:



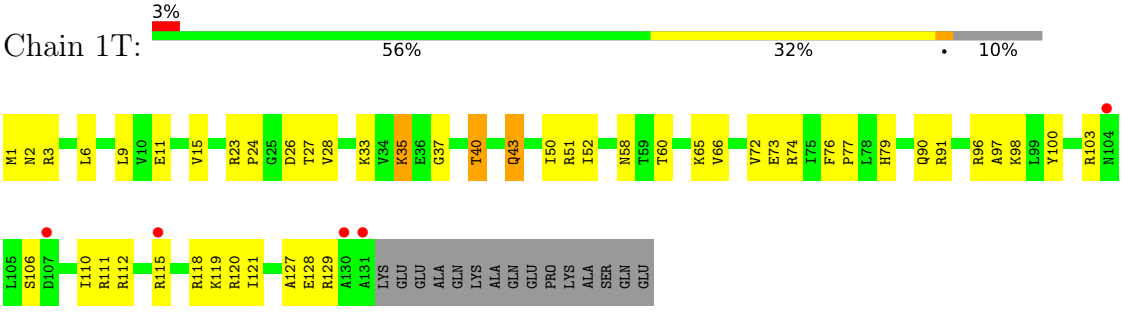

• Molecule 14: 50S ribosomal protein L18

Chain 2S:



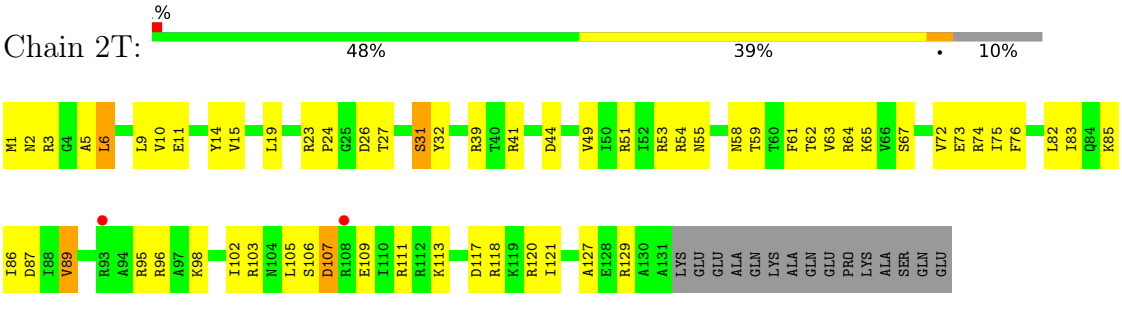

• Molecule 15: 50S ribosomal protein L19

Chain 1T:



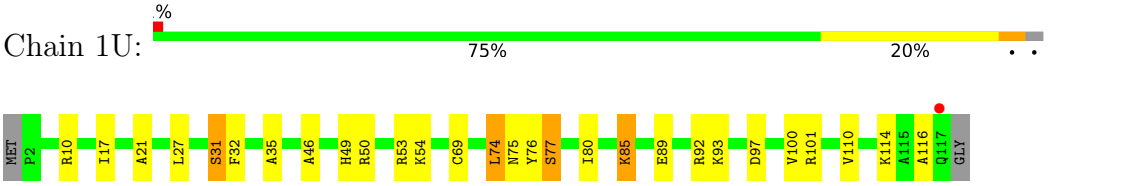

• Molecule 15: 50S ribosomal protein L19

Chain 2T:



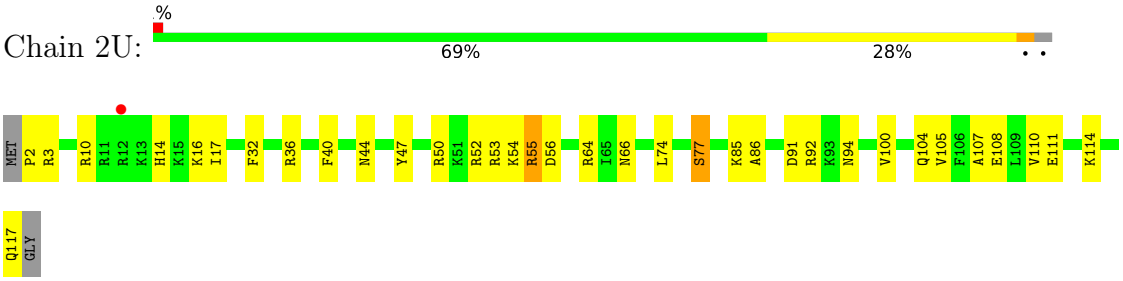

• Molecule 16: 50S ribosomal protein L20

Chain 1U:



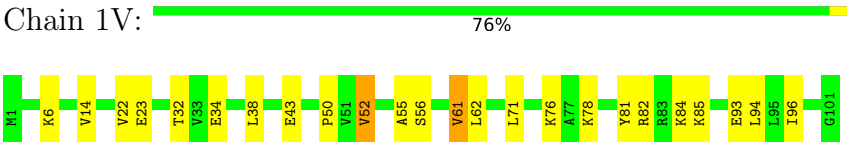

• Molecule 16: 50S ribosomal protein L20

Chain 2U:



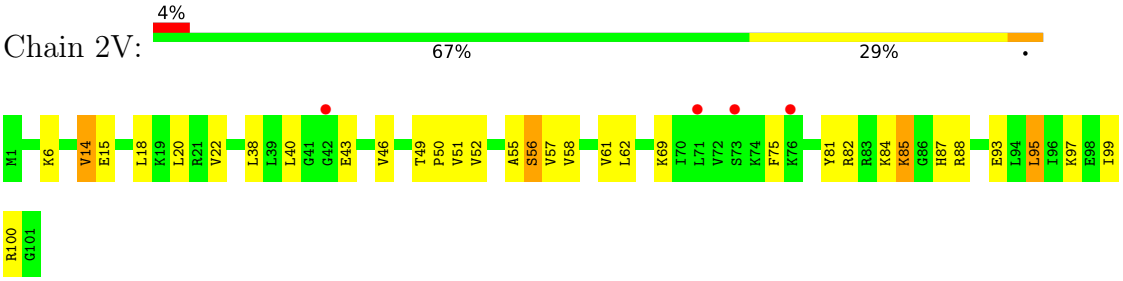

• Molecule 17: 50S ribosomal protein L21

Chain 1V:



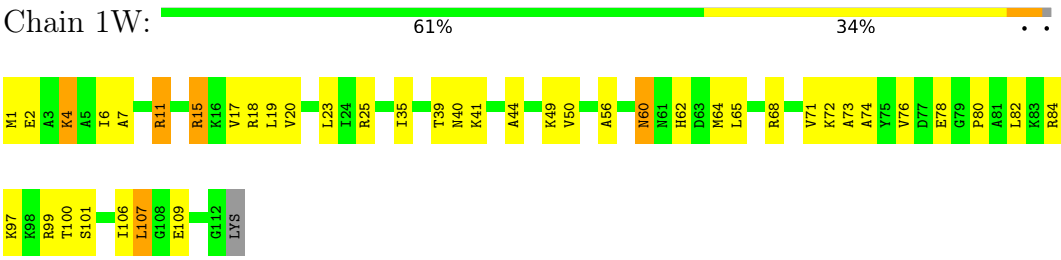

• Molecule 17: 50S ribosomal protein L21

Chain 2V:



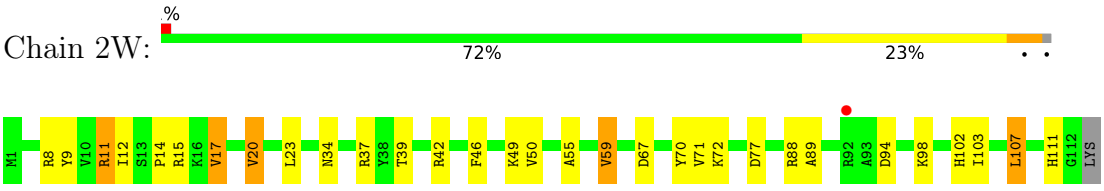

• Molecule 18: 50S ribosomal protein L22

Chain 1W:



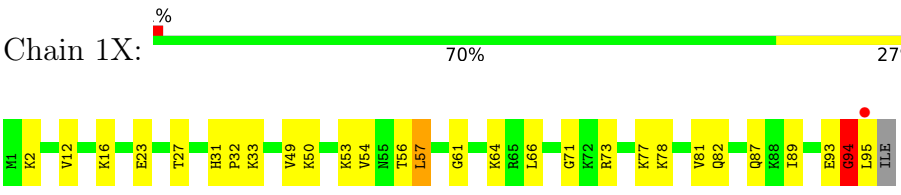

• Molecule 18: 50S ribosomal protein L22

Chain 2W:



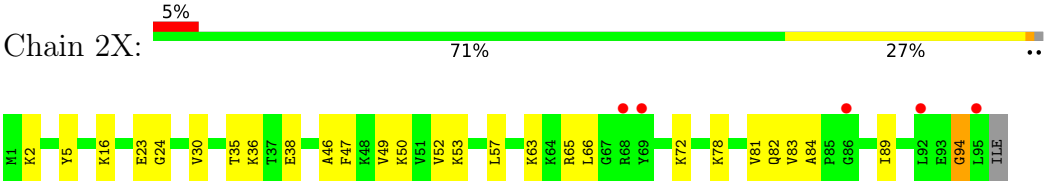

• Molecule 19: 50S ribosomal protein L23

Chain 1X:



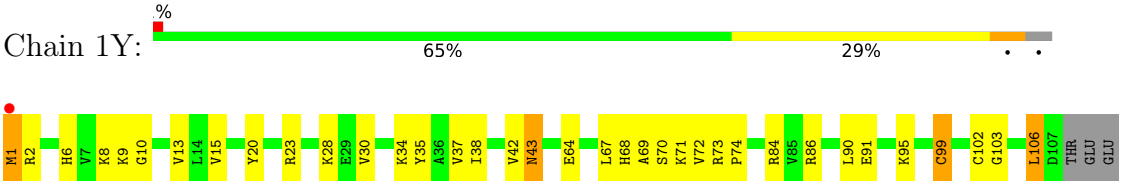
• Molecule 19: 50S ribosomal protein L23

Chain 2X:



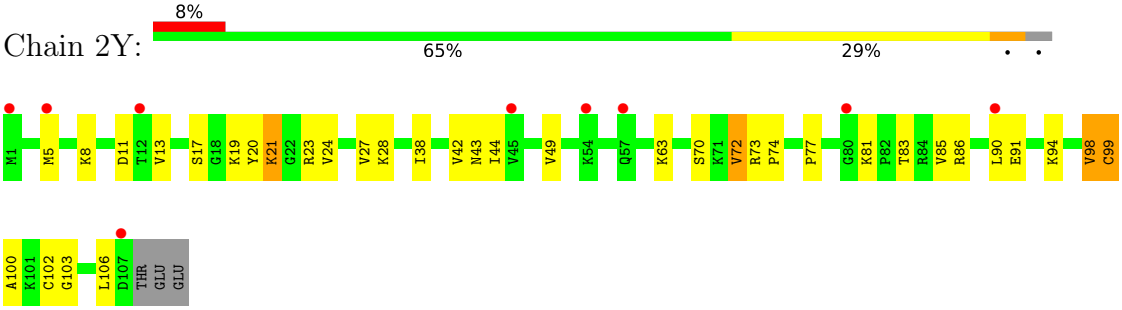

• Molecule 20: 50S ribosomal protein L24

Chain 1Y:



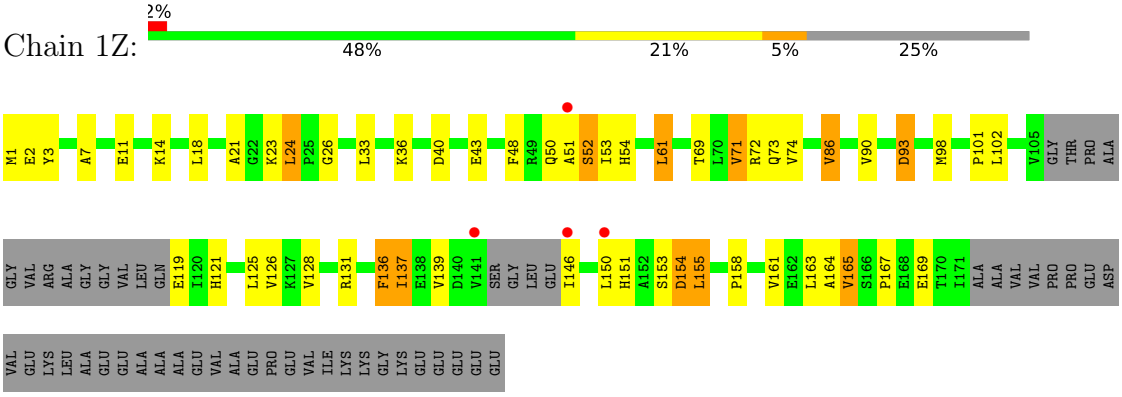

• Molecule 20: 50S ribosomal protein L24

Chain 2Y:



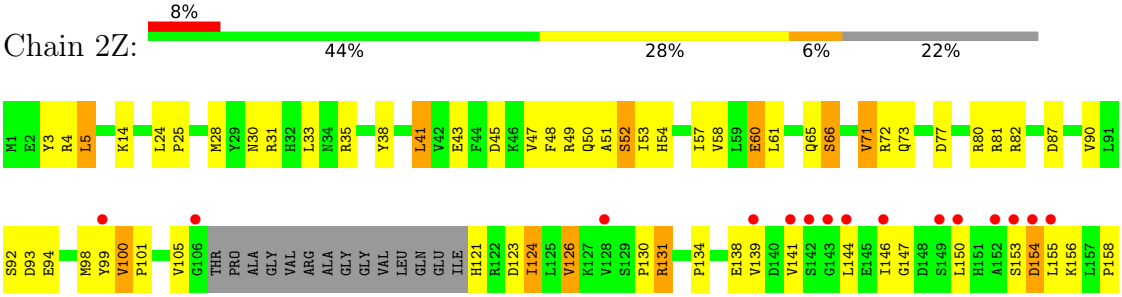

• Molecule 21: 50S ribosomal protein L25

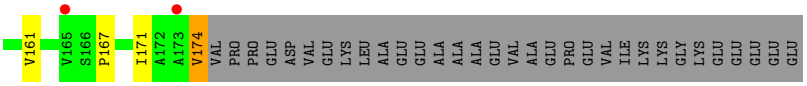
Chain 1Z:



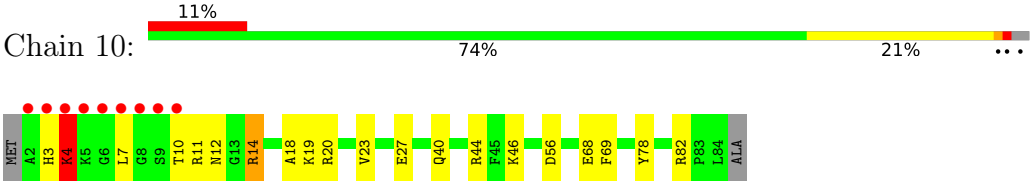

• Molecule 21: 50S ribosomal protein L25

Chain 2Z:

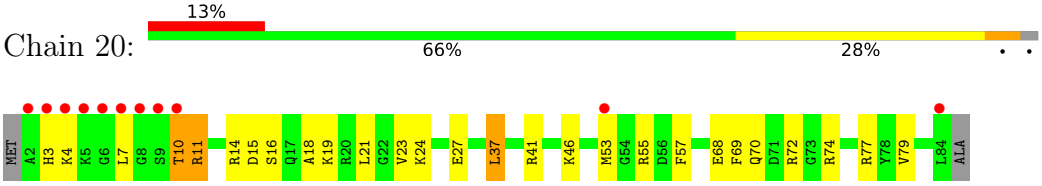




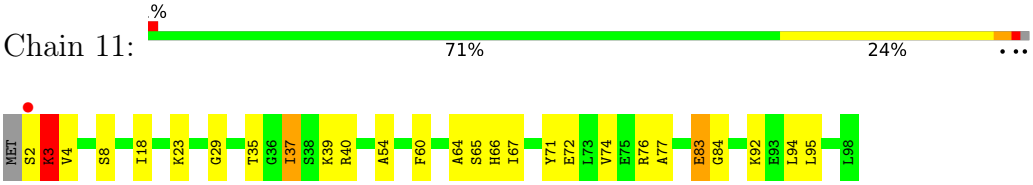

• Molecule 22: 50S ribosomal protein L27



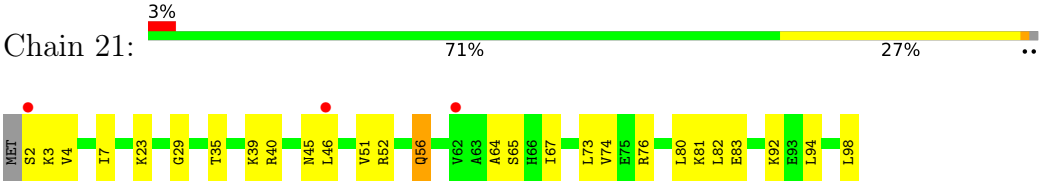

• Molecule 22: 50S ribosomal protein L27



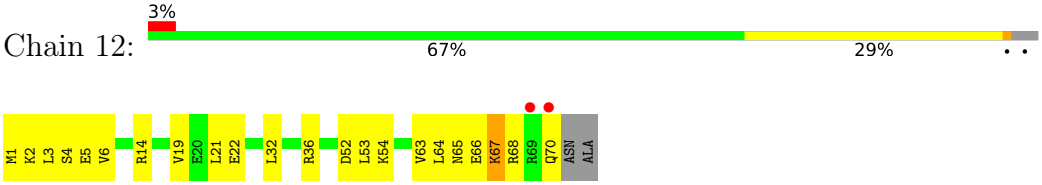

• Molecule 23: 50S ribosomal protein L28



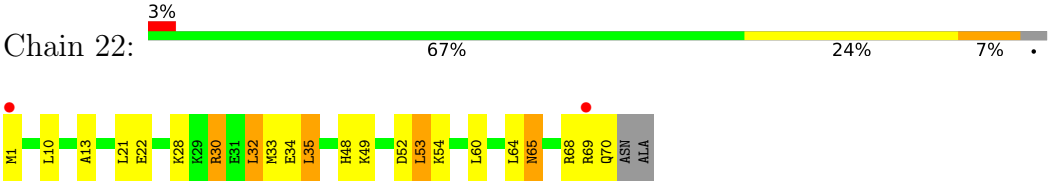

• Molecule 23: 50S ribosomal protein L28




• Molecule 24: 50S ribosomal protein L29

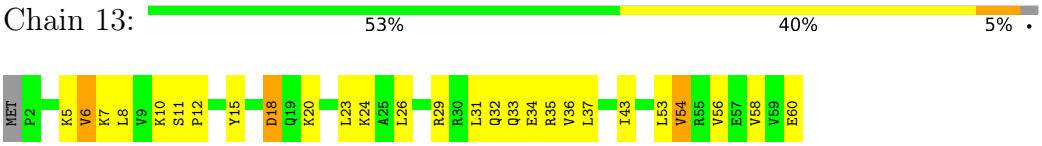



• Molecule 24: 50S ribosomal protein L29



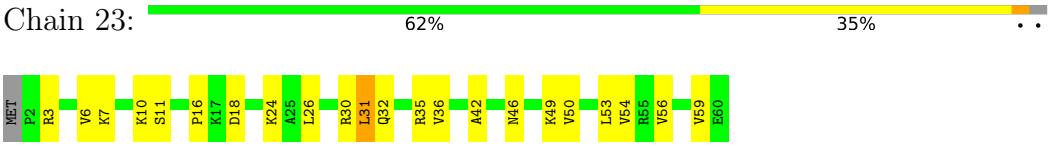

• Molecule 25: 50S ribosomal protein L30

Chain 13:



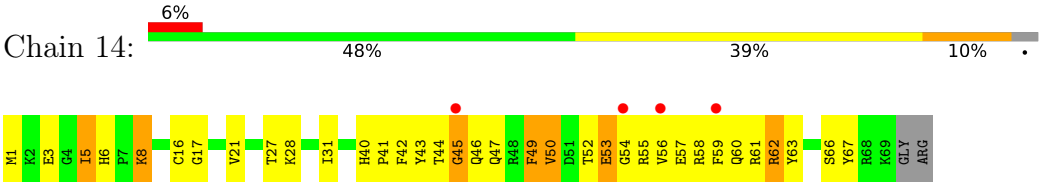

• Molecule 25: 50S ribosomal protein L30

Chain 23:



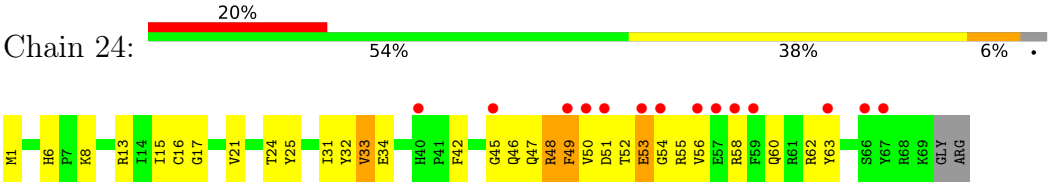

• Molecule 26: 50S ribosomal protein L31

Chain 14:



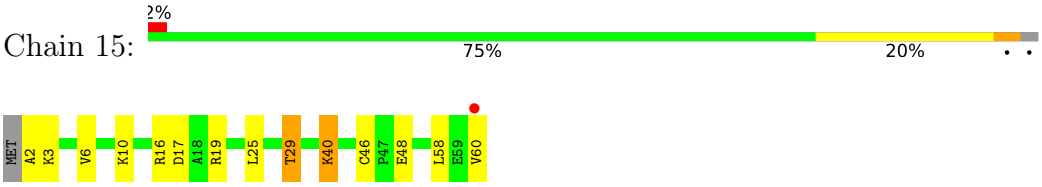

• Molecule 26: 50S ribosomal protein L31

Chain 24:



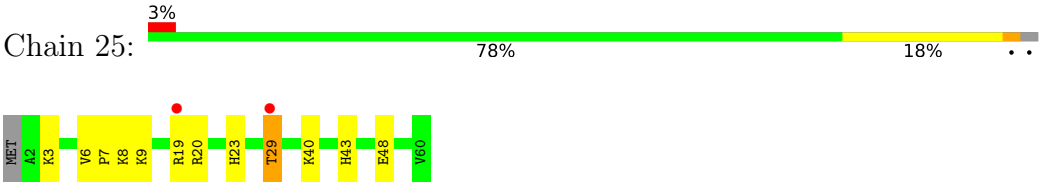

• Molecule 27: 50S ribosomal protein L32

Chain 15:



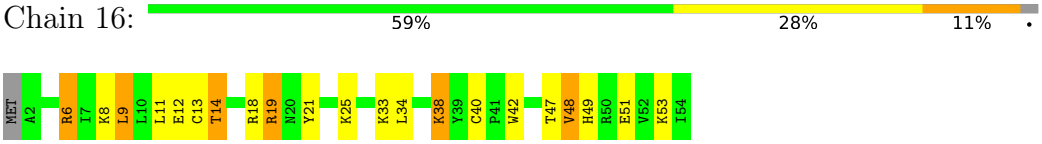

• Molecule 27: 50S ribosomal protein L32

Chain 25:



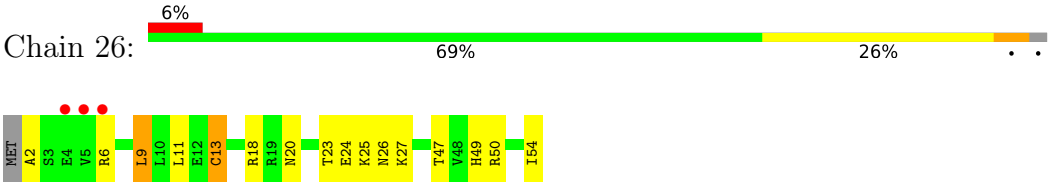

• Molecule 28: 50S ribosomal protein L33

Chain 16:



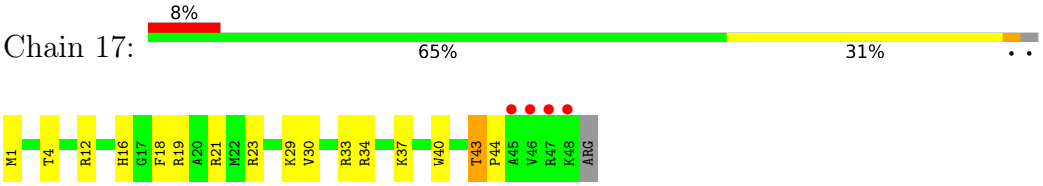

• Molecule 28: 50S ribosomal protein L33

Chain 26:



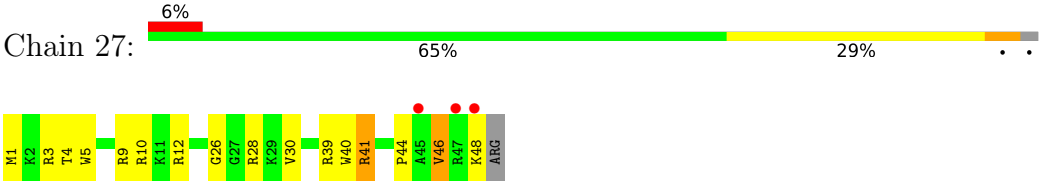

• Molecule 29: 50S ribosomal protein L34

Chain 17:



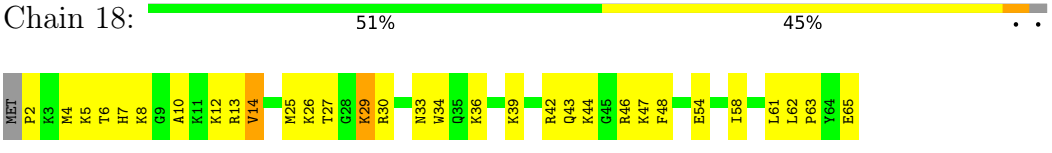

• Molecule 29: 50S ribosomal protein L34

Chain 27:



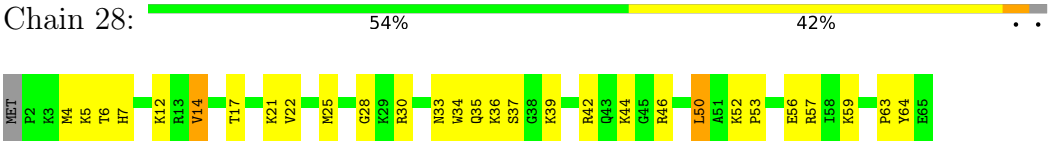

• Molecule 30: 50S ribosomal protein L35

Chain 18:



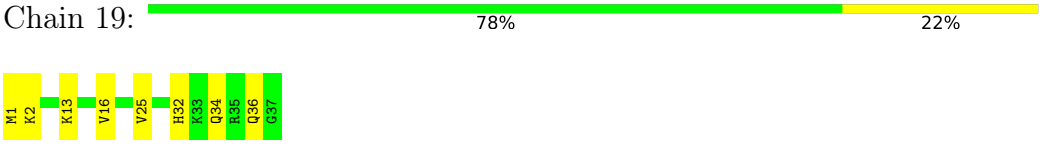

• Molecule 30: 50S ribosomal protein L35

Chain 28:



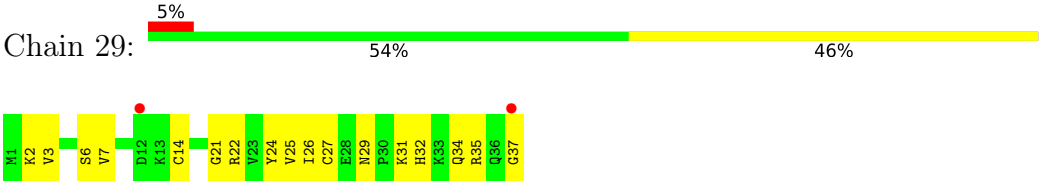

• Molecule 31: 50S ribosomal protein L36

Chain 19:



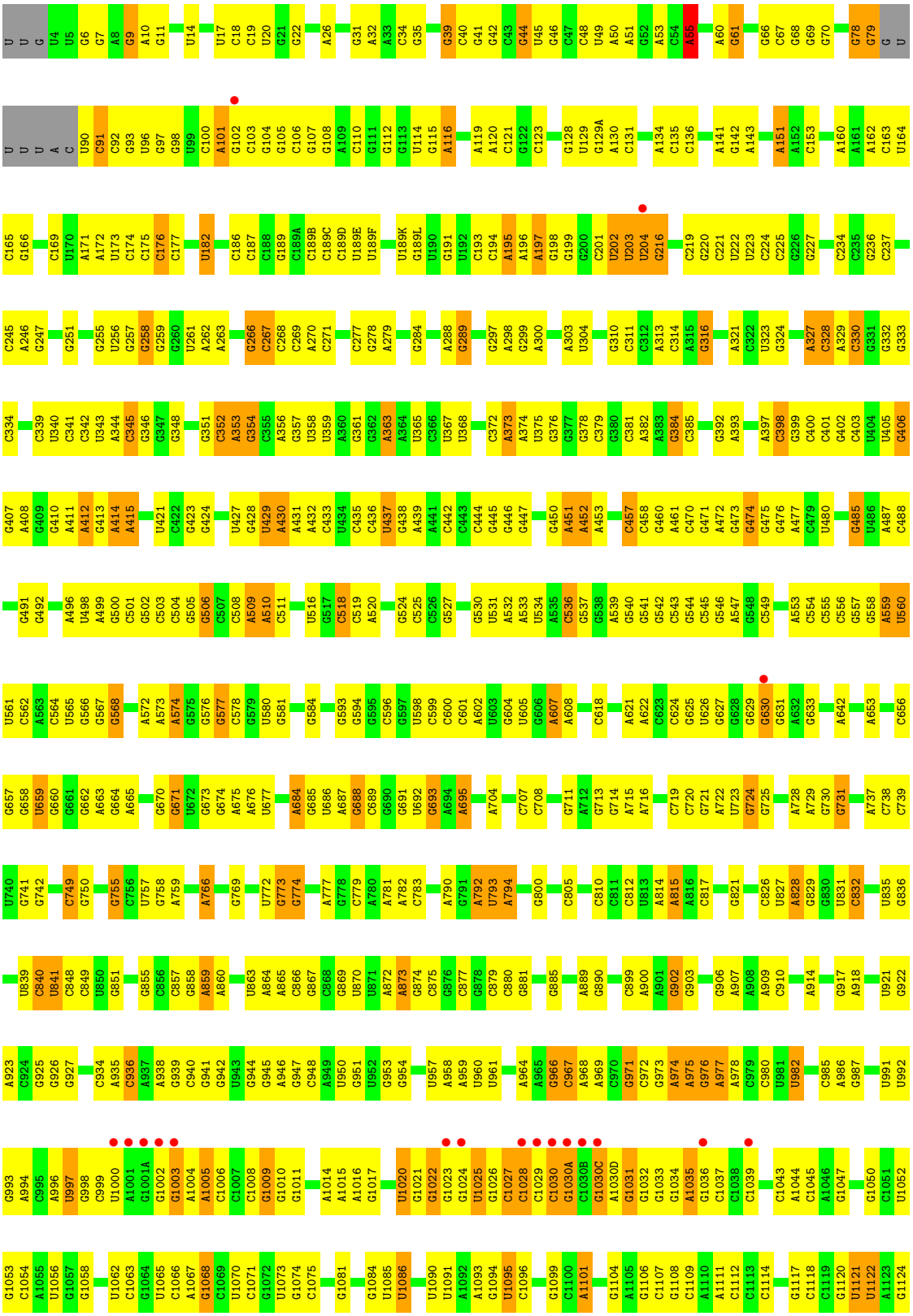

• Molecule 31: 50S ribosomal protein L36

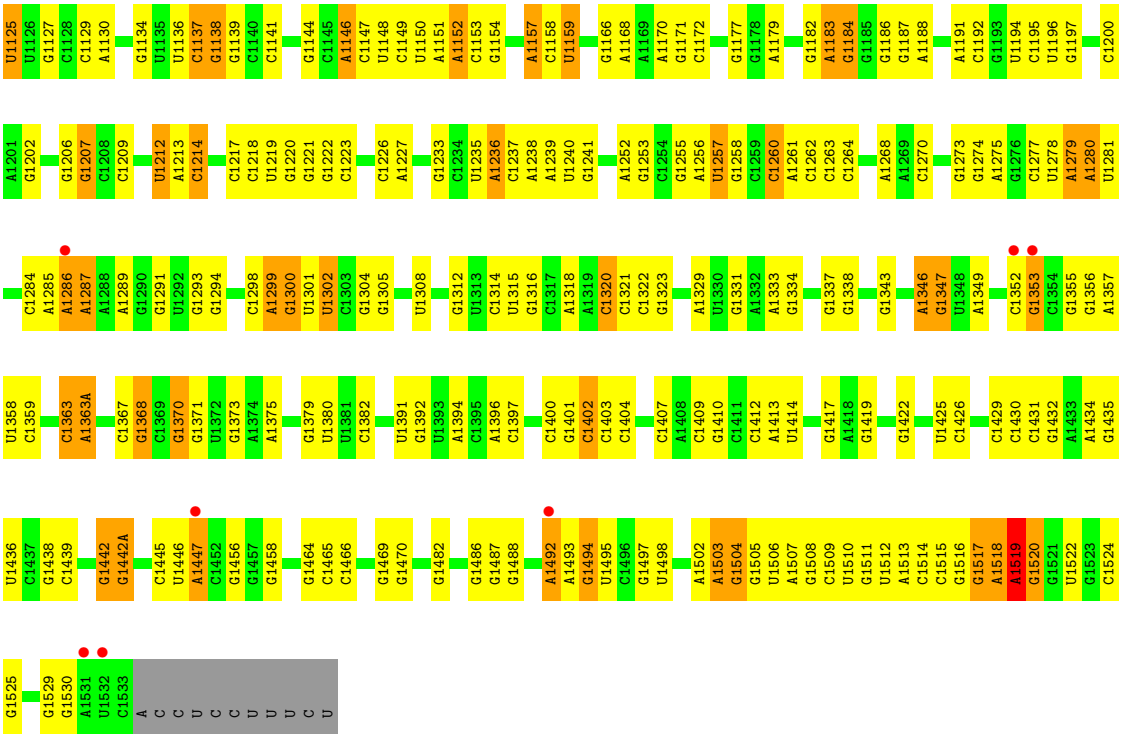
Chain 29:




• Molecule 32: 16S Ribosomal RNA

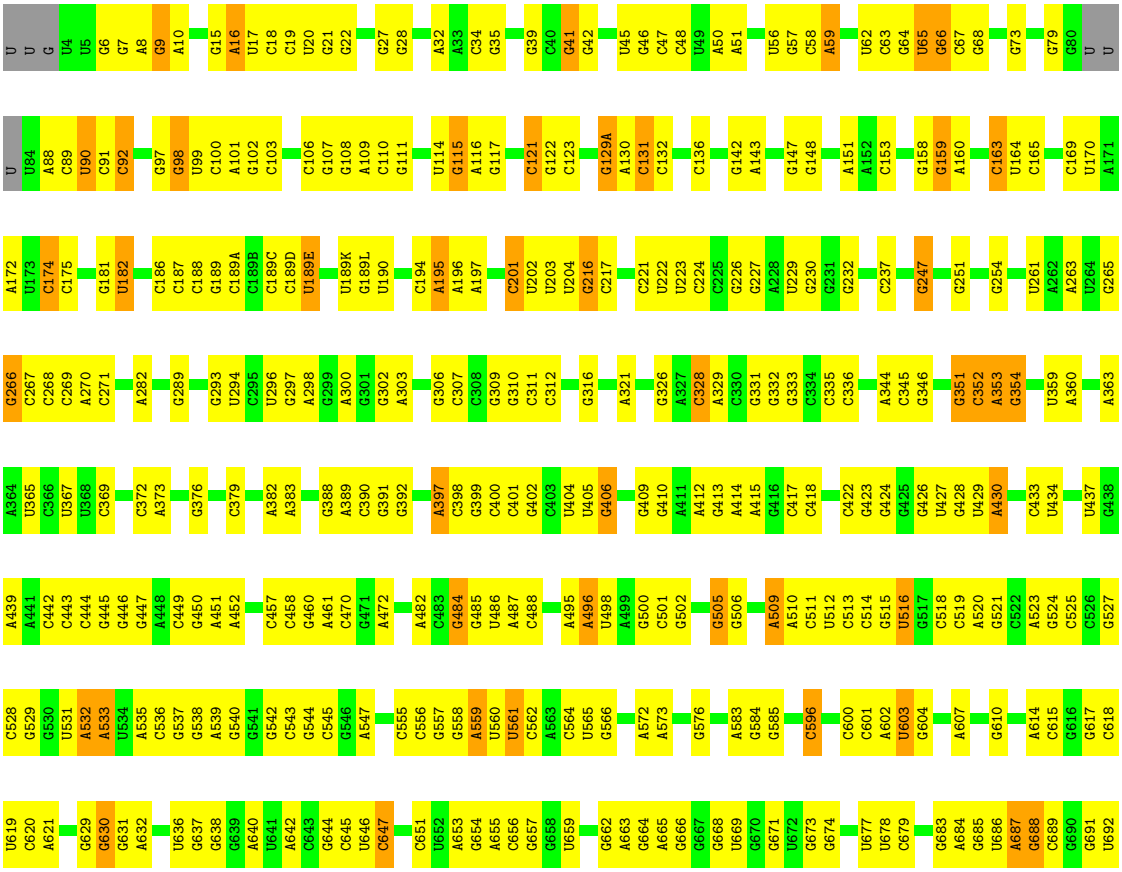
Chain 1a:

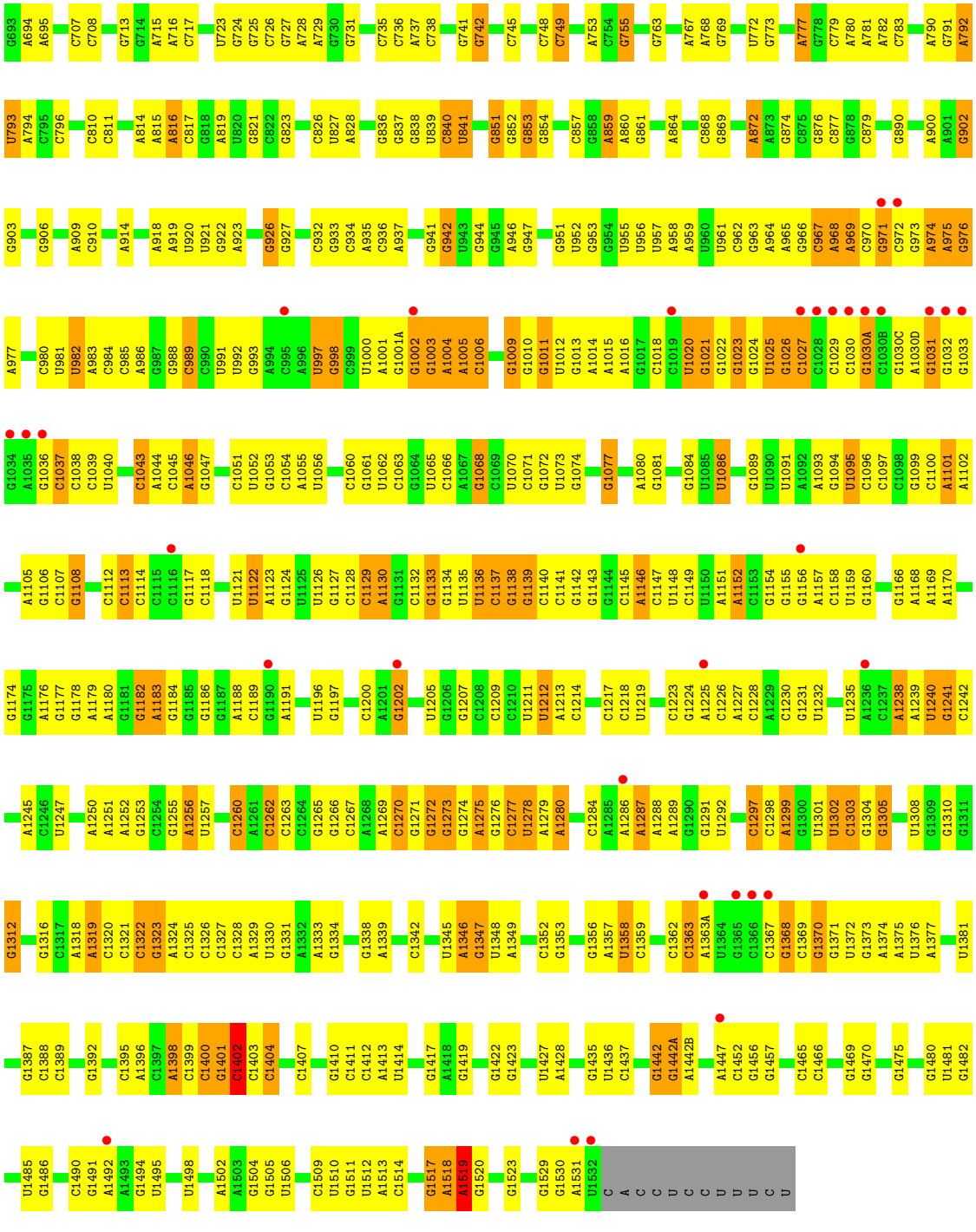




• Molecule 32: 16S Ribosomal RNA

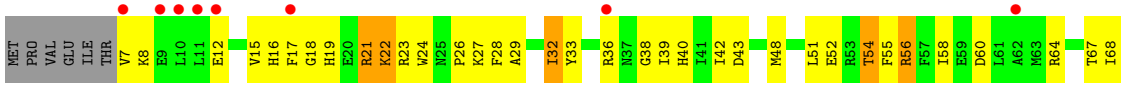
Chain 2a:

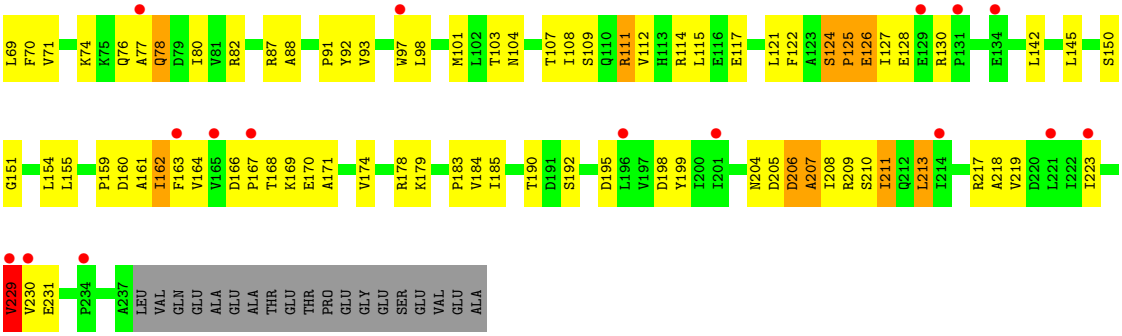




• Molecule 33: 30S ribosomal protein S2

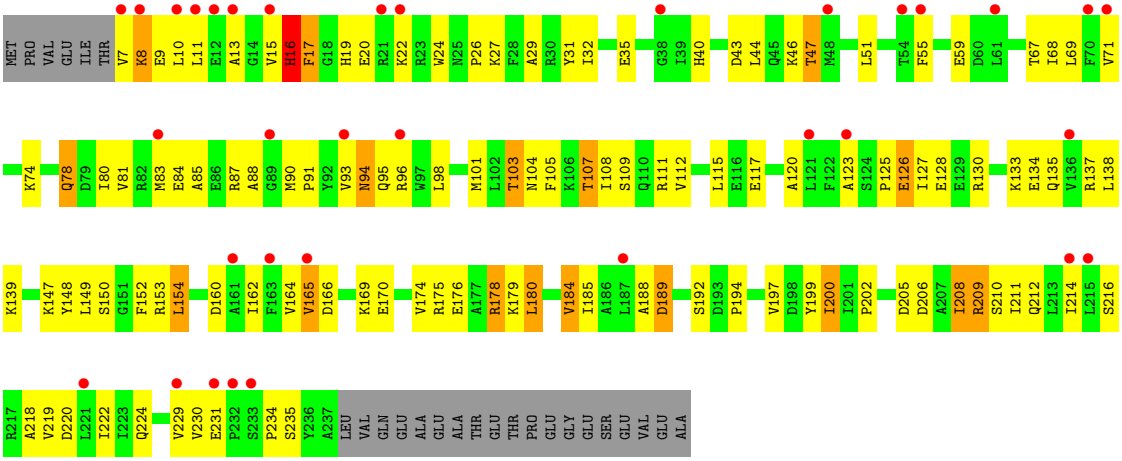
Chain 1b:





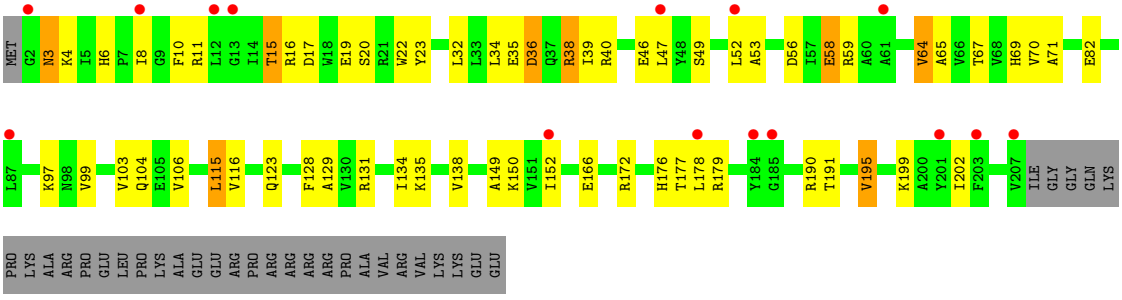
• Molecule 33: 30S ribosomal protein S2

Chain 2b:



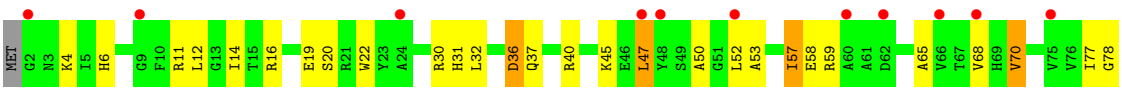
• Molecule 34: 30S ribosomal protein S3

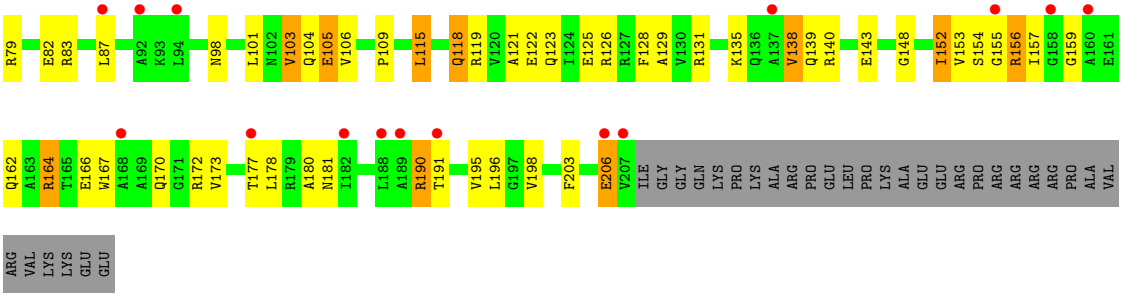
Chain 1c:



• Molecule 34: 30S ribosomal protein S3

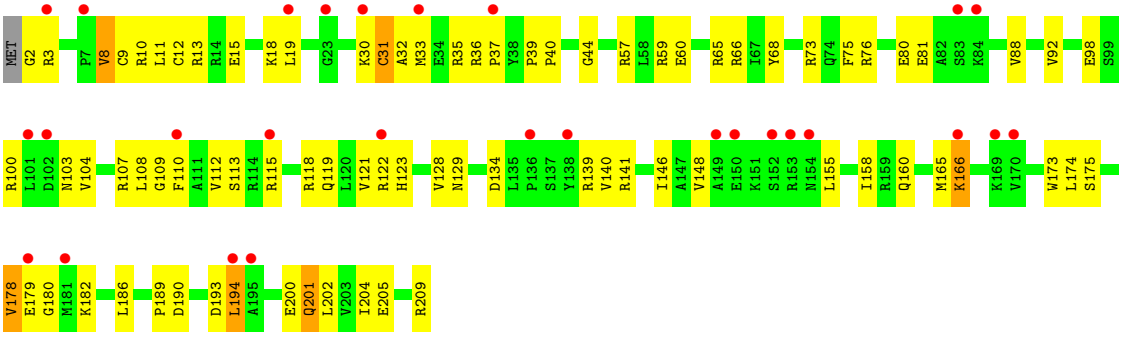
Chain 2c:





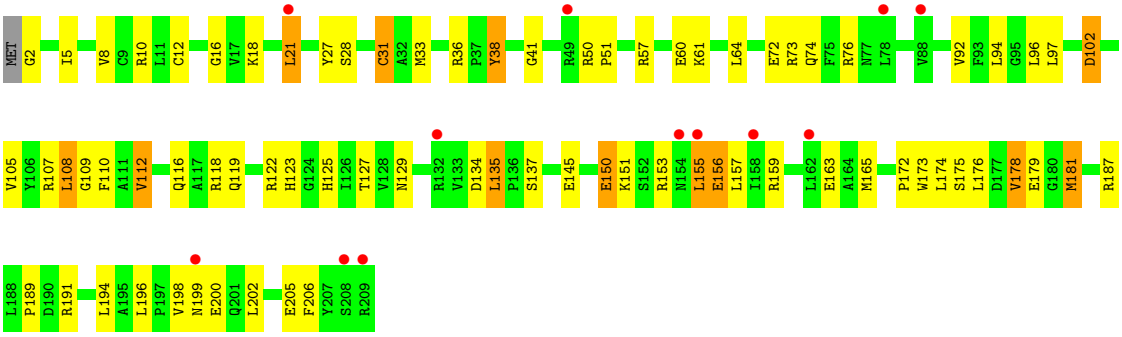

• Molecule 35: 30S ribosomal protein S4

Chain 1d:



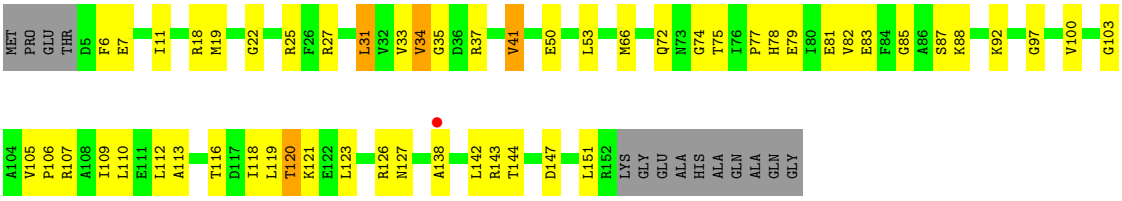

• Molecule 35: 30S ribosomal protein S4

Chain 2d:



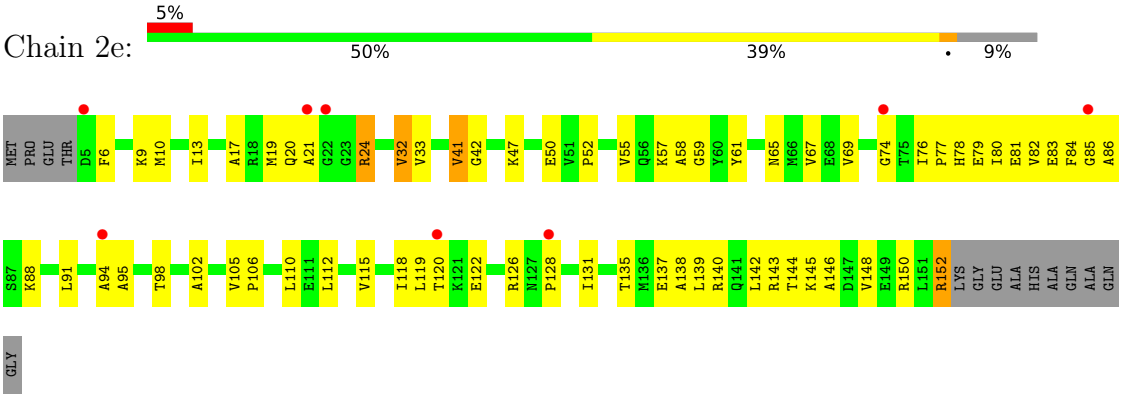

• Molecule 36: 30S ribosomal protein S5

Chain 1e:



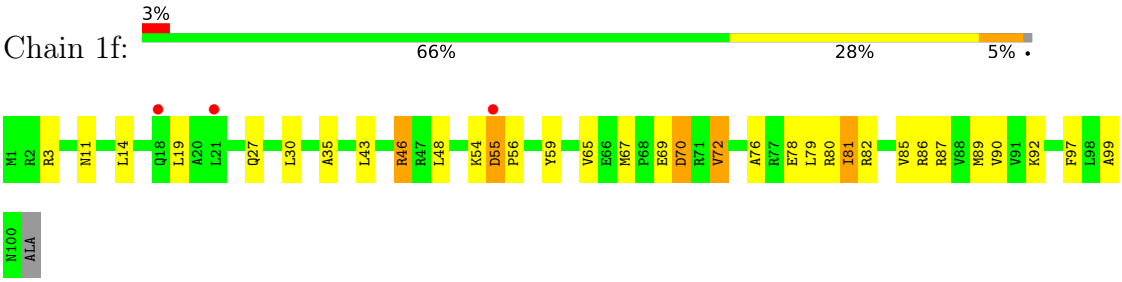

• Molecule 36: 30S ribosomal protein S5

Chain 2e:



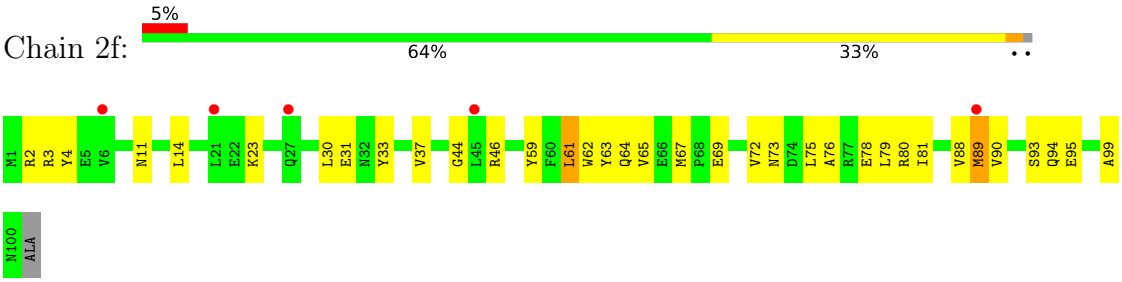

• Molecule 37: 30S ribosomal protein S6

Chain 1f:



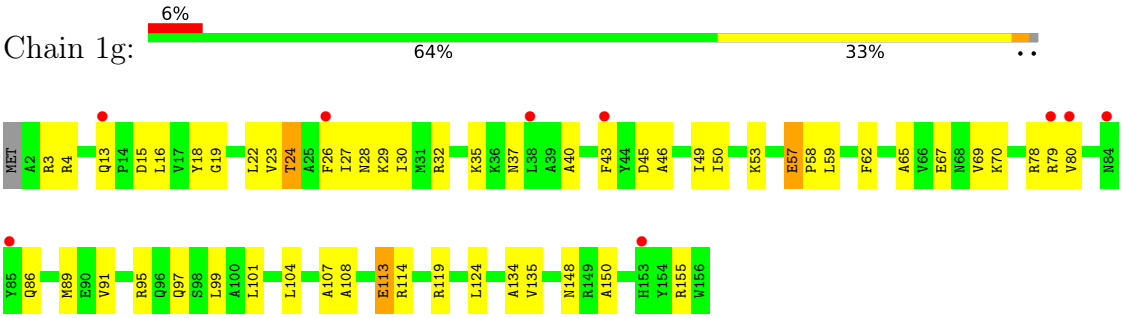

• Molecule 37: 30S ribosomal protein S6

Chain 2f:



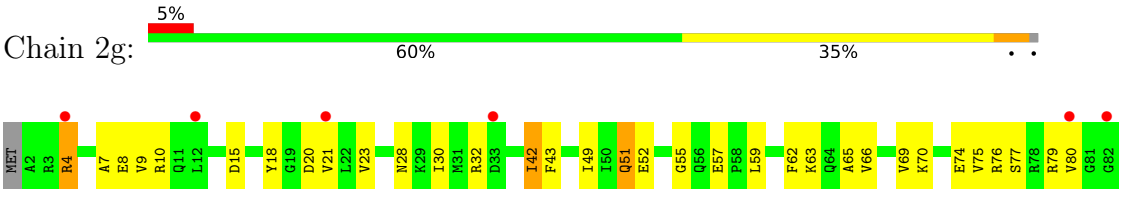

• Molecule 38: 30S ribosomal protein S7

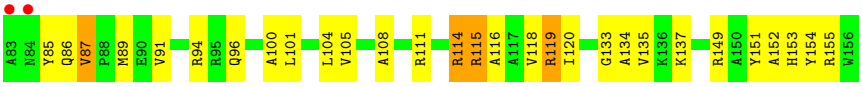
Chain 1g:




• Molecule 38: 30S ribosomal protein S7

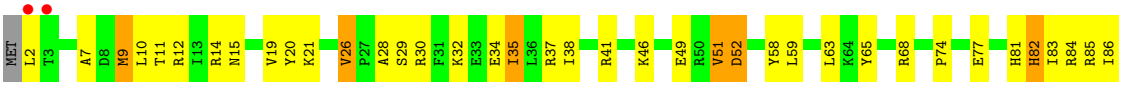
Chain 2g:

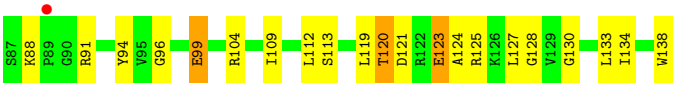




• Molecule 39: 30S ribosomal protein S8

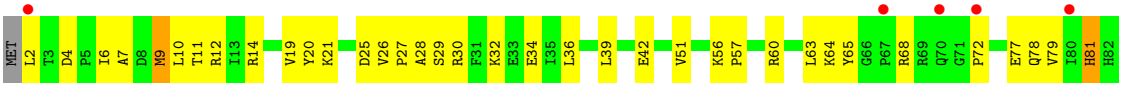
Chain 1h:





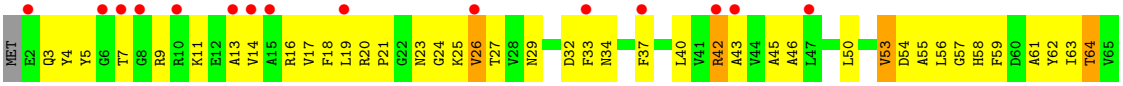
• Molecule 39: 30S ribosomal protein S8

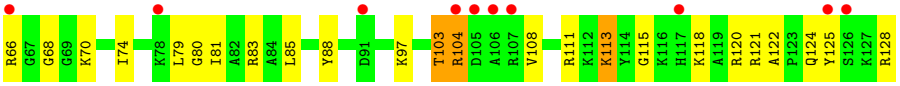
Chain 2h:



• Molecule 40: 30S ribosomal protein S9

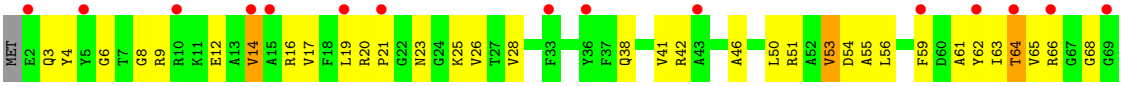
Chain 1i:

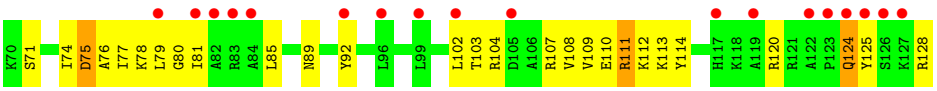




• Molecule 40: 30S ribosomal protein S9

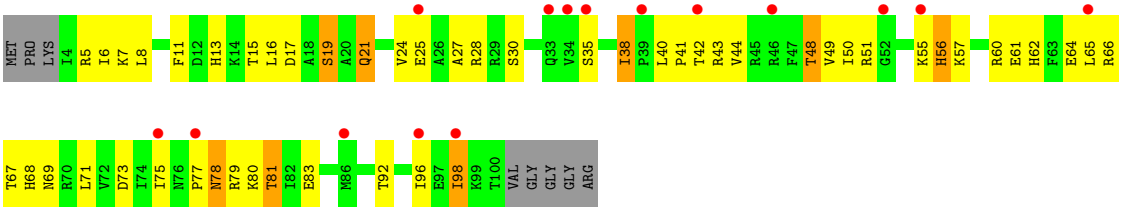
Chain 2i:



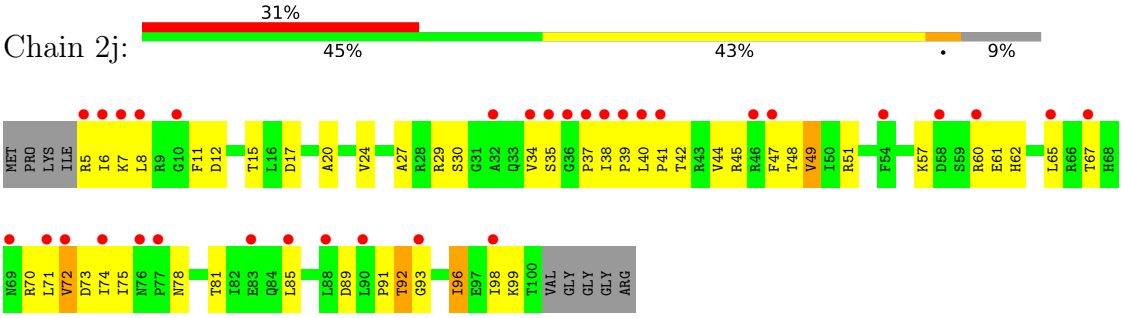


• Molecule 41: 30S ribosomal protein S10

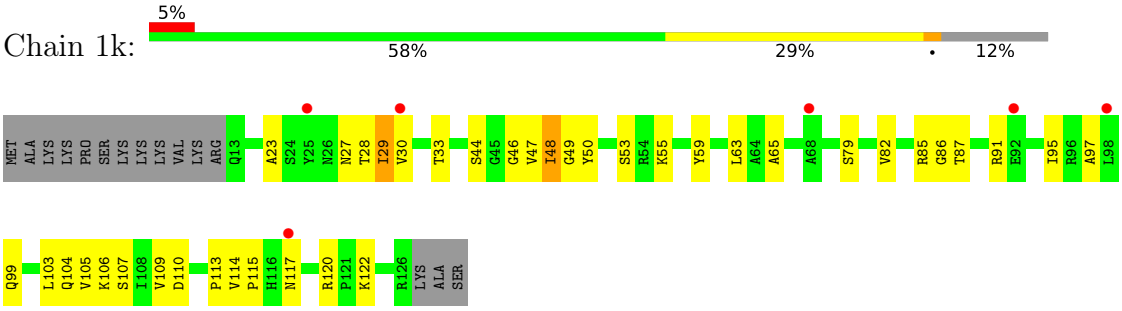
Chain 1j:



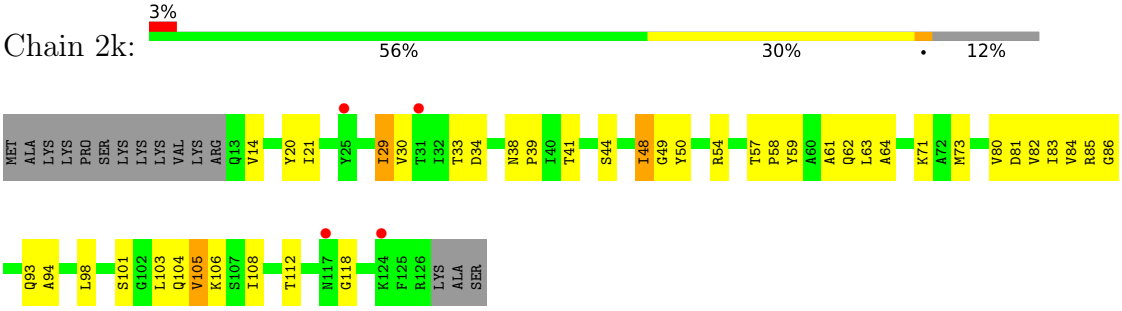

• Molecule 41: 30S ribosomal protein S10



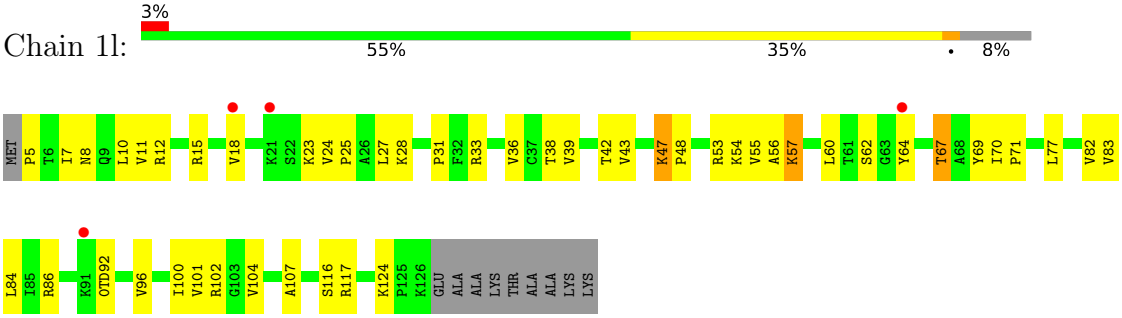

• Molecule 42: 30S ribosomal protein S11




• Molecule 42: 30S ribosomal protein S11

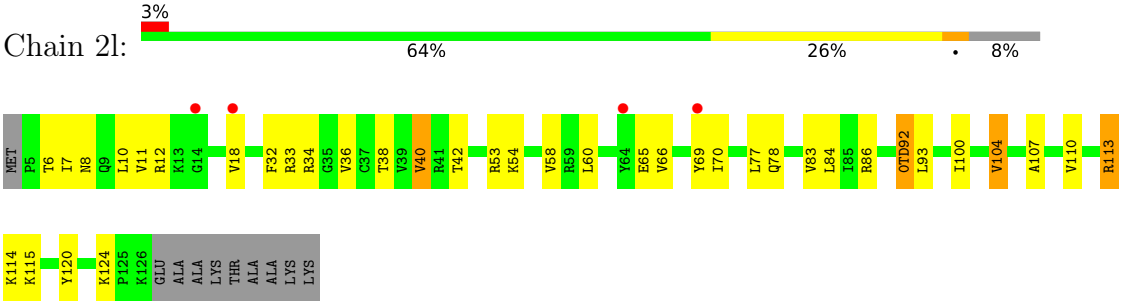



• Molecule 43: 30S ribosomal protein S12



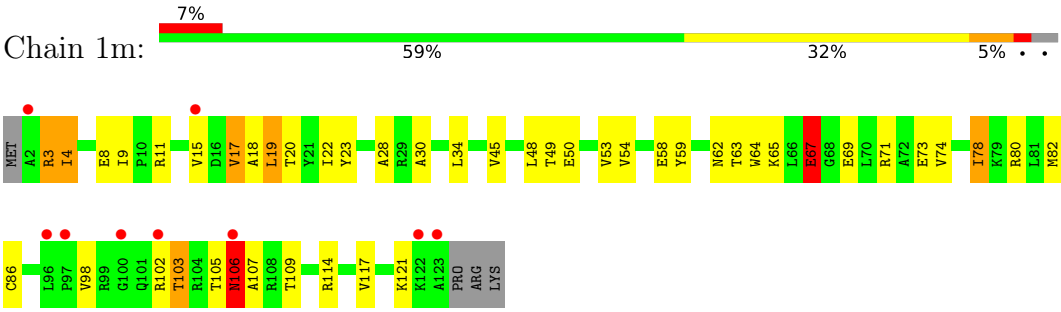
• Molecule 43: 30S ribosomal protein S12

Chain 2l:



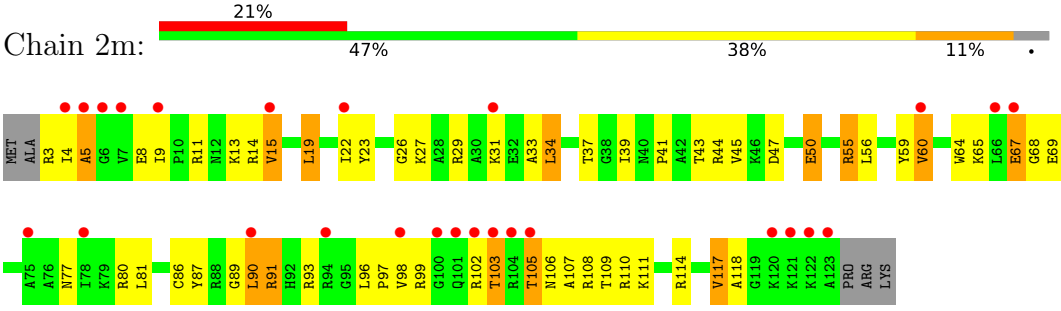

• Molecule 44: 30S ribosomal protein S13

Chain 1m:



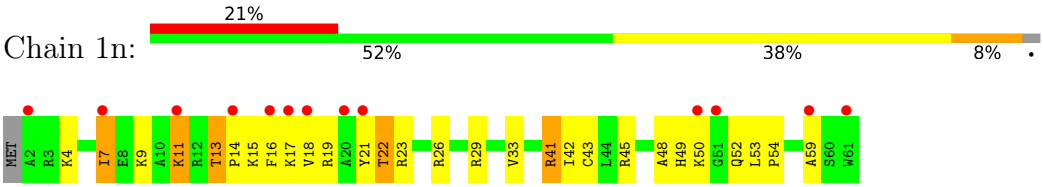

• Molecule 44: 30S ribosomal protein S13

Chain 2m:



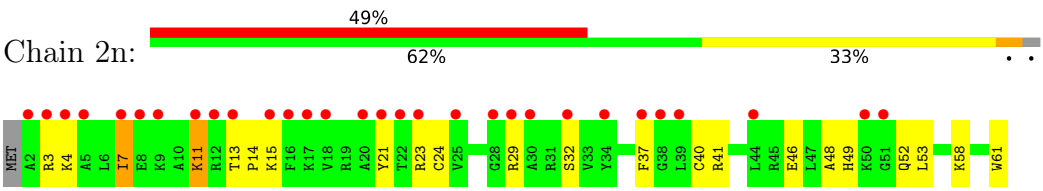

• Molecule 45: 30S ribosomal protein S14 type Z

Chain 1n:



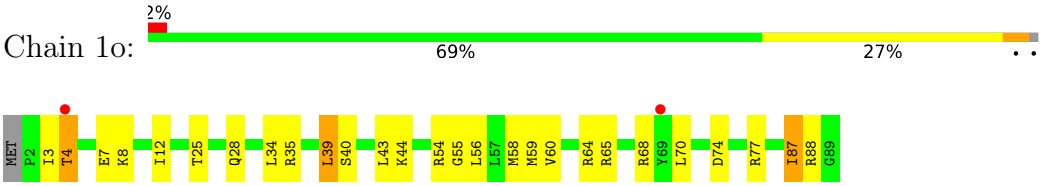

• Molecule 45: 30S ribosomal protein S14 type Z

Chain 2n:



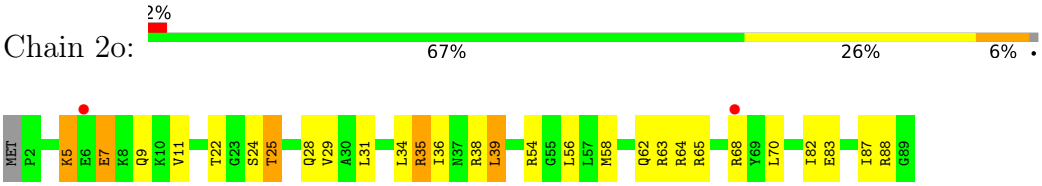

• Molecule 46: 30S ribosomal protein S15

Chain 1o:



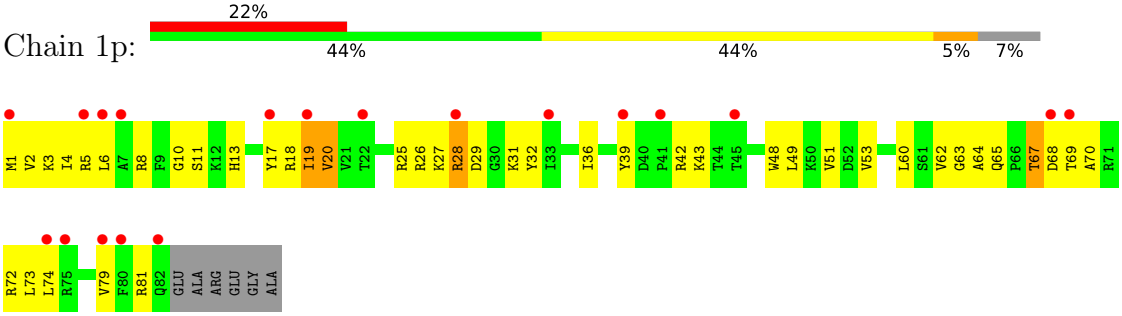

• Molecule 46: 30S ribosomal protein S15

Chain 2o:



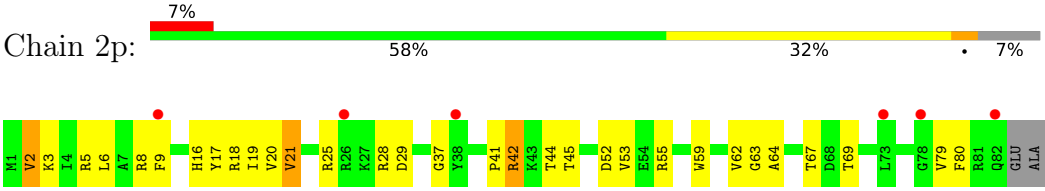

• Molecule 47: 30S ribosomal protein S16

Chain 1p:



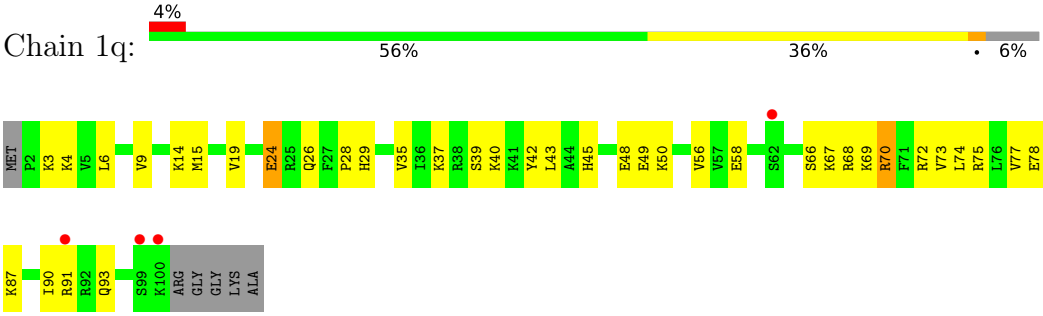

• Molecule 47: 30S ribosomal protein S16

Chain 2p:



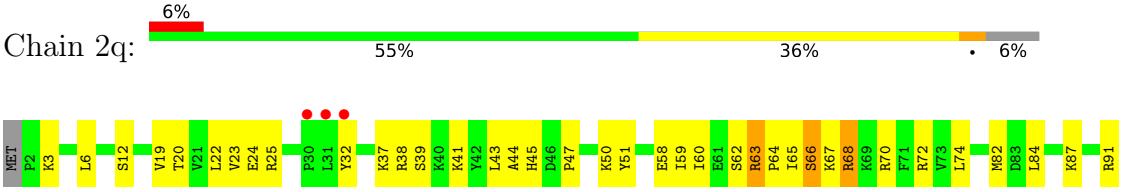

• Molecule 48: 30S ribosomal protein S17

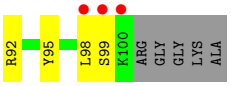
Chain 1q:




• Molecule 48: 30S ribosomal protein S17

Chain 2q:



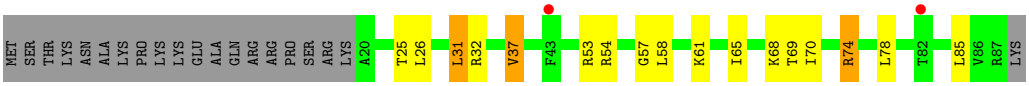



• Molecule 49: 30S ribosomal protein S18

Chain 1r:

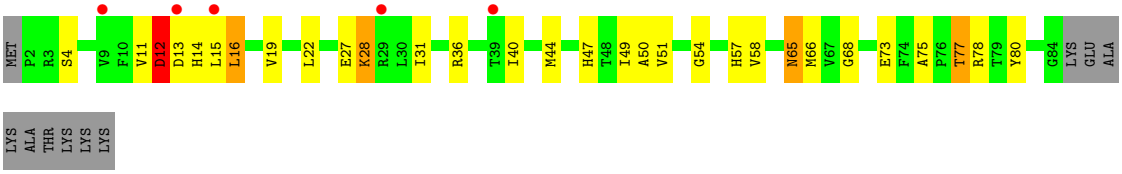
• Molecule 49: 30S ribosomal protein S18

Chain 2r:



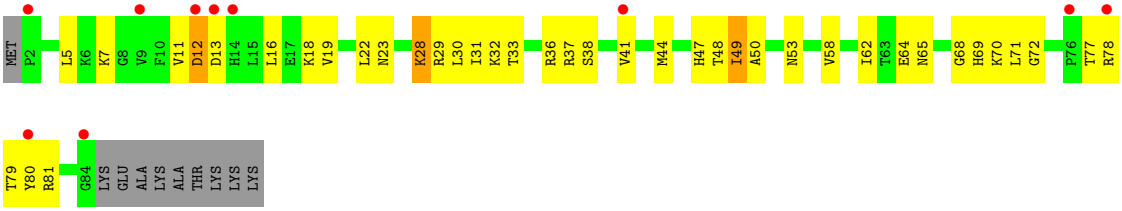

• Molecule 50: 30S ribosomal protein S19

Chain 1s:



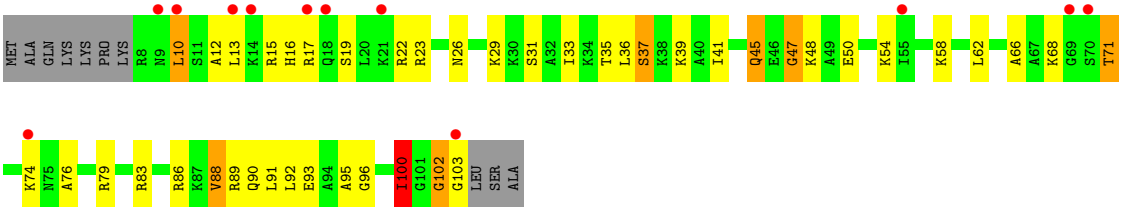

• Molecule 50: 30S ribosomal protein S19

Chain 2s:



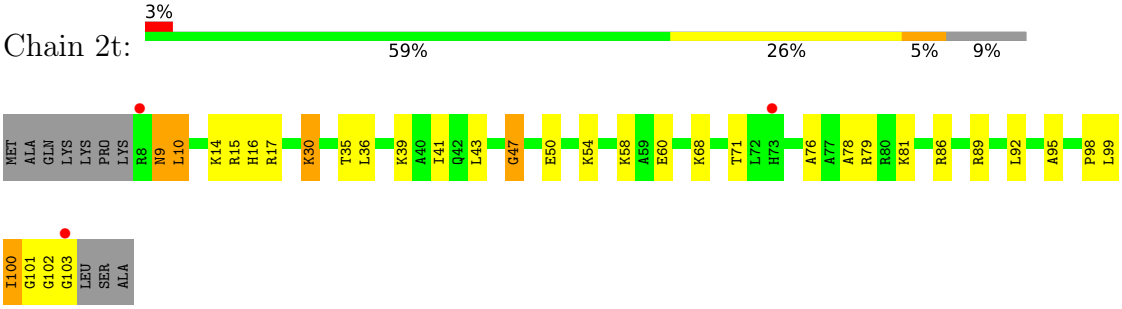

• Molecule 51: 30S ribosomal protein S20

Chain 1t:



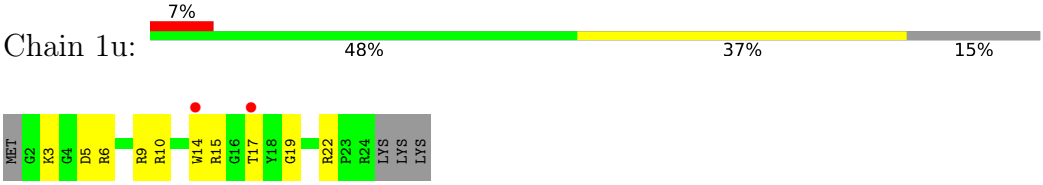
• Molecule 51: 30S ribosomal protein S20

Chain 2t:



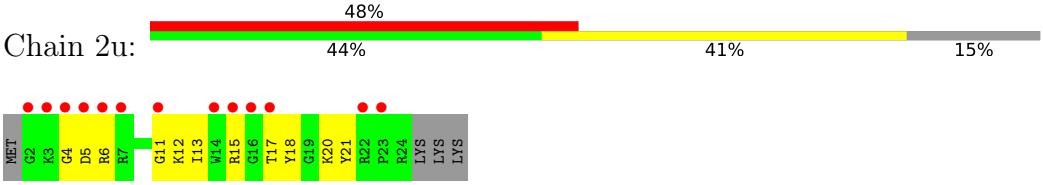

• Molecule 52: 30S ribosomal protein Thx

Chain 1u:



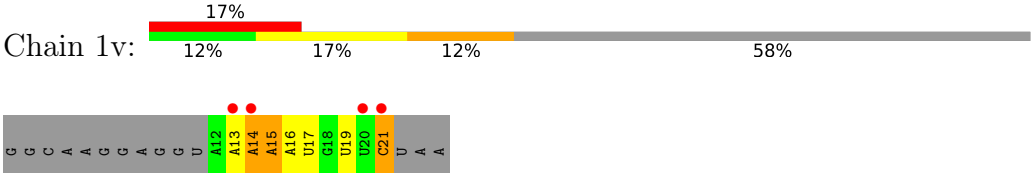

• Molecule 52: 30S ribosomal protein Thx

Chain 2u:




• Molecule 53: mRNA

Chain 1v:

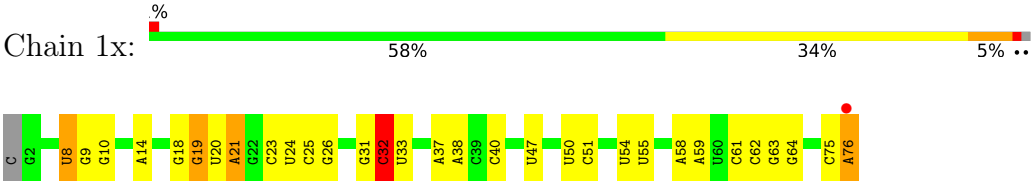



• Molecule 53: mRNA

Chain 2v:

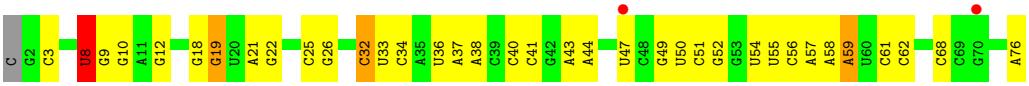
• Molecule 54: P-site tRNA

Chain 1x:




• Molecule 54: P-site tRNA

Chain 2x:


C
G2
C3
U8
G9
G10
A11
G12
G18
G19
U20
A21
G22
C25
G26
C32
U33
C34
A35
U36
A37
A38
C39
C40
C41
G42
A43
A44
U47
C48
G49
U50
C51
G52
G53
U54
U55
C56
A57
A58
A59
U60
C61
C62
C68
C69
G70
A76

# 4 Data and refinement statistics (i)

| Property | Value | Source |
|---|---|---|
| Space group | P 21 21 21 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 208.33Å 447.60Å 612.33Å<br>90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 75.46 – 2.80<br>75.46 – 2.80 | Depositor<br>EDS |
| % Data completeness<br>(in resolution range) | 98.3 (75.46-2.80)<br>98.3 (75.46-2.80) | Depositor<br>EDS |
| $R_{merge}$ | 0.21 | Depositor |
| $R_{sym}$ | (Not available) | Depositor |
| $< I/\sigma(I) >$ [1] | 1.21 (at 2.82Å) | Xtriage |
| Refinement program | PHENIX 1.8.2 | Depositor |
| R, $R_{free}$ | 0.225 , 0.276<br>0.226 , 0.275 | Depositor<br>DCC |
| $R_{free}$ test set | 68487 reflections (4.94%) | wwPDB-VP |
| Wilson B-factor (Å$^2$) | 54.7 | Xtriage |
| Anisotropy | 0.309 | Xtriage |
| Bulk solvent $k_{sol}$(e/Å$^3$), $B_{sol}$(Å$^2$) | 0.28 , 45.5 | EDS |
| L-test for twinning[2] | $< \|L\| > = 0.41$, $< L^2 > = 0.24$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| $F_o$,$F_c$ correlation | 0.92 | EDS |
| Total number of atoms | 292670 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 59.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.59% 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

## 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 2MA, OMG, 4OC, UR3, MG, V7A, 0TD, 5MC, MA6, SF4, ZN, M2G, 2MG, 5MU, 7MG, 2MU, 4SU, PSU

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

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #$\|Z\|$ >5 | RMSZ | #$\|Z\|$ >5 |
| 1 | 1A | 0.30 | 0/69009 | 0.46 | 1/107712 (0.0%) |
| 1 | 2A | 0.23 | 0/67293 | 0.41 | 2/105034 (0.0%) |
| 2 | 1B | 0.25 | 0/2882 | 0.41 | 0/4494 |
| 2 | 2B | 0.19 | 0/2879 | 0.39 | 0/4487 |
| 3 | 1D | 0.27 | 0/2186 | 0.50 | 0/2944 |
| 3 | 2D | 0.24 | 0/2186 | 0.46 | 0/2944 |
| 4 | 1E | 0.27 | 0/1592 | 0.52 | 0/2149 |
| 4 | 2E | 0.22 | 0/1592 | 0.45 | 0/2149 |
| 5 | 1F | 0.27 | 0/1619 | 0.49 | 0/2193 |
| 5 | 2F | 0.21 | 0/1615 | 0.47 | 2/2188 (0.1%) |
| 6 | 1G | 0.22 | 0/1448 | 0.45 | 0/1957 |
| 6 | 2G | 0.20 | 0/1453 | 0.46 | 0/1963 |
| 7 | 1H | 0.23 | 0/1356 | 0.43 | 0/1834 |
| 7 | 2H | 0.18 | 0/1356 | 0.37 | 0/1834 |
| 8 | 1I | 0.22 | 0/1112 | 0.44 | 0/1514 |
| 8 | 2I | 2.31 | 2/1079 (0.2%) | 0.77 | 4/1475 (0.3%) |
| 9 | 1N | 0.26 | 0/1144 | 0.46 | 0/1543 |
| 9 | 2N | 0.18 | 0/1144 | 0.40 | 0/1543 |
| 10 | 1O | 0.26 | 0/943 | 0.51 | 0/1269 |
| 10 | 2O | 0.23 | 0/943 | 0.47 | 0/1269 |
| 11 | 1P | 0.28 | 0/1152 | 0.56 | 0/1533 |
| 11 | 2P | 0.22 | 0/1152 | 0.50 | 0/1533 |
| 12 | 1Q | 0.27 | 0/1143 | 0.48 | 0/1527 |
| 12 | 2Q | 0.19 | 0/1143 | 0.42 | 0/1527 |
| 13 | 1R | 0.28 | 0/982 | 0.48 | 0/1312 |
| 13 | 2R | 0.20 | 0/982 | 0.44 | 0/1312 |
| 14 | 1S | 0.22 | 0/883 | 0.47 | 0/1176 |
| 14 | 2S | 0.19 | 0/880 | 0.44 | 0/1172 |
| 15 | 1T | 0.25 | 0/1105 | 0.48 | 0/1477 |
| 15 | 2T | 0.23 | 0/1097 | 0.44 | 0/1468 |
| 16 | 1U | 0.31 | 0/977 | 0.47 | 0/1301 |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 16 | 2U | 0.21 | 0/977 | 0.43 | 0/1301 |
| 17 | 1V | 0.24 | 0/782 | 0.46 | 0/1049 |
| 17 | 2V | 0.19 | 0/782 | 0.40 | 0/1049 |
| 18 | 1W | 0.28 | 0/897 | 0.45 | 0/1205 |
| 18 | 2W | 0.22 | 0/897 | 0.40 | 0/1205 |
| 19 | 1X | 0.27 | 0/764 | 0.52 | 2/1025 (0.2%) |
| 19 | 2X | 0.20 | 0/764 | 0.49 | 2/1025 (0.2%) |
| 20 | 1Y | 0.25 | 0/819 | 0.47 | 0/1095 |
| 20 | 2Y | 0.19 | 0/819 | 0.41 | 0/1095 |
| 21 | 1Z | 0.23 | 0/1267 | 0.48 | 0/1717 |
| 21 | 2Z | 0.20 | 0/1299 | 0.46 | 0/1763 |
| 22 | 10 | 0.28 | 0/662 | 0.49 | 0/881 |
| 22 | 20 | 0.22 | 0/662 | 0.48 | 0/881 |
| 23 | 11 | 0.26 | 0/762 | 0.46 | 0/1014 |
| 23 | 21 | 0.25 | 0/762 | 0.44 | 0/1014 |
| 24 | 12 | 0.25 | 0/590 | 0.44 | 0/781 |
| 24 | 22 | 0.19 | 0/590 | 0.37 | 0/781 |
| 25 | 13 | 0.26 | 0/474 | 0.46 | 0/635 |
| 25 | 23 | 0.25 | 0/469 | 0.46 | 0/630 |
| 26 | 14 | 0.27 | 0/565 | 0.58 | 0/761 |
| 26 | 24 | 0.27 | 0/545 | 0.65 | 1/737 (0.1%) |
| 27 | 15 | 0.32 | 0/469 | 0.53 | 0/635 |
| 27 | 25 | 0.23 | 0/469 | 0.41 | 0/635 |
| 28 | 16 | 0.29 | 0/460 | 0.51 | 0/613 |
| 28 | 26 | 0.20 | 0/456 | 0.42 | 0/608 |
| 29 | 17 | 0.30 | 0/426 | 0.53 | 0/561 |
| 29 | 27 | 0.24 | 0/426 | 0.48 | 0/561 |
| 30 | 18 | 0.29 | 0/525 | 0.53 | 0/691 |
| 30 | 28 | 0.22 | 0/525 | 0.42 | 0/691 |
| 31 | 19 | 0.25 | 0/310 | 0.50 | 0/407 |
| 31 | 29 | 0.20 | 0/310 | 0.45 | 0/407 |
| 32 | 1a | 0.35 | 10/35795 (0.0%) | 0.40 | 2/55864 (0.0%) |
| 32 | 2a | 0.19 | 0/35886 | 0.38 | 0/56005 |
| 33 | 1b | 0.22 | 0/1881 | 0.50 | 0/2542 |
| 33 | 2b | 0.23 | 0/1860 | 0.48 | 0/2518 |
| 34 | 1c | 0.18 | 0/1572 | 0.39 | 0/2126 |
| 34 | 2c | 0.21 | 0/1566 | 0.48 | 1/2119 (0.0%) |
| 35 | 1d | 0.21 | 0/1685 | 0.46 | 0/2262 |
| 35 | 2d | 0.20 | 0/1704 | 0.42 | 0/2284 |
| 36 | 1e | 0.21 | 0/1145 | 0.44 | 0/1543 |
| 36 | 2e | 0.21 | 0/1149 | 0.47 | 0/1548 |
| 37 | 1f | 0.18 | 0/823 | 0.39 | 0/1115 |
| 37 | 2f | 0.19 | 0/829 | 0.41 | 0/1123 |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 38 | 1g | 0.19 | 0/1250 | 0.43 | 0/1679 |
| 38 | 2g | 0.18 | 0/1254 | 0.41 | 0/1683 |
| 39 | 1h | 0.19 | 0/1108 | 0.42 | 0/1494 |
| 39 | 2h | 0.17 | 0/1108 | 0.40 | 0/1494 |
| 40 | 1i | 0.22 | 0/1002 | 0.48 | 0/1346 |
| 40 | 2i | 0.21 | 0/997 | 0.50 | 0/1343 |
| 41 | 1j | 0.19 | 0/722 | 0.42 | 0/982 |
| 41 | 2j | 0.20 | 0/727 | 0.44 | 0/988 |
| 42 | 1k | 0.20 | 0/844 | 0.49 | 0/1145 |
| 42 | 2k | 0.19 | 0/848 | 0.47 | 1/1149 (0.1%) |
| 43 | 1l | 0.20 | 0/937 | 0.43 | 0/1260 |
| 43 | 2l | 0.20 | 0/937 | 0.42 | 0/1260 |
| 44 | 1m | 0.23 | 0/961 | 0.49 | 0/1290 |
| 44 | 2m | 0.21 | 0/953 | 0.55 | 1/1279 (0.1%) |
| 45 | 1n | 0.19 | 0/501 | 0.44 | 0/664 |
| 45 | 2n | 0.20 | 0/501 | 0.46 | 0/664 |
| 46 | 1o | 0.19 | 0/739 | 0.40 | 0/985 |
| 46 | 2o | 0.18 | 0/739 | 0.37 | 0/985 |
| 47 | 1p | 0.21 | 0/697 | 0.44 | 0/939 |
| 47 | 2p | 0.19 | 0/693 | 0.45 | 0/935 |
| 48 | 1q | 0.19 | 0/836 | 0.45 | 0/1117 |
| 48 | 2q | 0.20 | 0/836 | 0.41 | 0/1117 |
| 49 | 1r | 0.20 | 0/560 | 0.42 | 0/746 |
| 49 | 2r | 0.19 | 0/560 | 0.41 | 0/746 |
| 50 | 1s | 0.20 | 0/667 | 0.48 | 0/900 |
| 50 | 2s | 0.23 | 0/661 | 0.55 | 0/893 |
| 51 | 1t | 0.20 | 0/730 | 0.45 | 0/965 |
| 51 | 2t | 0.21 | 0/729 | 0.49 | 0/965 |
| 52 | 1u | 0.19 | 0/203 | 0.47 | 0/266 |
| 52 | 2u | 0.23 | 0/203 | 0.49 | 0/266 |
| 53 | 1v | 0.23 | 0/238 | 0.38 | 0/368 |
| 53 | 2v | 0.27 | 0/126 | 0.41 | 0/195 |
| 54 | 1x | 0.26 | 0/1725 | 0.41 | 0/2689 |
| 54 | 2x | 0.24 | 0/1725 | 0.39 | 0/2689 |
| All | All | 0.29 | 12/310063 (0.0%) | 0.43 | 19/463821 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 21 | 1Z | 0 | 1 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 32 | 1a | 0 | 1 |
| 33 | 1b | 0 | 2 |
| All | All | 0 | 4 |

All (12) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 8 | 2I | 89 | TYR | CE1-CZ | 55.02 | 2.70 | 1.38 |
| 8 | 2I | 89 | TYR | CD2-CE2 | 51.24 | 2.92 | 1.38 |
| 32 | 1a | 55 | A | C5-C4 | 35.15 | 2.09 | 1.38 |
| 32 | 1a | 55 | A | N7-C5 | 15.61 | 1.70 | 1.39 |
| 32 | 1a | 55 | A | C8-N7 | 15.23 | 1.62 | 1.31 |
| 32 | 1a | 55 | A | N9-C8 | 14.83 | 1.67 | 1.37 |
| 32 | 1a | 55 | A | N9-C4 | 14.14 | 1.66 | 1.37 |
| 32 | 1a | 55 | A | C5-C6 | 13.25 | 1.67 | 1.41 |
| 32 | 1a | 55 | A | N3-C4 | 12.65 | 1.60 | 1.34 |
| 32 | 1a | 55 | A | C6-N1 | 12.64 | 1.60 | 1.35 |
| 32 | 1a | 55 | A | N1-C2 | 12.46 | 1.59 | 1.34 |
| 32 | 1a | 55 | A | C2-N3 | 11.88 | 1.57 | 1.33 |

All (19) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 8 | 2I | 89 | TYR | CZ-CE2-CD2 | -11.38 | 99.12 | 119.60 |
| 8 | 2I | 89 | TYR | CD1-CE1-CZ | 10.32 | 138.18 | 119.60 |
| 26 | 24 | 54 | GLY | N-CA-C | -9.43 | 103.85 | 115.08 |
| 8 | 2I | 89 | TYR | CG-CD2-CE2 | 8.93 | 134.59 | 121.20 |
| 32 | 1a | 357 | G | OP1-P-O3' | -8.67 | 81.98 | 108.00 |
| 44 | 2m | 91 | ARG | N-CA-C | -8.41 | 105.04 | 114.62 |
| 32 | 1a | 357 | G | OP2-P-O3' | -7.03 | 86.91 | 108.00 |
| 8 | 2I | 89 | TYR | CE1-CZ-CE2 | -6.63 | 107.04 | 120.30 |
| 42 | 2k | 118 | GLY | N-CA-C | 6.48 | 116.11 | 110.21 |
| 1 | 1A | 1992 | G | C2'-C3'-O3' | 5.54 | 117.81 | 109.50 |
| 34 | 2c | 139 | GLN | N-CA-C | -5.52 | 108.33 | 114.62 |
| 1 | 2A | 1992 | G | C2'-C3'-O3' | 5.50 | 117.75 | 109.50 |
| 19 | 2X | 94 | GLY | CA-C-N | 5.42 | 131.47 | 121.70 |
| 19 | 2X | 94 | GLY | C-N-CA | 5.42 | 131.47 | 121.70 |
| 19 | 1X | 94 | GLY | CA-C-N | 5.40 | 131.41 | 121.70 |
| 19 | 1X | 94 | GLY | C-N-CA | 5.40 | 131.41 | 121.70 |
| 5 | 2F | 21 | ALA | CA-C-N | 5.18 | 131.02 | 121.70 |
| 5 | 2F | 21 | ALA | C-N-CA | 5.18 | 131.02 | 121.70 |
| 1 | 2A | 271(M) | G | P-O3'-C3' | 5.13 | 125.85 | 119.70 |

There are no chirality outliers.

All (4) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 21 | 1Z | 136 | PHE | Peptide |
| 32 | 1a | 55 | A | Sidechain |
| 33 | 1b | 122 | PHE | Peptide |
| 33 | 1b | 126 | 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 | 31187 | 997 | 0 |
| 1 | 2A | 60322 | 0 | 30423 | 1063 | 0 |
| 2 | 1B | 2577 | 0 | 1305 | 39 | 0 |
| 2 | 2B | 2575 | 0 | 1303 | 60 | 0 |
| 3 | 1D | 2136 | 0 | 2218 | 69 | 0 |
| 3 | 2D | 2136 | 0 | 2218 | 66 | 0 |
| 4 | 1E | 1559 | 0 | 1618 | 37 | 0 |
| 4 | 2E | 1559 | 0 | 1618 | 62 | 0 |
| 5 | 1F | 1584 | 0 | 1625 | 61 | 0 |
| 5 | 2F | 1580 | 0 | 1619 | 59 | 0 |
| 6 | 1G | 1423 | 0 | 1436 | 42 | 0 |
| 6 | 2G | 1428 | 0 | 1438 | 70 | 0 |
| 7 | 1H | 1330 | 0 | 1407 | 35 | 0 |
| 7 | 2H | 1330 | 0 | 1407 | 33 | 0 |
| 8 | 1I | 1097 | 0 | 1140 | 38 | 0 |
| 8 | 2I | 1064 | 0 | 1082 | 60 | 12 |
| 9 | 1N | 1117 | 0 | 1184 | 21 | 0 |
| 9 | 2N | 1117 | 0 | 1184 | 23 | 0 |
| 10 | 1O | 933 | 0 | 996 | 24 | 0 |
| 10 | 2O | 933 | 0 | 996 | 38 | 0 |
| 11 | 1P | 1135 | 0 | 1212 | 61 | 0 |
| 11 | 2P | 1135 | 0 | 1212 | 46 | 0 |
| 12 | 1Q | 1122 | 0 | 1179 | 39 | 0 |
| 12 | 2Q | 1122 | 0 | 1179 | 37 | 0 |
| 13 | 1R | 968 | 0 | 1033 | 23 | 0 |
| 13 | 2R | 968 | 0 | 1033 | 26 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 14 | 1S | 873 | 0 | 927 | 36 | 0 |
| 14 | 2S | 870 | 0 | 923 | 41 | 0 |
| 15 | 1T | 1091 | 0 | 1151 | 33 | 0 |
| 15 | 2T | 1083 | 0 | 1136 | 45 | 0 |
| 16 | 1U | 959 | 0 | 1019 | 22 | 0 |
| 16 | 2U | 959 | 0 | 1019 | 26 | 0 |
| 17 | 1V | 771 | 0 | 830 | 12 | 0 |
| 17 | 2V | 771 | 0 | 830 | 22 | 0 |
| 18 | 1W | 886 | 0 | 940 | 28 | 0 |
| 18 | 2W | 886 | 0 | 940 | 22 | 0 |
| 19 | 1X | 750 | 0 | 814 | 17 | 0 |
| 19 | 2X | 750 | 0 | 814 | 13 | 0 |
| 20 | 1Y | 806 | 0 | 881 | 21 | 0 |
| 20 | 2Y | 806 | 0 | 881 | 21 | 0 |
| 21 | 1Z | 1240 | 0 | 1240 | 34 | 0 |
| 21 | 2Z | 1271 | 0 | 1273 | 52 | 0 |
| 22 | 10 | 653 | 0 | 674 | 15 | 0 |
| 22 | 20 | 653 | 0 | 674 | 21 | 0 |
| 23 | 11 | 755 | 0 | 826 | 19 | 0 |
| 23 | 21 | 755 | 0 | 826 | 17 | 0 |
| 24 | 12 | 588 | 0 | 643 | 11 | 0 |
| 24 | 22 | 588 | 0 | 643 | 14 | 0 |
| 25 | 13 | 469 | 0 | 518 | 17 | 0 |
| 25 | 23 | 464 | 0 | 514 | 12 | 0 |
| 26 | 14 | 552 | 0 | 533 | 26 | 0 |
| 26 | 24 | 532 | 0 | 503 | 24 | 0 |
| 27 | 15 | 455 | 0 | 465 | 10 | 0 |
| 27 | 25 | 455 | 0 | 465 | 9 | 0 |
| 28 | 16 | 453 | 0 | 473 | 16 | 0 |
| 28 | 26 | 449 | 0 | 469 | 9 | 0 |
| 29 | 17 | 418 | 0 | 467 | 13 | 0 |
| 29 | 27 | 418 | 0 | 467 | 13 | 0 |
| 30 | 18 | 517 | 0 | 582 | 34 | 0 |
| 30 | 28 | 517 | 0 | 582 | 25 | 0 |
| 31 | 19 | 307 | 0 | 335 | 5 | 0 |
| 31 | 29 | 307 | 0 | 335 | 11 | 0 |
| 32 | 1a | 32246 | 0 | 16295 | 626 | 12 |
| 32 | 2a | 32327 | 0 | 16339 | 656 | 0 |
| 33 | 1b | 1846 | 0 | 1867 | 77 | 0 |
| 33 | 2b | 1825 | 0 | 1828 | 70 | 0 |
| 34 | 1c | 1548 | 0 | 1535 | 45 | 0 |
| 34 | 2c | 1542 | 0 | 1517 | 50 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 35 | 1d | 1655 | 0 | 1672 | 67 | 0 |
| 35 | 2d | 1674 | 0 | 1714 | 59 | 0 |
| 36 | 1e | 1129 | 0 | 1185 | 42 | 0 |
| 36 | 2e | 1133 | 0 | 1191 | 48 | 0 |
| 37 | 1f | 810 | 0 | 804 | 26 | 0 |
| 37 | 2f | 816 | 0 | 808 | 20 | 0 |
| 38 | 1g | 1231 | 0 | 1238 | 38 | 0 |
| 38 | 2g | 1235 | 0 | 1249 | 42 | 0 |
| 39 | 1h | 1088 | 0 | 1126 | 44 | 0 |
| 39 | 2h | 1088 | 0 | 1126 | 44 | 0 |
| 40 | 1i | 983 | 0 | 986 | 50 | 0 |
| 40 | 2i | 978 | 0 | 966 | 54 | 0 |
| 41 | 1j | 709 | 0 | 650 | 44 | 0 |
| 41 | 2j | 714 | 0 | 672 | 37 | 0 |
| 42 | 1k | 829 | 0 | 825 | 25 | 0 |
| 42 | 2k | 833 | 0 | 836 | 23 | 0 |
| 43 | 1l | 932 | 0 | 981 | 31 | 0 |
| 43 | 2l | 932 | 0 | 981 | 23 | 0 |
| 44 | 1m | 951 | 0 | 995 | 30 | 0 |
| 44 | 2m | 943 | 0 | 981 | 49 | 0 |
| 45 | 1n | 492 | 0 | 529 | 28 | 0 |
| 45 | 2n | 492 | 0 | 529 | 17 | 0 |
| 46 | 1o | 728 | 0 | 760 | 19 | 0 |
| 46 | 2o | 728 | 0 | 760 | 24 | 0 |
| 47 | 1p | 681 | 0 | 697 | 32 | 0 |
| 47 | 2p | 677 | 0 | 686 | 22 | 0 |
| 48 | 1q | 823 | 0 | 891 | 28 | 0 |
| 48 | 2q | 823 | 0 | 891 | 26 | 0 |
| 49 | 1r | 555 | 0 | 618 | 15 | 0 |
| 49 | 2r | 555 | 0 | 618 | 9 | 0 |
| 50 | 1s | 652 | 0 | 662 | 28 | 0 |
| 50 | 2s | 646 | 0 | 644 | 28 | 0 |
| 51 | 1t | 728 | 0 | 798 | 28 | 0 |
| 51 | 2t | 727 | 0 | 796 | 25 | 0 |
| 52 | 1u | 199 | 0 | 208 | 6 | 0 |
| 52 | 2u | 199 | 0 | 208 | 8 | 0 |
| 53 | 1v | 213 | 0 | 108 | 5 | 0 |
| 53 | 2v | 113 | 0 | 54 | 1 | 0 |
| 54 | 1x | 1625 | 0 | 829 | 19 | 0 |
| 54 | 2x | 1625 | 0 | 829 | 21 | 0 |
| 55 | 10 | 5 | 0 | 0 | 0 | 0 |
| 55 | 11 | 4 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 55 | 12 | 2 | 0 | 0 | 0 | 0 |
| 55 | 13 | 3 | 0 | 0 | 0 | 0 |
| 55 | 15 | 5 | 0 | 0 | 0 | 0 |
| 55 | 16 | 1 | 0 | 0 | 0 | 0 |
| 55 | 17 | 4 | 0 | 0 | 0 | 0 |
| 55 | 18 | 6 | 0 | 0 | 0 | 0 |
| 55 | 19 | 1 | 0 | 0 | 0 | 0 |
| 55 | 1A | 1117 | 0 | 0 | 0 | 0 |
| 55 | 1B | 35 | 0 | 0 | 0 | 0 |
| 55 | 1D | 13 | 0 | 0 | 0 | 0 |
| 55 | 1E | 11 | 0 | 0 | 0 | 0 |
| 55 | 1F | 11 | 0 | 0 | 0 | 0 |
| 55 | 1G | 4 | 0 | 0 | 0 | 0 |
| 55 | 1N | 4 | 0 | 0 | 0 | 0 |
| 55 | 1O | 4 | 0 | 0 | 0 | 0 |
| 55 | 1P | 3 | 0 | 0 | 0 | 0 |
| 55 | 1Q | 7 | 0 | 0 | 0 | 0 |
| 55 | 1R | 2 | 0 | 0 | 0 | 0 |
| 55 | 1S | 1 | 0 | 0 | 0 | 0 |
| 55 | 1T | 3 | 0 | 0 | 0 | 0 |
| 55 | 1U | 7 | 0 | 0 | 0 | 0 |
| 55 | 1V | 4 | 0 | 0 | 0 | 0 |
| 55 | 1W | 5 | 0 | 0 | 0 | 0 |
| 55 | 1X | 6 | 0 | 0 | 0 | 0 |
| 55 | 1Y | 4 | 0 | 0 | 0 | 0 |
| 55 | 1Z | 2 | 0 | 0 | 0 | 0 |
| 55 | 1a | 234 | 0 | 0 | 0 | 0 |
| 55 | 1b | 1 | 0 | 0 | 0 | 0 |
| 55 | 1e | 2 | 0 | 0 | 0 | 0 |
| 55 | 1f | 2 | 0 | 0 | 0 | 0 |
| 55 | 1l | 4 | 0 | 0 | 0 | 0 |
| 55 | 1n | 2 | 0 | 0 | 0 | 0 |
| 55 | 1t | 1 | 0 | 0 | 0 | 0 |
| 55 | 1v | 2 | 0 | 0 | 0 | 0 |
| 55 | 1x | 13 | 0 | 0 | 0 | 0 |
| 55 | 20 | 1 | 0 | 0 | 0 | 0 |
| 55 | 23 | 1 | 0 | 0 | 0 | 0 |
| 55 | 25 | 2 | 0 | 0 | 0 | 0 |
| 55 | 26 | 1 | 0 | 0 | 0 | 0 |
| 55 | 27 | 1 | 0 | 0 | 0 | 0 |
| 55 | 28 | 3 | 0 | 0 | 0 | 0 |
| 55 | 2A | 862 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 55 | 2B | 19 | 0 | 0 | 0 | 0 |
| 55 | 2D | 3 | 0 | 0 | 0 | 0 |
| 55 | 2E | 9 | 0 | 0 | 0 | 0 |
| 55 | 2F | 6 | 0 | 0 | 0 | 0 |
| 55 | 2G | 1 | 0 | 0 | 0 | 0 |
| 55 | 2N | 2 | 0 | 0 | 0 | 0 |
| 55 | 2O | 2 | 0 | 0 | 0 | 0 |
| 55 | 2P | 2 | 0 | 0 | 0 | 0 |
| 55 | 2Q | 4 | 0 | 0 | 0 | 0 |
| 55 | 2R | 2 | 0 | 0 | 0 | 0 |
| 55 | 2T | 3 | 0 | 0 | 0 | 0 |
| 55 | 2U | 2 | 0 | 0 | 0 | 0 |
| 55 | 2V | 3 | 0 | 0 | 0 | 0 |
| 55 | 2W | 2 | 0 | 0 | 0 | 0 |
| 55 | 2X | 2 | 0 | 0 | 0 | 0 |
| 55 | 2Z | 1 | 0 | 0 | 0 | 0 |
| 55 | 2a | 209 | 0 | 0 | 0 | 0 |
| 55 | 2d | 2 | 0 | 0 | 0 | 0 |
| 55 | 2e | 1 | 0 | 0 | 0 | 0 |
| 55 | 2f | 2 | 0 | 0 | 0 | 0 |
| 55 | 2g | 1 | 0 | 0 | 0 | 0 |
| 55 | 2i | 1 | 0 | 0 | 0 | 0 |
| 55 | 2j | 2 | 0 | 0 | 0 | 0 |
| 55 | 2l | 3 | 0 | 0 | 0 | 0 |
| 55 | 2p | 1 | 0 | 0 | 0 | 0 |
| 55 | 2q | 1 | 0 | 0 | 0 | 0 |
| 55 | 2r | 1 | 0 | 0 | 0 | 0 |
| 55 | 2t | 1 | 0 | 0 | 0 | 0 |
| 55 | 2x | 5 | 0 | 0 | 0 | 0 |
| 56 | 14 | 1 | 0 | 0 | 0 | 0 |
| 56 | 15 | 1 | 0 | 0 | 0 | 0 |
| 56 | 16 | 1 | 0 | 0 | 0 | 0 |
| 56 | 19 | 1 | 0 | 0 | 0 | 0 |
| 56 | 1Y | 1 | 0 | 0 | 0 | 0 |
| 56 | 1n | 1 | 0 | 0 | 0 | 0 |
| 56 | 24 | 1 | 0 | 0 | 0 | 0 |
| 56 | 25 | 1 | 0 | 0 | 0 | 0 |
| 56 | 26 | 1 | 0 | 0 | 0 | 0 |
| 56 | 29 | 1 | 0 | 0 | 0 | 0 |
| 56 | 2Y | 1 | 0 | 0 | 0 | 0 |
| 56 | 2n | 1 | 0 | 0 | 0 | 0 |
| 57 | 1a | 35 | 0 | 0 | 2 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 57 | 2a | 35 | 0 | 0 | 4 | 0 |
| 58 | 1d | 8 | 0 | 0 | 3 | 0 |
| 58 | 2d | 8 | 0 | 0 | 1 | 0 |
| 59 | 10 | 8 | 0 | 0 | 1 | 0 |
| 59 | 11 | 7 | 0 | 0 | 1 | 0 |
| 59 | 12 | 1 | 0 | 0 | 0 | 0 |
| 59 | 13 | 4 | 0 | 0 | 0 | 0 |
| 59 | 15 | 7 | 0 | 0 | 0 | 0 |
| 59 | 16 | 2 | 0 | 0 | 0 | 0 |
| 59 | 17 | 6 | 0 | 0 | 3 | 0 |
| 59 | 18 | 9 | 0 | 0 | 1 | 0 |
| 59 | 1A | 1716 | 0 | 0 | 124 | 0 |
| 59 | 1B | 47 | 0 | 0 | 1 | 0 |
| 59 | 1D | 21 | 0 | 0 | 3 | 0 |
| 59 | 1E | 25 | 0 | 0 | 1 | 0 |
| 59 | 1F | 13 | 0 | 0 | 0 | 0 |
| 59 | 1G | 2 | 0 | 0 | 0 | 0 |
| 59 | 1H | 2 | 0 | 0 | 0 | 0 |
| 59 | 1I | 2 | 0 | 0 | 0 | 0 |
| 59 | 1N | 3 | 0 | 0 | 1 | 0 |
| 59 | 1O | 7 | 0 | 0 | 0 | 0 |
| 59 | 1P | 17 | 0 | 0 | 1 | 0 |
| 59 | 1Q | 6 | 0 | 0 | 0 | 0 |
| 59 | 1R | 9 | 0 | 0 | 0 | 0 |
| 59 | 1S | 1 | 0 | 0 | 0 | 0 |
| 59 | 1T | 8 | 0 | 0 | 0 | 0 |
| 59 | 1U | 13 | 0 | 0 | 1 | 0 |
| 59 | 1V | 9 | 0 | 0 | 0 | 0 |
| 59 | 1W | 8 | 0 | 0 | 0 | 0 |
| 59 | 1X | 6 | 0 | 0 | 0 | 0 |
| 59 | 1Y | 2 | 0 | 0 | 1 | 0 |
| 59 | 1a | 294 | 0 | 0 | 23 | 0 |
| 59 | 1b | 1 | 0 | 0 | 0 | 0 |
| 59 | 1d | 3 | 0 | 0 | 0 | 0 |
| 59 | 1e | 1 | 0 | 0 | 0 | 0 |
| 59 | 1i | 1 | 0 | 0 | 0 | 0 |
| 59 | 1j | 1 | 0 | 0 | 0 | 0 |
| 59 | 1l | 4 | 0 | 0 | 0 | 0 |
| 59 | 1m | 1 | 0 | 0 | 0 | 0 |
| 59 | 1o | 1 | 0 | 0 | 0 | 0 |
| 59 | 1q | 2 | 0 | 0 | 0 | 0 |
| 59 | 1v | 4 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 59 | 1x | 17 | 0 | 0 | 2 | 0 |
| 59 | 20 | 3 | 0 | 0 | 0 | 0 |
| 59 | 21 | 8 | 0 | 0 | 0 | 0 |
| 59 | 22 | 1 | 0 | 0 | 0 | 0 |
| 59 | 25 | 1 | 0 | 0 | 0 | 0 |
| 59 | 27 | 1 | 0 | 0 | 0 | 0 |
| 59 | 28 | 3 | 0 | 0 | 0 | 0 |
| 59 | 29 | 1 | 0 | 0 | 0 | 0 |
| 59 | 2A | 867 | 0 | 0 | 80 | 0 |
| 59 | 2B | 14 | 0 | 0 | 3 | 0 |
| 59 | 2D | 16 | 0 | 0 | 0 | 0 |
| 59 | 2E | 8 | 0 | 0 | 1 | 0 |
| 59 | 2F | 13 | 0 | 0 | 0 | 0 |
| 59 | 2I | 1 | 0 | 0 | 0 | 0 |
| 59 | 2N | 1 | 0 | 0 | 0 | 0 |
| 59 | 2O | 1 | 0 | 0 | 0 | 0 |
| 59 | 2P | 4 | 0 | 0 | 0 | 0 |
| 59 | 2Q | 2 | 0 | 0 | 0 | 0 |
| 59 | 2R | 2 | 0 | 0 | 0 | 0 |
| 59 | 2T | 4 | 0 | 0 | 0 | 0 |
| 59 | 2U | 3 | 0 | 0 | 1 | 0 |
| 59 | 2W | 5 | 0 | 0 | 1 | 0 |
| 59 | 2X | 2 | 0 | 0 | 0 | 0 |
| 59 | 2Z | 1 | 0 | 0 | 0 | 0 |
| 59 | 2a | 146 | 0 | 0 | 11 | 0 |
| 59 | 2g | 1 | 0 | 0 | 0 | 0 |
| 59 | 2j | 2 | 0 | 0 | 0 | 0 |
| 59 | 2l | 4 | 0 | 0 | 1 | 0 |
| 59 | 2p | 1 | 0 | 0 | 0 | 0 |
| 59 | 2r | 1 | 0 | 0 | 0 | 0 |
| 59 | 2t | 1 | 0 | 0 | 0 | 0 |
| 59 | 2v | 1 | 0 | 0 | 0 | 0 |
| 59 | 2x | 6 | 0 | 0 | 0 | 0 |
| All | All | 292670 | 0 | 193346 | 5696 | 12 |

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 13.

All (5696) 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) |
|---|---|---|---|
| 32:1a:55:A:C5 | 32:1a:55:A:N7 | 1.70 | 1.56 |
| 32:1a:55:A:C5 | 32:1a:55:A:C4 | 2.09 | 1.39 |
| 1:1A:1082:U:H3 | 1:1A:1086:A:N6 | 1.39 | 1.17 |
| 1:2A:2138:C:N4 | 1:2A:2153:G:H1 | 1.51 | 1.07 |
| 1:1A:1059:G:H1 | 1:1A:1079:C:N4 | 1.56 | 1.03 |
| 1:1A:1082:U:O4 | 1:1A:1086:A:N1 | 1.92 | 1.02 |
| 1:1A:1062:G:H1 | 1:1A:1077:A:H61 | 1.08 | 0.98 |
| 1:1A:2822:G:OP2 | 59:1A:4213:HOH:O | 1.81 | 0.97 |
| 1:1A:2128:C:H42 | 1:1A:2160:G:H1 | 1.09 | 0.96 |
| 1:1A:1054:A:N6 | 1:1A:1105:U:H3 | 1.63 | 0.95 |
| 32:2a:1133:G:H1 | 32:2a:1141:C:H42 | 0.96 | 0.95 |
| 50:2s:28:LYS:HB2 | 50:2s:29:ARG:HA | 1.46 | 0.95 |
| 1:2A:2129:C:H42 | 1:2A:2159:G:H1 | 0.96 | 0.94 |
| 1:2A:2104:G:H1 | 1:2A:2185:C:H42 | 1.04 | 0.94 |
| 1:1A:1054:A:H61 | 1:1A:1105:U:H3 | 1.05 | 0.92 |
| 1:1A:2099:U:H3 | 1:1A:2190:G:H1 | 0.94 | 0.92 |
| 32:2a:1133:G:H1 | 32:2a:1141:C:N4 | 1.66 | 0.91 |
| 32:1a:559:A:H4' | 32:1a:560:U:H3' | 1.51 | 0.91 |
| 1:1A:1059:G:H1 | 1:1A:1079:C:H42 | 0.91 | 0.91 |
| 1:1A:1082:U:N3 | 1:1A:1086:A:N6 | 2.07 | 0.91 |
| 21:2Z:156:LYS:HE3 | 21:2Z:158:PRO:HD3 | 1.53 | 0.91 |
| 1:1A:1670:C:OP2 | 59:1A:4214:HOH:O | 1.88 | 0.91 |
| 1:2A:2129:C:N4 | 1:2A:2159:G:H1 | 1.69 | 0.90 |
| 32:2a:656:C:O2' | 46:2o:28:GLN:NE2 | 2.05 | 0.89 |
| 1:1A:2821:A:OP2 | 59:1A:4213:HOH:O | 1.89 | 0.89 |
| 33:1b:16:HIS:HB2 | 33:1b:204:ASN:HB3 | 1.56 | 0.88 |
| 32:2a:975:A:H4' | 32:2a:976:G:H5" | 1.55 | 0.88 |
| 1:1A:2096:U:H3 | 1:1A:2193:G:H1 | 1.22 | 0.86 |
| 1:1A:826:U:OP1 | 59:1A:4215:HOH:O | 1.94 | 0.86 |
| 1:1A:2123:G:H1 | 1:1A:2175:C:H42 | 1.19 | 0.86 |
| 32:1a:987:G:H1 | 32:1a:1218:C:H42 | 1.22 | 0.86 |
| 32:2a:1025:U:H3 | 32:2a:1036:G:H1 | 1.24 | 0.86 |
| 32:2a:1055:A:N7 | 32:2a:1200:C:N4 | 2.24 | 0.85 |
| 8:2I:92:VAL:HG23 | 8:2I:96:ASP:HB3 | 1.59 | 0.85 |
| 50:1s:27:GLU:HB2 | 50:1s:28:LYS:HA | 1.59 | 0.85 |
| 32:2a:1086:U:H3 | 32:2a:1099:G:H22 | 1.23 | 0.85 |
| 1:1A:1264:G:OP1 | 27:15:19:ARG:NH2 | 2.07 | 0.85 |
| 1:2A:2138:C:N3 | 1:2A:2153:G:N2 | 2.25 | 0.85 |
| 21:2Z:141:VAL:HG13 | 21:2Z:144:LEU:HB3 | 1.59 | 0.84 |
| 10:2O:48:PRO:HB3 | 32:2a:1422:G:H5" | 1.59 | 0.83 |
| 21:2Z:4:ARG:HG2 | 21:2Z:58:VAL:HB | 1.59 | 0.83 |
| 1:2A:2592:G:OP1 | 59:2A:3905:HOH:O | 1.95 | 0.83 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 32:2a:559:A:H4' | 32:2a:560:U:H3' | 1.59 | 0.83 |
| 32:2a:1000:U:H2' | 32:2a:1001:A:H8 | 1.41 | 0.83 |
| 1:1A:2136:C:N3 | 1:1A:2155:G:N2 | 2.26 | 0.83 |
| 10:2O:24:VAL:HG13 | 10:2O:33:ALA:HB2 | 1.60 | 0.83 |
| 32:2a:1256:A:H61 | 32:2a:1278:U:H1' | 1.43 | 0.83 |
| 19:1X:57:LEU:HD11 | 19:1X:78:LYS:HE2 | 1.59 | 0.83 |
| 22:10:11:ARG:O | 22:10:14:ARG:NH2 | 2.11 | 0.83 |
| 32:1a:945:G:OP2 | 59:1a:1903:HOH:O | 1.97 | 0.83 |
| 11:1P:50:ARG:HD3 | 30:18:7:HIS:CD2 | 2.14 | 0.83 |
| 32:1a:1030(C):G:N7 | 32:1a:1031:G:N2 | 2.26 | 0.82 |
| 11:2P:56:SER:HB2 | 11:2P:61:ARG:HD2 | 1.59 | 0.82 |
| 1:2A:2104:G:H1 | 1:2A:2185:C:N4 | 1.78 | 0.82 |
| 32:1a:501:C:OP1 | 43:1l:117:ARG:NH2 | 2.13 | 0.82 |
| 32:2a:584:G:H5' | 48:2q:91:ARG:HH12 | 1.44 | 0.81 |
| 1:1A:279:C:H42 | 1:1A:361:G:H1 | 1.26 | 0.81 |
| 10:1O:48:PRO:HB3 | 32:1a:1422:G:H5" | 1.63 | 0.81 |
| 44:2m:34:LEU:HD13 | 44:2m:41:PRO:HB3 | 1.62 | 0.81 |
| 1:1A:2592:G:OP1 | 59:1A:4217:HOH:O | 1.98 | 0.81 |
| 1:1A:1970:A:OP1 | 59:1A:4216:HOH:O | 1.98 | 0.81 |
| 1:1A:2756:U:O4 | 1:1A:2758:A:N6 | 2.14 | 0.81 |
| 1:1A:956:G:O6 | 59:1A:4220:HOH:O | 1.99 | 0.80 |
| 1:2A:631:A:OP1 | 11:2P:65:ARG:NH1 | 2.13 | 0.80 |
| 35:1d:107:ARG:HH21 | 35:1d:194:LEU:HD21 | 1.43 | 0.80 |
| 32:2a:363:A:OP2 | 43:2l:34:ARG:NH1 | 2.15 | 0.80 |
| 32:2a:1030(A):G:N2 | 32:2a:1030(D):A:OP2 | 2.14 | 0.80 |
| 19:2X:57:LEU:HD11 | 19:2X:78:LYS:HE2 | 1.63 | 0.80 |
| 32:1a:975:A:H4' | 32:1a:976:G:H5" | 1.62 | 0.80 |
| 8:2I:89:TYR:CE1 | 8:2I:89:TYR:CZ | 2.70 | 0.80 |
| 1:1A:2427:C:OP1 | 59:1A:4215:HOH:O | 1.99 | 0.80 |
| 15:1T:35:LYS:HG2 | 15:1T:40:THR:HG22 | 1.63 | 0.80 |
| 34:2c:79:ARG:H | 34:2c:82:GLU:HB3 | 1.47 | 0.80 |
| 1:1A:762:U:OP1 | 59:1A:4218:HOH:O | 1.98 | 0.79 |
| 1:1A:2128:C:N4 | 1:1A:2160:G:H1 | 1.80 | 0.79 |
| 4:2E:127:ASP:OD2 | 59:2E:401:HOH:O | 2.00 | 0.79 |
| 8:2I:69:LYS:HD2 | 8:2I:138:ILE:HG12 | 1.63 | 0.79 |
| 1:1A:2453:A:OP1 | 59:1A:4219:HOH:O | 1.99 | 0.79 |
| 28:16:25:LYS:NZ | 28:16:51:GLU:OE2 | 2.15 | 0.79 |
| 32:1a:407:G:H5" | 35:1d:115:ARG:HG2 | 1.64 | 0.79 |
| 1:2A:1670:C:OP1 | 59:2A:3907:HOH:O | 2.00 | 0.79 |
| 32:2a:1274:G:N2 | 32:2a:1275:A:N7 | 2.26 | 0.79 |
| 41:2j:35:SER:HB3 | 41:2j:73:ASP:HB2 | 1.64 | 0.79 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 26:14:55:ARG:H | 26:14:56:VAL:HA | 1.46 | 0.79 |
| 32:1a:1008:C:N3 | 32:1a:1021:G:O6 | 2.14 | 0.79 |
| 51:2t:50:GLU:HG3 | 51:2t:100:ILE:HD11 | 1.63 | 0.79 |
| 34:2c:118:GLN:HA | 34:2c:121:ALA:HB3 | 1.63 | 0.79 |
| 1:1A:2136:C:N4 | 1:1A:2155:G:N1 | 2.30 | 0.79 |
| 1:2A:994:C:OP1 | 16:2U:53:ARG:NH2 | 2.15 | 0.79 |
| 1:1A:1669:A:OP2 | 59:1A:4214:HOH:O | 2.01 | 0.79 |
| 59:1A:4213:HOH:O | 4:1E:110:GLY:O | 2.00 | 0.79 |
| 1:2A:2682:U:O2' | 15:2T:58:ASN:ND2 | 2.15 | 0.79 |
| 1:1A:392:C:OP1 | 59:1A:4221:HOH:O | 1.99 | 0.79 |
| 44:1m:58:GLU:O | 44:1m:62:ASN:ND2 | 2.15 | 0.79 |
| 5:2F:53:THR:HG23 | 5:2F:55:GLY:H | 1.47 | 0.79 |
| 11:1P:52:GLU:OE1 | 11:1P:55:ARG:NH1 | 2.15 | 0.78 |
| 32:1a:1086:U:H3 | 32:1a:1099:G:H22 | 1.31 | 0.78 |
| 43:2l:32:PHE:HB3 | 43:2l:84:LEU:HD11 | 1.65 | 0.78 |
| 3:1D:180:GLY:HA3 | 3:1D:275:LYS:HG2 | 1.65 | 0.78 |
| 1:2A:1785:A:OP1 | 59:2A:3906:HOH:O | 2.00 | 0.78 |
| 1:1A:301:G:OP2 | 20:1Y:84:ARG:NH2 | 2.17 | 0.78 |
| 1:1A:1014:U:OP2 | 59:1A:4224:HOH:O | 2.02 | 0.78 |
| 1:1A:2163:C:OP1 | 1:1A:2165:G:N2 | 2.17 | 0.78 |
| 32:1a:1314:C:OP2 | 50:1s:4:SER:OG | 2.00 | 0.78 |
| 1:1A:1653:G:H3' | 13:1R:2:ARG:HD3 | 1.65 | 0.78 |
| 1:1A:1059:G:N2 | 1:1A:1079:C:N3 | 2.31 | 0.78 |
| 1:1A:1604:C:OP2 | 59:1A:4223:HOH:O | 2.02 | 0.78 |
| 32:1a:877:C:OP1 | 39:1h:88:LYS:NZ | 2.13 | 0.78 |
| 1:1A:272(G):C:H42 | 1:1A:363(C):G:H1 | 1.32 | 0.77 |
| 32:1a:1004:A:H5" | 32:1a:1024:G:H22 | 1.49 | 0.77 |
| 32:1a:1027:C:C2 | 32:1a:1034:G:N2 | 2.52 | 0.77 |
| 6:2G:73:ALA:HB3 | 6:2G:85:GLY:H | 1.47 | 0.77 |
| 32:1a:506:G:OP1 | 59:1a:1904:HOH:O | 2.01 | 0.77 |
| 1:1A:272(J):C:H2' | 1:1A:274:G:H8 | 1.50 | 0.77 |
| 1:1A:2405:G:H5" | 11:1P:75:ILE:HG21 | 1.66 | 0.77 |
| 1:1A:792:G:O6 | 59:1A:4222:HOH:O | 2.01 | 0.77 |
| 32:2a:953:G:H5' | 32:2a:965:A:H61 | 1.47 | 0.77 |
| 1:1A:2123:G:H2' | 1:1A:2124:G:H8 | 1.50 | 0.77 |
| 1:2A:64:A:N6 | 1:2A:90:U:O4 | 2.17 | 0.77 |
| 36:1e:144:THR:H | 36:1e:147:ASP:HB2 | 1.50 | 0.77 |
| 1:2A:888:C:OP1 | 44:2m:93:ARG:NH1 | 2.18 | 0.77 |
| 32:2a:1402:4OC:HM22 | 32:2a:1403:C:H5' | 1.64 | 0.77 |
| 35:1d:12:CYS:HB2 | 58:1d:501:SF4:S2 | 2.25 | 0.77 |
| 1:2A:228:A:OP1 | 11:2P:76:LYS:NZ | 2.17 | 0.77 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:2A:2404:C:O3' | 11:2P:77:ARG:NH2 | 2.18 | 0.77 |
| 1:2A:2162:G:H4' | 1:2A:2172:U:H2' | 1.67 | 0.76 |
| 12:1Q:18:LYS:O | 12:1Q:98:LYS:NZ | 2.15 | 0.76 |
| 43:1l:84:LEU:HB3 | 43:1l:104:VAL:HG21 | 1.67 | 0.76 |
| 51:1t:89:ARG:HH22 | 51:1t:103:GLY:HA3 | 1.51 | 0.76 |
| 6:1G:27:ASN:HB3 | 6:1G:30:GLU:HG3 | 1.67 | 0.76 |
| 1:2A:601:C:O2' | 5:2F:104:LYS:NZ | 2.19 | 0.76 |
| 48:2q:67:LYS:HA | 48:2q:70:ARG:HH12 | 1.50 | 0.76 |
| 1:2A:857:C:OP2 | 22:20:77:ARG:NH2 | 2.19 | 0.76 |
| 8:2I:52:ARG:HA | 8:2I:55:ALA:HB3 | 1.67 | 0.76 |
| 32:2a:376:G:H5" | 47:2p:5:ARG:HB2 | 1.68 | 0.76 |
| 1:2A:987:G:O2' | 1:2A:1000:A:N3 | 2.17 | 0.76 |
| 1:2A:2297:C:O2 | 1:2A:2321:G:N2 | 2.14 | 0.76 |
| 1:2A:2807:G:N1 | 1:2A:2893:G:O6 | 2.18 | 0.76 |
| 45:1n:4:LYS:HA | 45:1n:7:ILE:HG23 | 1.68 | 0.76 |
| 1:1A:568:U:O2' | 59:1A:4226:HOH:O | 2.03 | 0.76 |
| 1:1A:1968:G:OP1 | 59:1A:4217:HOH:O | 2.04 | 0.76 |
| 1:2A:587:C:OP2 | 11:2P:21:ARG:NH2 | 2.19 | 0.76 |
| 9:2N:20:GLY:HA2 | 9:2N:61:ARG:HD2 | 1.68 | 0.76 |
| 44:1m:65:LYS:HB2 | 44:1m:69:GLU:HG2 | 1.68 | 0.75 |
| 2:1B:31:C:O2 | 2:1B:53:A:N6 | 2.20 | 0.75 |
| 42:1k:99:GLN:HE21 | 42:1k:105:VAL:HG11 | 1.51 | 0.75 |
| 47:1p:67:THR:H | 47:1p:70:ALA:HB3 | 1.50 | 0.75 |
| 1:2A:2127:G:O2' | 1:2A:2173:A:N3 | 2.17 | 0.75 |
| 40:1i:50:LEU:HD13 | 40:1i:56:LEU:HA | 1.68 | 0.75 |
| 1:1A:1990:C:OP2 | 59:1A:4225:HOH:O | 2.03 | 0.75 |
| 1:2A:568:U:O4 | 59:2A:3911:HOH:O | 2.05 | 0.75 |
| 1:2A:752:A:H3' | 29:27:1:MET:HE1 | 1.68 | 0.75 |
| 33:2b:88:ALA:HB2 | 33:2b:219:VAL:HG13 | 1.67 | 0.75 |
| 1:1A:1648:C:OP1 | 59:1A:4227:HOH:O | 2.03 | 0.75 |
| 1:1A:2683:C:O2 | 10:1O:70:LYS:NZ | 2.15 | 0.75 |
| 40:1i:21:PRO:HA | 40:1i:59:PHE:HA | 1.68 | 0.75 |
| 42:1k:85:ARG:HD3 | 42:1k:113:PRO:HD3 | 1.67 | 0.75 |
| 1:2A:2821:A:OP2 | 59:2A:3908:HOH:O | 2.03 | 0.75 |
| 32:2a:1000:U:H2' | 32:2a:1001:A:C8 | 2.21 | 0.75 |
| 4:1E:28:ALA:HB3 | 4:1E:93:VAL:HG12 | 1.69 | 0.75 |
| 1:1A:441:U:O2 | 5:1F:46:ARG:NH2 | 2.20 | 0.74 |
| 32:1a:55:A:C5 | 32:1a:55:A:C8 | 2.75 | 0.74 |
| 1:2A:1968:G:OP1 | 59:2A:3905:HOH:O | 2.04 | 0.74 |
| 2:1B:66:A:H61 | 2:1B:109:C:H5' | 1.52 | 0.74 |
| 25:13:10:LYS:NZ | 25:13:15:TYR:OH | 2.20 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:2A:2448:A:OP1 | 59:2A:3909:HOH:O | 2.04 | 0.74 |
| 14:2S:83:LYS:HB2 | 14:2S:111:GLU:HG3 | 1.67 | 0.74 |
| 32:2a:1129:C:O2' | 32:2a:1130:A:N7 | 2.18 | 0.74 |
| 1:1A:631:A:OP1 | 11:1P:65:ARG:NH1 | 2.21 | 0.74 |
| 42:2k:62:GLN:OE1 | 42:2k:93:GLN:NE2 | 2.21 | 0.74 |
| 1:2A:2364:C:OP1 | 22:20:55:ARG:NH1 | 2.20 | 0.74 |
| 4:2E:143:ASN:HD22 | 4:2E:147:PRO:HD3 | 1.51 | 0.74 |
| 1:1A:1185:C:OP2 | 59:1A:4228:HOH:O | 2.04 | 0.74 |
| 33:1b:21:ARG:HH22 | 33:1b:23:ARG:HD2 | 1.51 | 0.74 |
| 32:2a:959:A:HO2' | 32:2a:984:C:HO2' | 1.26 | 0.74 |
| 32:2a:1128:C:H1' | 32:2a:1147:C:H42 | 1.53 | 0.74 |
| 26:14:16:CYS:SG | 26:14:17:GLY:N | 2.61 | 0.74 |
| 1:2A:218:A:OP2 | 59:2A:3912:HOH:O | 2.05 | 0.74 |
| 23:21:23:LYS:HB3 | 23:21:29:GLY:HA3 | 1.68 | 0.74 |
| 32:2a:151:A:N6 | 32:2a:170:U:O2 | 2.18 | 0.74 |
| 1:1A:1418:G:N7 | 59:1A:4292:HOH:O | 2.20 | 0.74 |
| 1:1A:2839:G:H5' | 13:1R:46:GLY:HA2 | 1.69 | 0.74 |
| 1:1A:298:G:OP2 | 59:1A:4229:HOH:O | 2.05 | 0.74 |
| 32:1a:518:C:O2' | 32:1a:1492:A:N6 | 2.21 | 0.74 |
| 44:2m:37:THR:O | 44:2m:55:ARG:NH1 | 2.21 | 0.74 |
| 1:1A:1930:G:O6 | 59:1A:4232:HOH:O | 2.05 | 0.74 |
| 32:1a:584:G:H5' | 48:1q:91:ARG:HH22 | 1.53 | 0.74 |
| 35:2d:122:ARG:NH1 | 35:2d:134:ASP:O | 2.20 | 0.74 |
| 36:1e:78:HIS:HE1 | 36:1e:143:ARG:H | 1.36 | 0.73 |
| 1:2A:1633:G:OP2 | 59:2A:3910:HOH:O | 2.05 | 0.73 |
| 2:2B:48:A:H4' | 14:2S:95:HIS:HD2 | 1.52 | 0.73 |
| 8:2I:78:THR:HG1 | 8:2I:143:SER:HG | 1.24 | 0.73 |
| 33:1b:69:LEU:HB3 | 33:1b:162:ILE:HG22 | 1.69 | 0.73 |
| 11:2P:126:VAL:HG12 | 11:2P:148:LEU:HD22 | 1.69 | 0.73 |
| 2:2B:54:G:OP2 | 59:2B:301:HOH:O | 2.07 | 0.73 |
| 20:2Y:77:PRO:HD2 | 20:2Y:106:LEU:HD22 | 1.70 | 0.73 |
| 34:2c:52:LEU:HD13 | 34:2c:68:VAL:HG13 | 1.67 | 0.73 |
| 1:1A:833:U:O2 | 11:1P:55:ARG:NH2 | 2.20 | 0.73 |
| 32:1a:642:A:N3 | 39:1h:113:SER:OG | 2.21 | 0.73 |
| 32:2a:742:G:OP2 | 46:2o:35:ARG:NH1 | 2.22 | 0.73 |
| 1:1A:422:A:OP2 | 59:1A:4233:HOH:O | 2.06 | 0.73 |
| 1:1A:1865:G:OP1 | 59:1A:4230:HOH:O | 2.05 | 0.73 |
| 21:1Z:139:VAL:HG22 | 21:1Z:155:LEU:HD11 | 1.71 | 0.73 |
| 1:2A:2138:C:H42 | 1:2A:2153:G:H1 | 0.79 | 0.73 |
| 40:2i:46:ALA:HA | 40:2i:78:LYS:HB2 | 1.71 | 0.73 |
| 1:2A:2436:G:O6 | 59:2A:3913:HOH:O | 2.06 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 11:1P:50:ARG:HD3 | 30:18:7:HIS:HD2 | 1.53 | 0.73 |
| 32:1a:14:U:OP2 | 59:1a:1905:HOH:O | 2.07 | 0.72 |
| 32:1a:1021:G:O2' | 32:1a:1022:G:O5' | 2.07 | 0.72 |
| 50:2s:11:VAL:O | 50:2s:13:ASP:N | 2.21 | 0.72 |
| 1:1A:467:G:OP1 | 29:17:33:ARG:NH1 | 2.22 | 0.72 |
| 1:1A:637:A:H8 | 11:1P:117:GLU:HG3 | 1.52 | 0.72 |
| 1:1A:2452:C:OP1 | 59:1A:4234:HOH:O | 2.07 | 0.72 |
| 2:1B:89:G:OP1 | 59:1B:301:HOH:O | 2.06 | 0.72 |
| 1:2A:2057:A:OP2 | 59:2A:3915:HOH:O | 2.07 | 0.72 |
| 1:2A:2589:A:OP1 | 59:2A:3914:HOH:O | 2.07 | 0.72 |
| 3:2D:71:ASP:HB2 | 3:2D:103:ARG:HH12 | 1.53 | 0.72 |
| 1:2A:602:G:O2' | 1:2A:655:A:N6 | 2.23 | 0.72 |
| 35:1d:15:GLU:OE2 | 35:1d:66:ARG:NH1 | 2.22 | 0.72 |
| 39:1h:119:LEU:HB3 | 39:1h:123:GLU:HB2 | 1.71 | 0.72 |
| 44:1m:80:ARG:NH1 | 50:1s:65:ASN:O | 2.21 | 0.72 |
| 46:2o:87:ILE:HG22 | 46:2o:88:ARG:H | 1.55 | 0.72 |
| 1:2A:1204:A:H2 | 1:2A:1241:A:H62 | 1.36 | 0.72 |
| 1:2A:1689:A:H62 | 1:2A:1698:A:H2 | 1.37 | 0.72 |
| 21:2Z:45:ASP:OD1 | 21:2Z:49:ARG:NH1 | 2.21 | 0.72 |
| 24:22:32:LEU:HD11 | 24:22:54:LYS:HG3 | 1.70 | 0.72 |
| 40:2i:23:ASN:HD21 | 40:2i:25:LYS:HG2 | 1.55 | 0.72 |
| 1:1A:918:A:N3 | 2:1B:80:U:O2' | 2.22 | 0.72 |
| 8:1I:79:ILE:HD13 | 8:1I:92:VAL:HG21 | 1.71 | 0.72 |
| 32:2a:642:A:N3 | 39:2h:113:SER:OG | 2.23 | 0.72 |
| 32:1a:1435:G:H2' | 32:1a:1436:U:C6 | 2.25 | 0.72 |
| 21:2Z:100:VAL:HG21 | 21:2Z:134:PRO:HG2 | 1.72 | 0.72 |
| 43:1l:70:ILE:HG12 | 43:1l:100:ILE:HD12 | 1.70 | 0.72 |
| 15:2T:41:ARG:NH2 | 32:2a:346:G:OP1 | 2.22 | 0.72 |
| 32:2a:1232:U:OP1 | 40:2i:124:GLN:NE2 | 2.23 | 0.72 |
| 3:1D:8:PRO:HB3 | 3:1D:14:ARG:HB3 | 1.72 | 0.72 |
| 17:1V:76:LYS:HB2 | 17:1V:81:TYR:HB3 | 1.71 | 0.72 |
| 32:1a:812:C:N3 | 59:1a:1919:HOH:O | 2.22 | 0.72 |
| 1:2A:994:C:H3' | 16:2U:54:LYS:HE3 | 1.71 | 0.72 |
| 32:2a:1381:U:H1' | 38:2g:79:ARG:HE | 1.55 | 0.72 |
| 1:2A:637:A:H8 | 11:2P:117:GLU:HG3 | 1.54 | 0.71 |
| 1:2A:2552:2MU:OP2 | 59:2A:3917:HOH:O | 2.08 | 0.71 |
| 1:1A:530:G:N1 | 1:1A:2023:G:OP1 | 2.22 | 0.71 |
| 1:1A:1062:G:P | 1:1A:1070:A:H1' | 2.30 | 0.71 |
| 1:1A:2100:G:H1 | 1:1A:2189:U:H3 | 0.76 | 0.71 |
| 33:1b:69:LEU:HD23 | 33:1b:91:PRO:HB2 | 1.72 | 0.71 |
| 46:1o:54:ARG:HG2 | 46:1o:58:MET:HE2 | 1.72 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:2A:2296:U:OP2 | 14:2S:9:ARG:NH2 | 2.23 | 0.71 |
| 32:2a:823:G:H1 | 32:2a:877:C:H42 | 1.36 | 0.71 |
| 1:1A:307:G:N7 | 59:1A:4306:HOH:O | 2.23 | 0.71 |
| 1:1A:2749:A:OP1 | 7:1H:3:ARG:NH1 | 2.22 | 0.71 |
| 3:1D:71:ASP:HB3 | 3:1D:103:ARG:HH12 | 1.54 | 0.71 |
| 32:1a:559:A:OP1 | 36:1e:126:ARG:NH2 | 2.22 | 0.71 |
| 32:1a:1108:G:O6 | 59:1a:1906:HOH:O | 2.07 | 0.71 |
| 32:2a:401:C:OP2 | 35:2d:73:ARG:NH2 | 2.23 | 0.71 |
| 32:2a:1027:C:N4 | 32:2a:1036:G:O6 | 2.22 | 0.71 |
| 12:1Q:111:GLU:OE2 | 12:1Q:133:ARG:NH2 | 2.23 | 0.71 |
| 32:1a:1445:C:O2' | 32:1a:1447:A:N6 | 2.24 | 0.71 |
| 1:1A:448:U:OP2 | 59:1A:4237:HOH:O | 2.09 | 0.71 |
| 34:1c:131:ARG:HH11 | 34:1c:166:GLU:HG3 | 1.53 | 0.71 |
| 39:2h:34:GLU:HB3 | 39:2h:118:VAL:HG11 | 1.72 | 0.71 |
| 44:2m:31:LYS:HA | 44:2m:34:LEU:HD12 | 1.72 | 0.71 |
| 1:1A:2646:C:OP2 | 1:1A:2732:G:O2' | 2.07 | 0.71 |
| 32:1a:719:C:H1' | 49:1r:49:LYS:HB3 | 1.73 | 0.71 |
| 1:2A:586:A:N1 | 1:2A:809:G:O2' | 2.22 | 0.71 |
| 1:2A:761:A:OP2 | 59:2A:3923:HOH:O | 2.09 | 0.71 |
| 1:2A:2292:C:OP1 | 14:2S:17:ARG:NH2 | 2.21 | 0.71 |
| 1:1A:248:G:OP1 | 59:1A:4236:HOH:O | 2.08 | 0.71 |
| 1:1A:2379:G:O2' | 14:1S:17:ARG:NH1 | 2.20 | 0.71 |
| 1:1A:1058:G:H1 | 1:1A:1080:C:H42 | 1.36 | 0.71 |
| 32:1a:574:A:OP2 | 59:1a:1909:HOH:O | 2.09 | 0.71 |
| 1:2A:222:A:OP1 | 59:2A:3920:HOH:O | 2.09 | 0.71 |
| 1:2A:1975:G:OP2 | 59:2A:3919:HOH:O | 2.09 | 0.71 |
| 1:1A:918:A:O2' | 2:1B:97:G:N2 | 2.24 | 0.70 |
| 1:1A:2123:G:H1 | 1:1A:2175:C:N4 | 1.89 | 0.70 |
| 39:1h:9:MET:HE3 | 39:1h:32:LYS:HB3 | 1.72 | 0.70 |
| 1:2A:882:G:H1 | 1:2A:894:C:H42 | 1.39 | 0.70 |
| 5:2F:21:ALA:HB3 | 5:2F:22:ALA:HA | 1.73 | 0.70 |
| 32:2a:1011:G:H1 | 32:2a:1018:C:N4 | 1.88 | 0.70 |
| 41:2j:6:ILE:HG12 | 41:2j:98:ILE:HG22 | 1.72 | 0.70 |
| 1:2A:2206:G:H3' | 1:2A:2207:G:C8 | 2.26 | 0.70 |
| 1:2A:2518:A:OP2 | 59:2A:3916:HOH:O | 2.08 | 0.70 |
| 32:2a:117:G:OP2 | 59:2a:3302:HOH:O | 2.08 | 0.70 |
| 32:2a:1133:G:N2 | 32:2a:1141:C:N3 | 2.37 | 0.70 |
| 35:2d:18:LYS:NZ | 35:2d:31:CYS:SG | 2.64 | 0.70 |
| 39:2h:119:LEU:HB3 | 39:2h:123:GLU:HG3 | 1.72 | 0.70 |
| 1:1A:1784:A:OP2 | 59:1A:4241:HOH:O | 2.09 | 0.70 |
| 1:2A:2126:A:N6 | 1:2A:2162:G:O2' | 2.23 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1A:86:C:H4' | 1:1A:104:U:H1' | 1.72 | 0.70 |
| 3:1D:242:ARG:O | 59:1D:401:HOH:O | 2.08 | 0.70 |
| 18:2W:34:ASN:OD1 | 18:2W:37:ARG:NH2 | 2.25 | 0.70 |
| 44:2m:33:ALA:O | 44:2m:37:THR:OG1 | 2.08 | 0.70 |
| 1:1A:2059:A:OP2 | 59:1A:4235:HOH:O | 2.08 | 0.70 |
| 1:1A:2153:G:H2' | 1:1A:2154:G:H8 | 1.56 | 0.70 |
| 1:1A:2855:C:H2' | 1:1A:2856:C:H6 | 1.56 | 0.70 |
| 1:1A:2156:G:H2' | 1:1A:2157:G:C2 | 2.27 | 0.70 |
| 23:11:77:ALA:HB2 | 23:11:94:LEU:HD21 | 1.73 | 0.70 |
| 32:1a:766:A:OP2 | 59:1a:1907:HOH:O | 2.08 | 0.70 |
| 1:2A:198:C:OP2 | 59:2A:3903:HOH:O | 2.10 | 0.70 |
| 1:2A:2049:G:N7 | 59:2A:3976:HOH:O | 2.25 | 0.70 |
| 32:1a:558:G:OP1 | 59:1a:1908:HOH:O | 2.09 | 0.70 |
| 51:1t:83:ARG:HA | 51:1t:86:ARG:HH11 | 1.57 | 0.70 |
| 1:1A:995:C:OP2 | 16:1U:54:LYS:NZ | 2.25 | 0.70 |
| 1:1A:2327:A:H2' | 1:1A:2328:A:C8 | 2.27 | 0.70 |
| 5:1F:32:LEU:HD13 | 5:1F:112:MET:HE1 | 1.73 | 0.70 |
| 1:2A:2547:U:O2 | 10:2O:23:ARG:NH2 | 2.25 | 0.70 |
| 32:2a:903:G:OP1 | 59:2a:3303:HOH:O | 2.10 | 0.70 |
| 32:2a:1273:G:H3' | 32:2a:1274:G:H8 | 1.56 | 0.70 |
| 22:10:27:GLU:HG3 | 22:10:68:GLU:HA | 1.73 | 0.69 |
| 44:1m:3:ARG:HG2 | 44:1m:8:GLU:HA | 1.72 | 0.69 |
| 1:1A:1332:G:OP1 | 59:1A:4243:HOH:O | 2.09 | 0.69 |
| 1:2A:2502:G:OP2 | 59:2A:3918:HOH:O | 2.08 | 0.69 |
| 1:1A:615:G:OP2 | 5:1F:43:LYS:NZ | 2.24 | 0.69 |
| 1:1A:2589:A:OP1 | 59:1A:4240:HOH:O | 2.09 | 0.69 |
| 32:1a:1008:C:O2 | 32:1a:1021:G:N1 | 2.21 | 0.69 |
| 54:1x:8:4SU:O2 | 54:1x:21:A:H2 | 1.75 | 0.69 |
| 1:2A:1604:C:OP1 | 59:2A:3922:HOH:O | 2.09 | 0.69 |
| 1:2A:1671:U:OP2 | 59:2A:3907:HOH:O | 2.10 | 0.69 |
| 32:2a:9:G:H2' | 32:2a:10:A:H8 | 1.58 | 0.69 |
| 32:1a:1002:G:H3' | 32:1a:1003:G:H4' | 1.75 | 0.69 |
| 30:28:33:ASN:HA | 30:28:36:LYS:HD2 | 1.74 | 0.69 |
| 1:1A:962:G:OP1 | 59:1A:4242:HOH:O | 2.09 | 0.69 |
| 11:1P:42:SER:O | 59:1P:302:HOH:O | 2.10 | 0.69 |
| 49:1r:32:ARG:HA | 49:1r:69:THR:HG21 | 1.74 | 0.69 |
| 1:2A:745:G:O6 | 59:2A:3925:HOH:O | 2.10 | 0.69 |
| 1:2A:2242:G:OP1 | 59:2A:3927:HOH:O | 2.10 | 0.69 |
| 7:2H:33:LEU:HD21 | 7:2H:136:ILE:HB | 1.75 | 0.69 |
| 38:2g:115:ARG:HG2 | 38:2g:118:VAL:HG23 | 1.74 | 0.69 |
| 1:1A:1324:G:OP2 | 59:1A:4246:HOH:O | 2.10 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 39:1h:10:LEU:HD22 | 39:1h:83:ILE:HD11 | 1.73 | 0.69 |
| 1:1A:511:U:OP2 | 59:1A:4249:HOH:O | 2.11 | 0.69 |
| 1:1A:1010:A:OP2 | 59:1A:4247:HOH:O | 2.10 | 0.69 |
| 26:14:58:ARG:HG3 | 50:1s:68:GLY:H | 1.56 | 0.69 |
| 32:1a:1356:G:H2' | 32:1a:1357:A:C8 | 2.28 | 0.69 |
| 1:2A:1434:A:H61 | 1:2A:1558:A:H62 | 1.40 | 0.69 |
| 7:2H:15:VAL:HG12 | 7:2H:29:PRO:HD3 | 1.74 | 0.69 |
| 23:21:2:SER:HB3 | 23:21:46:LEU:HD12 | 1.74 | 0.69 |
| 32:2a:316:G:OP2 | 32:2a:351:G:O2' | 2.10 | 0.69 |
| 1:1A:399:G:OP2 | 59:1A:4244:HOH:O | 2.09 | 0.69 |
| 1:1A:1244:G:OP2 | 59:1A:4239:HOH:O | 2.09 | 0.69 |
| 1:1A:2131:G:N2 | 1:1A:2133:G:N3 | 2.41 | 0.69 |
| 9:1N:77:GLY:O | 59:1N:301:HOH:O | 2.09 | 0.69 |
| 52:1u:17:THR:O | 52:1u:22:ARG:NH1 | 2.26 | 0.69 |
| 1:2A:637:A:H5" | 11:2P:117:GLU:HG2 | 1.73 | 0.69 |
| 32:2a:596:C:O2 | 32:2a:644:G:N2 | 2.17 | 0.69 |
| 41:2j:49:VAL:HG23 | 45:2n:41:ARG:HB2 | 1.75 | 0.69 |
| 1:1A:2206:G:H3' | 1:1A:2207:G:C8 | 2.29 | 0.69 |
| 35:1d:100:ARG:HH22 | 35:1d:118:ARG:HH21 | 1.39 | 0.69 |
| 44:1m:23:TYR:HB3 | 44:1m:67:GLU:HA | 1.74 | 0.69 |
| 1:2A:1383:C:O2 | 59:2A:3924:HOH:O | 2.09 | 0.69 |
| 32:2a:539:A:H2' | 32:2a:540:G:C8 | 2.28 | 0.69 |
| 1:1A:773:U:OP1 | 59:1A:4238:HOH:O | 2.09 | 0.68 |
| 16:1U:27:LEU:HB3 | 16:1U:31:SER:HB3 | 1.72 | 0.68 |
| 31:29:25:VAL:HB | 31:29:34:GLN:HB2 | 1.75 | 0.68 |
| 1:1A:602:G:O2' | 1:1A:655:A:N6 | 2.26 | 0.68 |
| 1:1A:2499:C:OP1 | 59:1A:4253:HOH:O | 2.11 | 0.68 |
| 1:2A:2042:A:OP1 | 59:2A:3931:HOH:O | 2.12 | 0.68 |
| 41:2j:17:ASP:OD1 | 41:2j:70:ARG:NE | 2.25 | 0.68 |
| 44:2m:107:ALA:HB3 | 44:2m:111:LYS:HE3 | 1.74 | 0.68 |
| 1:1A:1047:G:H2' | 1:1A:1110:G:H22 | 1.56 | 0.68 |
| 1:1A:1997:G:OP2 | 59:1A:4248:HOH:O | 2.11 | 0.68 |
| 1:1A:2285:C:OP2 | 28:16:6:ARG:NH1 | 2.26 | 0.68 |
| 35:1d:88:VAL:HA | 36:1e:97:GLY:HA3 | 1.74 | 0.68 |
| 54:2x:40:C:H2' | 54:2x:41:C:H6 | 1.58 | 0.68 |
| 1:1A:400:G:N7 | 59:1A:4321:HOH:O | 2.25 | 0.68 |
| 1:1A:2550:G:OP1 | 59:1A:4214:HOH:O | 2.10 | 0.68 |
| 1:2A:271(H):G:H5' | 23:21:81:LYS:HE3 | 1.74 | 0.68 |
| 1:2A:370:G:OP2 | 59:2A:3928:HOH:O | 2.11 | 0.68 |
| 4:2E:105:THR:OG1 | 4:2E:199:ARG:NH2 | 2.25 | 0.68 |
| 12:2Q:26:TYR:O | 12:2Q:67:ARG:NH1 | 2.26 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1A:1453:U:O2' | 1:1A:1455:G:N7 | 2.27 | 0.68 |
| 3:1D:12:SER:HB3 | 3:1D:208:LYS:HB3 | 1.74 | 0.68 |
| 8:1I:129:THR:HG22 | 8:1I:139:GLN:HE22 | 1.59 | 0.68 |
| 15:2T:85:LYS:NZ | 15:2T:87:ASP:OD2 | 2.25 | 0.68 |
| 32:2a:1011:G:H1 | 32:2a:1018:C:H42 | 1.40 | 0.68 |
| 32:2a:1245:A:H61 | 32:2a:1292:U:H3 | 1.41 | 0.68 |
| 30:18:6:THR:HG22 | 30:18:63:PRO:HD2 | 1.76 | 0.68 |
| 35:1d:3:ARG:HD3 | 35:1d:118:ARG:HD2 | 1.75 | 0.68 |
| 34:2c:47:LEU:HB3 | 34:2c:52:LEU:HB2 | 1.75 | 0.68 |
| 1:1A:2763:G:OP2 | 59:1A:4251:HOH:O | 2.11 | 0.68 |
| 41:1j:38:ILE:HG13 | 41:1j:71:LEU:HB3 | 1.76 | 0.68 |
| 1:2A:89:G:H3' | 1:2A:90:U:H5" | 1.76 | 0.68 |
| 32:2a:1029:C:N4 | 32:2a:1031:G:O6 | 2.27 | 0.68 |
| 43:2l:60:LEU:HD11 | 43:2l:66:VAL:HG22 | 1.75 | 0.68 |
| 20:1Y:15:VAL:HG21 | 20:1Y:42:VAL:HG11 | 1.76 | 0.68 |
| 37:1f:89:MET:HE1 | 49:1r:72:ARG:HB3 | 1.74 | 0.68 |
| 47:1p:53:VAL:HG13 | 47:1p:79:VAL:HG22 | 1.76 | 0.68 |
| 21:2Z:48:PHE:HE1 | 21:2Z:71:VAL:HG11 | 1.58 | 0.68 |
| 1:1A:2366:A:OP1 | 59:1A:4250:HOH:O | 2.11 | 0.68 |
| 32:1a:330:C:O2 | 59:1a:1910:HOH:O | 2.12 | 0.68 |
| 13:2R:97:VAL:HG22 | 13:2R:114:VAL:HG13 | 1.76 | 0.68 |
| 1:1A:1448:G:O2' | 1:1A:1528(A):A:N1 | 2.28 | 0.67 |
| 20:1Y:30:VAL:HG22 | 20:1Y:37:VAL:HG12 | 1.76 | 0.67 |
| 32:1a:356:A:N3 | 32:1a:368:U:O2' | 2.26 | 0.67 |
| 51:1t:29:LYS:HD2 | 51:1t:71:THR:HG21 | 1.74 | 0.67 |
| 1:2A:761:A:OP1 | 59:2A:3930:HOH:O | 2.12 | 0.67 |
| 1:2A:782:A:OP2 | 59:2A:3933:HOH:O | 2.12 | 0.67 |
| 1:2A:870:A:OP1 | 12:2Q:6:ARG:NE | 2.26 | 0.67 |
| 32:2a:737:A:H1' | 37:2f:73:ASN:HD21 | 1.59 | 0.67 |
| 1:1A:2483:C:N3 | 12:1Q:124:LYS:NZ | 2.39 | 0.67 |
| 4:1E:12:THR:HG21 | 15:1T:11:GLU:HG2 | 1.76 | 0.67 |
| 32:1a:1075:C:OP1 | 33:1b:179:LYS:NZ | 2.22 | 0.67 |
| 36:1e:7:GLU:OE2 | 36:1e:37:ARG:NH2 | 2.27 | 0.67 |
| 1:2A:2746:U:OP1 | 7:2H:85:LYS:NZ | 2.26 | 0.67 |
| 3:2D:2:ALA:N | 3:2D:200:ASP:OD2 | 2.28 | 0.67 |
| 5:2F:18:ARG:NH1 | 5:2F:127:GLU:OE2 | 2.27 | 0.67 |
| 21:2Z:31:ARG:HH11 | 21:2Z:94:GLU:HG2 | 1.58 | 0.67 |
| 32:2a:677:U:H3 | 32:2a:713:G:H22 | 1.42 | 0.67 |
| 33:2b:87:ARG:HH11 | 33:2b:219:VAL:HG12 | 1.60 | 0.67 |
| 36:2e:122:GLU:O | 36:2e:126:ARG:NH1 | 2.26 | 0.67 |
| 3:1D:37:LEU:HD13 | 3:1D:62:TYR:HB2 | 1.77 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 32:1a:987:G:H1 | 32:1a:1218:C:N4 | 1.92 | 0.67 |
| 1:2A:1264:G:OP1 | 27:25:19:ARG:NH2 | 2.25 | 0.67 |
| 8:2I:38:LEU:H | 8:2I:38:LEU:HD12 | 1.60 | 0.67 |
| 21:2Z:153:SER:HB2 | 21:2Z:167:PRO:HB3 | 1.76 | 0.67 |
| 32:2a:1348:U:H4' | 40:2i:120:ARG:HD2 | 1.76 | 0.67 |
| 1:2A:2808:U:O2 | 1:2A:2892:A:N6 | 2.28 | 0.67 |
| 21:2Z:41:LEU:HD11 | 21:2Z:82:ARG:HH12 | 1.59 | 0.67 |
| 32:2a:890:G:O2' | 32:2a:906:G:O6 | 2.13 | 0.67 |
| 33:2b:179:LYS:HD3 | 39:2h:72:PRO:HG3 | 1.76 | 0.67 |
| 1:2A:1507:A:O2' | 1:2A:1508:A:O4' | 2.12 | 0.67 |
| 1:2A:2839:G:H5' | 13:2R:46:GLY:HA2 | 1.76 | 0.67 |
| 34:1c:19:GLU:O | 34:1c:40:ARG:NH2 | 2.28 | 0.67 |
| 1:2A:2608:G:N7 | 59:2A:3992:HOH:O | 2.28 | 0.67 |
| 4:2E:28:ALA:HB3 | 4:2E:93:VAL:HG12 | 1.77 | 0.67 |
| 32:2a:976:G:H5' | 32:2a:1358:U:O2' | 1.95 | 0.67 |
| 1:1A:1069:A:H1' | 1:1A:1096:A:H4' | 1.76 | 0.67 |
| 1:1A:1113:U:H2' | 1:1A:1114:G:C8 | 2.29 | 0.67 |
| 6:1G:5:VAL:HG23 | 6:1G:8:LYS:HE2 | 1.76 | 0.67 |
| 43:1l:47:LYS:HG2 | 43:1l:48:PRO:HA | 1.77 | 0.67 |
| 1:2A:1713:U:H2' | 1:2A:1714:G:H8 | 1.60 | 0.67 |
| 1:1A:1183:G:O2' | 25:13:29:ARG:NH1 | 2.28 | 0.67 |
| 1:1A:2445:G:OP1 | 5:1F:74:ARG:NH2 | 2.28 | 0.67 |
| 34:2c:70:VAL:O | 34:2c:106:VAL:N | 2.26 | 0.67 |
| 32:1a:1009:G:O6 | 32:1a:1020:U:O2 | 2.13 | 0.67 |
| 33:1b:82:ARG:NH1 | 33:1b:92:TYR:OH | 2.28 | 0.67 |
| 1:2A:1376:C:OP2 | 59:2A:3929:HOH:O | 2.11 | 0.67 |
| 32:2a:664:G:H22 | 32:2a:741:G:H1 | 1.39 | 0.67 |
| 32:2a:1060:C:H5" | 41:2j:51:ARG:HG2 | 1.77 | 0.67 |
| 5:2F:24:LEU:HD23 | 5:2F:115:ALA:HA | 1.76 | 0.67 |
| 35:2d:156:GLU:HA | 35:2d:159:ARG:HE | 1.59 | 0.67 |
| 32:1a:1352:C:OP1 | 52:1u:3:LYS:NZ | 2.23 | 0.66 |
| 1:2A:1339:G:H5" | 19:2X:16:LYS:HD3 | 1.77 | 0.66 |
| 1:2A:1939:5MU:OP1 | 1:2A:2604:U:O2' | 2.14 | 0.66 |
| 1:1A:527:C:OP1 | 59:1A:4260:HOH:O | 2.14 | 0.66 |
| 1:2A:1648:C:OP1 | 59:2A:3934:HOH:O | 2.12 | 0.66 |
| 1:2A:2759:G:OP2 | 59:2A:3932:HOH:O | 2.12 | 0.66 |
| 1:1A:1064:C:H1' | 1:1A:1076:C:H5 | 1.60 | 0.66 |
| 1:1A:2331:G:N7 | 59:1A:4331:HOH:O | 2.27 | 0.66 |
| 3:1D:2:ALA:N | 59:1D:403:HOH:O | 2.28 | 0.66 |
| 34:1c:56:ASP:HB2 | 34:1c:67:THR:HB | 1.76 | 0.66 |
| 1:2A:2327:A:H2' | 1:2A:2328:A:C8 | 2.29 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:2A:2445:G:OP1 | 5:2F:74:ARG:NH2 | 2.29 | 0.66 |
| 32:2a:1345:U:OP2 | 59:2a:3305:HOH:O | 2.14 | 0.66 |
| 1:1A:2140:C:N3 | 1:1A:2151:G:O6 | 2.28 | 0.66 |
| 2:1B:13:A:N1 | 2:1B:69:G:O2' | 2.24 | 0.66 |
| 24:12:32:LEU:HD11 | 24:12:54:LYS:HG3 | 1.75 | 0.66 |
| 43:2l:84:LEU:HB3 | 43:2l:104:VAL:HG21 | 1.76 | 0.66 |
| 1:1A:249:C:O2 | 30:18:12:LYS:NZ | 2.22 | 0.66 |
| 1:1A:1315:C:OP2 | 59:1A:4243:HOH:O | 2.12 | 0.66 |
| 1:1A:2099:U:O2 | 1:1A:2190:G:N2 | 2.23 | 0.66 |
| 2:1B:105:A:OP1 | 21:1Z:72:ARG:NH1 | 2.27 | 0.66 |
| 3:1D:241:PRO:O | 59:1D:402:HOH:O | 2.12 | 0.66 |
| 8:1I:75:LEU:HD22 | 8:1I:105:HIS:HD2 | 1.59 | 0.66 |
| 32:1a:1047:G:H5" | 45:1n:4:LYS:HD3 | 1.75 | 0.66 |
| 1:2A:2206:G:H5" | 1:2A:2207:G:N7 | 2.11 | 0.66 |
| 32:2a:369:C:H42 | 32:2a:392:G:H1 | 1.44 | 0.66 |
| 1:1A:1890:A:OP2 | 59:1A:4264:HOH:O | 2.14 | 0.66 |
| 3:2D:180:GLY:HA3 | 3:2D:275:LYS:HG2 | 1.77 | 0.66 |
| 15:2T:51:ARG:HB2 | 15:2T:98:LYS:HD2 | 1.76 | 0.66 |
| 34:2c:11:ARG:NH2 | 34:2c:177:THR:O | 2.29 | 0.66 |
| 13:1R:53:HIS:ND1 | 13:1R:94:TYR:OH | 2.27 | 0.66 |
| 22:10:10:THR:HG22 | 22:10:12:ASN:H | 1.60 | 0.66 |
| 15:2T:27:THR:HB | 15:2T:89:VAL:HG22 | 1.77 | 0.66 |
| 32:2a:1347:G:H5" | 40:2i:107:ARG:HB3 | 1.78 | 0.66 |
| 1:1A:1252:G:OP2 | 59:1A:4255:HOH:O | 2.13 | 0.66 |
| 1:1A:1658:C:OP1 | 59:1A:4254:HOH:O | 2.12 | 0.66 |
| 1:1A:2130:U:H2' | 1:1A:2158:A:H61 | 1.61 | 0.66 |
| 1:1A:2155:G:H3' | 1:1A:2156:G:H8 | 1.60 | 0.66 |
| 1:1A:2588:G:OP1 | 59:1A:4257:HOH:O | 2.13 | 0.66 |
| 3:1D:17:THR:O | 3:1D:211:ARG:NH2 | 2.27 | 0.66 |
| 18:1W:4:LYS:HD2 | 18:1W:6:ILE:HD11 | 1.77 | 0.66 |
| 3:2D:146:GLU:HB2 | 3:2D:189:CYS:HB3 | 1.78 | 0.66 |
| 1:1A:1930:G:O2' | 1:1A:1968:G:O6 | 2.11 | 0.66 |
| 33:1b:162:ILE:HD11 | 33:1b:184:VAL:HG22 | 1.78 | 0.66 |
| 1:2A:1299:G:OP1 | 59:2A:3936:HOH:O | 2.14 | 0.66 |
| 7:2H:125:VAL:HG22 | 7:2H:131:VAL:HG22 | 1.79 | 0.66 |
| 1:1A:1528:A:OP2 | 59:1A:4267:HOH:O | 2.15 | 0.65 |
| 1:1A:1859:A:N6 | 1:1A:1883:G:O2' | 2.29 | 0.65 |
| 1:2A:465:G:O6 | 59:2A:3926:HOH:O | 2.10 | 0.65 |
| 34:2c:148:GLY:HA3 | 34:2c:203:PHE:HB3 | 1.79 | 0.65 |
| 1:1A:2400:G:O6 | 59:1A:4258:HOH:O | 2.13 | 0.65 |
| 1:2A:463:G:OP2 | 59:2A:3938:HOH:O | 2.14 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:2A:1022:G:N2 | 1:2A:1023:U:O4 | 2.29 | 0.65 |
| 2:2B:26:A:O2' | 59:2B:302:HOH:O | 2.14 | 0.65 |
| 5:2F:155:LEU:HB2 | 5:2F:189:THR:HG21 | 1.78 | 0.65 |
| 1:1A:1105:U:H2' | 1:1A:1106:G:C8 | 2.32 | 0.65 |
| 8:1I:92:VAL:HG13 | 8:1I:120:ILE:HB | 1.79 | 0.65 |
| 1:1A:449:A:N7 | 59:1A:4351:HOH:O | 2.29 | 0.65 |
| 4:1E:105:THR:OG1 | 4:1E:199:ARG:NH2 | 2.30 | 0.65 |
| 32:1a:1159:U:O4' | 32:1a:1182:G:N2 | 2.30 | 0.65 |
| 46:1o:74:ASP:HB3 | 46:1o:77:ARG:HB2 | 1.76 | 0.65 |
| 1:2A:1688:U:O2 | 1:2A:1700:A:H5' | 1.95 | 0.65 |
| 1:1A:578:A:OP2 | 59:1A:4259:HOH:O | 2.13 | 0.65 |
| 24:12:63:VAL:HA | 24:12:66:GLU:HG2 | 1.79 | 0.65 |
| 28:16:11:LEU:HB2 | 28:16:21:TYR:HB2 | 1.77 | 0.65 |
| 32:1a:412:A:OP2 | 35:1d:35:ARG:NH2 | 2.29 | 0.65 |
| 46:1o:55:GLY:HA2 | 46:1o:58:MET:HE3 | 1.78 | 0.65 |
| 11:2P:62:LEU:HD11 | 30:28:50:LEU:HD11 | 1.78 | 0.65 |
| 1:1A:217:G:OP2 | 59:1A:4269:HOH:O | 2.15 | 0.65 |
| 26:14:55:ARG:N | 26:14:56:VAL:HA | 2.10 | 0.65 |
| 1:2A:2248:C:OP2 | 59:2A:3939:HOH:O | 2.15 | 0.65 |
| 40:2i:16:ARG:HB2 | 40:2i:64:THR:HG22 | 1.77 | 0.65 |
| 8:1I:77:LEU:HB3 | 8:1I:142:VAL:HG12 | 1.79 | 0.65 |
| 2:2B:22:U:H3 | 2:2B:61:G:H1 | 1.45 | 0.65 |
| 32:2a:560:U:OP2 | 59:2a:3307:HOH:O | 2.14 | 0.65 |
| 1:1A:761:A:N7 | 59:1A:4358:HOH:O | 2.29 | 0.65 |
| 1:1A:2176:A:H2' | 1:1A:2177:C:C6 | 2.32 | 0.65 |
| 1:1A:2532:G:O2' | 1:1A:2657:A:N1 | 2.30 | 0.65 |
| 32:1a:1010:G:N2 | 32:1a:1020:U:O2' | 2.30 | 0.65 |
| 32:2a:1280:A:H5' | 41:2j:41:PRO:HD2 | 1.79 | 0.65 |
| 1:1A:2867:G:OP2 | 15:1T:119:LYS:NZ | 2.22 | 0.65 |
| 32:1a:103:C:O2' | 32:1a:172:A:N1 | 2.27 | 0.65 |
| 32:1a:452:A:H4' | 47:1p:72:ARG:CZ | 2.26 | 0.65 |
| 32:1a:1070:U:H2' | 32:1a:1071:C:H6 | 1.62 | 0.65 |
| 46:1o:39:LEU:HD13 | 46:1o:56:LEU:HB2 | 1.76 | 0.65 |
| 1:2A:1603:A:OP1 | 59:2A:3937:HOH:O | 2.14 | 0.65 |
| 32:2a:610:G:OP2 | 59:2a:3306:HOH:O | 2.14 | 0.65 |
| 33:2b:74:LYS:NZ | 33:2b:205:ASP:O | 2.29 | 0.65 |
| 24:12:32:LEU:HD22 | 24:12:36:ARG:HH11 | 1.62 | 0.65 |
| 32:1a:673:G:H2' | 32:1a:674:G:C8 | 2.32 | 0.65 |
| 34:2c:119:ARG:HE | 34:2c:140:ARG:NH2 | 1.95 | 0.65 |
| 37:2f:99:ALA:HB2 | 49:2r:31:LEU:HD11 | 1.78 | 0.65 |
| 44:2m:33:ALA:HB2 | 44:2m:64:TRP:HH2 | 1.62 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 49:2r:32:ARG:HA | 49:2r:69:THR:HG21 | 1.79 | 0.65 |
| 1:1A:1358:G:OP2 | 59:1A:4263:HOH:O | 2.14 | 0.64 |
| 34:1c:64:VAL:HG12 | 34:1c:99:VAL:HA | 1.78 | 0.64 |
| 41:1j:27:ALA:HA | 41:1j:81:THR:HG21 | 1.79 | 0.64 |
| 1:2A:783:A:OP2 | 59:2A:3914:HOH:O | 2.14 | 0.64 |
| 1:2A:796:C:H2' | 1:2A:797:C:C6 | 2.32 | 0.64 |
| 11:2P:89:ALA:HA | 11:2P:121:LYS:HD3 | 1.79 | 0.64 |
| 14:2S:104:GLY:HA2 | 14:2S:107:GLU:HB2 | 1.80 | 0.64 |
| 32:2a:790:A:OP1 | 54:2x:38:A:O2' | 2.15 | 0.64 |
| 1:1A:2350:C:OP2 | 59:1A:4268:HOH:O | 2.15 | 0.64 |
| 32:1a:972:C:OP2 | 41:1j:57:LYS:NZ | 2.23 | 0.64 |
| 1:2A:2741:A:OP1 | 31:29:22:ARG:NH2 | 2.27 | 0.64 |
| 8:2I:78:THR:O | 8:2I:104:GLN:NE2 | 2.30 | 0.64 |
| 10:2O:115:VAL:HG13 | 10:2O:121:VAL:HG21 | 1.78 | 0.64 |
| 32:2a:1490:C:H2' | 32:2a:1491:G:O4' | 1.98 | 0.64 |
| 34:2c:32:LEU:HD21 | 34:2c:59:ARG:HD2 | 1.78 | 0.64 |
| 1:1A:1456:G:OP2 | 59:1A:4266:HOH:O | 2.14 | 0.64 |
| 1:1A:1828:G:OP2 | 59:1A:4256:HOH:O | 2.13 | 0.64 |
| 1:1A:2280:G:O2' | 1:1A:2388:A:N1 | 2.30 | 0.64 |
| 1:1A:2304:G:H22 | 1:1A:2312:U:H3 | 1.44 | 0.64 |
| 1:1A:2502:G:OP2 | 59:1A:4261:HOH:O | 2.14 | 0.64 |
| 40:1i:13:ALA:HB2 | 40:1i:68:GLY:HA3 | 1.79 | 0.64 |
| 1:1A:2815:C:H5' | 27:15:29:THR:HG21 | 1.80 | 0.64 |
| 11:1P:29:LYS:HD3 | 11:1P:30:THR:HG23 | 1.79 | 0.64 |
| 33:1b:29:ALA:HA | 33:1b:32:ILE:HG13 | 1.78 | 0.64 |
| 1:2A:253:C:OP2 | 30:28:5:LYS:NZ | 2.24 | 0.64 |
| 1:1A:1975:G:OP2 | 59:1A:4265:HOH:O | 2.14 | 0.64 |
| 1:1A:2123:G:H2' | 1:1A:2124:G:C8 | 2.33 | 0.64 |
| 1:1A:2242:G:OP1 | 59:1A:4270:HOH:O | 2.15 | 0.64 |
| 21:1Z:21:ALA:O | 21:1Z:23:LYS:NZ | 2.30 | 0.64 |
| 23:11:18:ILE:HG12 | 23:11:37:ILE:HG23 | 1.79 | 0.64 |
| 32:1a:936:C:O2 | 32:1a:1382:C:N4 | 2.30 | 0.64 |
| 39:1h:96:GLY:N | 39:1h:99:GLU:OE1 | 2.30 | 0.64 |
| 54:1x:75:C:OP1 | 59:1x:201:HOH:O | 2.15 | 0.64 |
| 17:2V:62:LEU:HD21 | 17:2V:95:LEU:HB2 | 1.80 | 0.64 |
| 1:1A:1518:U:H2' | 1:1A:1519:G:O4' | 1.97 | 0.64 |
| 4:1E:170:LEU:HB3 | 4:1E:184:VAL:HG22 | 1.80 | 0.64 |
| 32:1a:1305:G:N2 | 32:1a:1331:G:H1' | 2.13 | 0.64 |
| 32:1a:1510:U:H2' | 32:1a:1511:G:C8 | 2.33 | 0.64 |
| 32:1a:1518:MA6:N6 | 32:1a:1519:MA6:H103 | 2.12 | 0.64 |
| 1:2A:1814:G:H5" | 3:2D:54:ARG:HH21 | 1.63 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 33:2b:104:ASN:OD1 | 33:2b:107:THR:OG1 | 2.14 | 0.64 |
| 40:2i:85:LEU:O | 40:2i:89:ASN:N | 2.31 | 0.64 |
| 1:1A:1816:G:O6 | 3:1D:35:LYS:NZ | 2.28 | 0.64 |
| 11:1P:126:VAL:HG12 | 11:1P:148:LEU:HD22 | 1.80 | 0.64 |
| 23:11:65:SER:OG | 23:11:66:HIS:ND1 | 2.24 | 0.64 |
| 32:1a:974:A:OP2 | 45:1n:41:ARG:NH2 | 2.29 | 0.64 |
| 32:1a:1035:A:N3 | 32:1a:1036:G:N2 | 2.46 | 0.64 |
| 1:2A:2189:U:H2' | 1:2A:2190:G:C8 | 2.33 | 0.64 |
| 6:2G:42:GLY:O | 6:2G:44:GLY:N | 2.30 | 0.64 |
| 34:2c:53:ALA:HB2 | 34:2c:115:LEU:HD13 | 1.80 | 0.64 |
| 35:2d:50:ARG:HD3 | 35:2d:51:PRO:HD2 | 1.79 | 0.64 |
| 1:2A:1226:A:OP1 | 17:2V:84:LYS:NZ | 2.27 | 0.64 |
| 1:2A:2615:U:OP1 | 59:2A:3940:HOH:O | 2.15 | 0.64 |
| 6:2G:120:LEU:N | 6:2G:179:PRO:O | 2.29 | 0.64 |
| 8:2I:84:GLY:H | 8:2I:87:LYS:HG2 | 1.62 | 0.64 |
| 1:1A:286:C:H2' | 1:1A:287:C:C6 | 2.33 | 0.64 |
| 32:1a:67:C:H2' | 32:1a:68:G:C8 | 2.33 | 0.64 |
| 33:1b:24:TRP:HZ3 | 33:1b:29:ALA:HB2 | 1.61 | 0.64 |
| 1:2A:531:C:OP1 | 1:2A:561:G:N1 | 2.29 | 0.64 |
| 33:2b:69:LEU:HB3 | 33:2b:162:ILE:HG22 | 1.79 | 0.64 |
| 41:2j:30:SER:O | 41:2j:81:THR:OG1 | 2.14 | 0.64 |
| 1:1A:952:G:OP1 | 12:1Q:16:ARG:NH2 | 2.31 | 0.63 |
| 35:1d:31:CYS:SG | 35:1d:32:ALA:N | 2.70 | 0.63 |
| 1:2A:1693:U:O2' | 3:2D:14:ARG:NH2 | 2.30 | 0.63 |
| 32:2a:373:A:O2' | 32:2a:451:A:N7 | 2.30 | 0.63 |
| 32:2a:1327:C:OP1 | 52:2u:12:LYS:NZ | 2.31 | 0.63 |
| 39:2h:10:LEU:HD22 | 39:2h:83:ILE:HD11 | 1.80 | 0.63 |
| 11:1P:63:PRO:HG2 | 30:18:25:MET:HB2 | 1.79 | 0.63 |
| 32:1a:67:C:H2' | 32:1a:68:G:H8 | 1.63 | 0.63 |
| 32:1a:1286:A:H2' | 32:1a:1287:A:H4' | 1.79 | 0.63 |
| 1:1A:807:U:OP2 | 11:1P:41:ARG:NH2 | 2.31 | 0.63 |
| 32:1a:1036:G:H5" | 32:1a:1037:C:C5 | 2.32 | 0.63 |
| 1:2A:2801(A):A:H5' | 1:2A:2802:G:C8 | 2.33 | 0.63 |
| 32:2a:266:G:H5" | 32:2a:268:C:H41 | 1.63 | 0.63 |
| 32:2a:328:C:H4' | 32:2a:329:A:H5' | 1.80 | 0.63 |
| 38:2g:20:ASP:HB3 | 38:2g:23:VAL:HB | 1.80 | 0.63 |
| 1:1A:1300:U:H4' | 1:1A:1301:A:H5" | 1.80 | 0.63 |
| 1:1A:1603:A:OP1 | 59:1A:4223:HOH:O | 2.16 | 0.63 |
| 1:2A:1025:G:C4 | 1:2A:1135:C:H1' | 2.33 | 0.63 |
| 5:2F:155:LEU:HD23 | 5:2F:192:LEU:HD13 | 1.79 | 0.63 |
| 1:1A:583:G:N7 | 59:1A:4369:HOH:O | 2.31 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 32:1a:1456:G:O6 | 51:1t:54:LYS:NZ | 2.29 | 0.63 |
| 1:2A:882:G:H1 | 1:2A:894:C:N4 | 1.97 | 0.63 |
| 1:2A:2141:G:O6 | 1:2A:2150:U:O2 | 2.16 | 0.63 |
| 5:2F:185:ASP:HA | 5:2F:188:ARG:HD3 | 1.79 | 0.63 |
| 11:2P:37:GLY:O | 11:2P:40:SER:OG | 2.14 | 0.63 |
| 33:2b:95:GLN:HG3 | 33:2b:147:LYS:HG3 | 1.80 | 0.63 |
| 1:1A:2079:U:O3' | 23:11:35:THR:OG1 | 2.17 | 0.63 |
| 23:11:54:ALA:HB1 | 23:11:83:GLU:HG3 | 1.80 | 0.63 |
| 1:2A:2065:C:H4' | 1:2A:2251:OMG:HM23 | 1.80 | 0.63 |
| 1:2A:2405:G:H5" | 11:2P:75:ILE:HG21 | 1.79 | 0.63 |
| 1:2A:2815:C:H5' | 27:25:29:THR:HG21 | 1.80 | 0.63 |
| 32:2a:56:U:H2' | 32:2a:57:G:C8 | 2.34 | 0.63 |
| 32:2a:501:C:H2' | 32:2a:502:G:H8 | 1.63 | 0.63 |
| 1:1A:955:C:OP1 | 12:1Q:87:LYS:HE3 | 1.98 | 0.63 |
| 1:1A:1153:C:OP2 | 59:1A:4271:HOH:O | 2.16 | 0.63 |
| 32:1a:128:G:O2' | 48:1q:3:LYS:NZ | 2.31 | 0.63 |
| 32:1a:1035:A:H2' | 32:1a:1036:G:H21 | 1.64 | 0.63 |
| 1:2A:1815:A:P | 3:2D:54:ARG:HH22 | 2.21 | 0.63 |
| 1:2A:1865:G:N2 | 1:2A:1877:A:OP2 | 2.31 | 0.63 |
| 1:2A:2562:U:H1' | 10:2O:23:ARG:HE | 1.64 | 0.63 |
| 13:2R:117:VAL:HG12 | 13:2R:118:GLU:H | 1.62 | 0.63 |
| 17:2V:40:LEU:HB2 | 17:2V:46:VAL:HB | 1.80 | 0.63 |
| 41:1j:8:LEU:HD22 | 41:1j:96:ILE:HG22 | 1.80 | 0.63 |
| 1:2A:2129:C:N3 | 1:2A:2159:G:N2 | 2.45 | 0.63 |
| 9:2N:104:LYS:HA | 9:2N:107:LEU:HD12 | 1.79 | 0.63 |
| 26:24:16:CYS:SG | 26:24:17:GLY:N | 2.71 | 0.63 |
| 7:1H:149:ARG:NH1 | 7:1H:167:GLU:OE2 | 2.30 | 0.63 |
| 50:1s:50:ALA:HB1 | 50:1s:57:HIS:HB3 | 1.79 | 0.63 |
| 1:2A:2313:C:H2' | 1:2A:2314:C:H6 | 1.63 | 0.63 |
| 10:2O:49:ARG:NH2 | 32:2a:1423:G:OP1 | 2.29 | 0.63 |
| 11:2P:89:ALA:O | 11:2P:121:LYS:NZ | 2.32 | 0.63 |
| 32:2a:1209:C:O2' | 32:2a:1214:C:N4 | 2.30 | 0.63 |
| 11:1P:59:LEU:HD11 | 30:18:10:ALA:HB2 | 1.81 | 0.62 |
| 32:1a:45:U:H2' | 32:1a:46:G:C8 | 2.34 | 0.62 |
| 32:1a:299:G:O6 | 59:1a:1908:HOH:O | 2.12 | 0.62 |
| 32:1a:1030:C:N4 | 32:1a:1030(A):G:N3 | 2.47 | 0.62 |
| 38:1g:69:VAL:HG21 | 38:1g:104:LEU:HD11 | 1.80 | 0.62 |
| 1:2A:1670:C:O2 | 4:2E:129:HIS:NE2 | 2.29 | 0.62 |
| 1:2A:2086:U:H2' | 1:2A:2087:G:C8 | 2.34 | 0.62 |
| 5:2F:157:VAL:HB | 5:2F:194:MET:HG2 | 1.81 | 0.62 |
| 32:2a:501:C:H2' | 32:2a:502:G:C8 | 2.33 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 32:2a:1338:G:H21 | 54:2x:41:C:H1' | 1.62 | 0.62 |
| 1:1A:2611:U:C4 | 27:15:3:LYS:HG2 | 2.34 | 0.62 |
| 32:1a:40:C:H2' | 32:1a:41:G:H8 | 1.64 | 0.62 |
| 1:2A:995:C:O2 | 9:2N:3:THR:OG1 | 2.16 | 0.62 |
| 8:2I:31:LEU:HD21 | 8:2I:38:LEU:HG | 1.81 | 0.62 |
| 32:1a:730:G:N2 | 32:1a:766:A:OP1 | 2.28 | 0.62 |
| 33:1b:104:ASN:OD1 | 33:1b:107:THR:OG1 | 2.16 | 0.62 |
| 1:2A:2198:A:O2' | 1:2A:2224:G:N2 | 2.29 | 0.62 |
| 34:2c:131:ARG:NH2 | 36:2e:50:GLU:HG3 | 2.14 | 0.62 |
| 35:2d:38:TYR:HD2 | 35:2d:38:TYR:H | 1.46 | 0.62 |
| 21:1Z:128:VAL:HG23 | 21:1Z:161:VAL:HG12 | 1.82 | 0.62 |
| 41:1j:16:LEU:HD23 | 41:1j:68:HIS:HB2 | 1.82 | 0.62 |
| 44:1m:9:ILE:HB | 44:1m:18:ALA:HB1 | 1.80 | 0.62 |
| 32:2a:662:G:H2' | 32:2a:663:A:C8 | 2.34 | 0.62 |
| 33:2b:200:ILE:HD12 | 33:2b:202:PRO:HD3 | 1.81 | 0.62 |
| 45:2n:7:ILE:HA | 45:2n:23:ARG:HD3 | 1.82 | 0.62 |
| 1:1A:586:A:H5' | 5:1F:89:VAL:HG21 | 1.81 | 0.62 |
| 36:1e:35:GLY:HA3 | 36:1e:112:LEU:HB3 | 1.80 | 0.62 |
| 41:1j:5:ARG:HD3 | 41:1j:71:LEU:HD11 | 1.81 | 0.62 |
| 1:2A:2313:C:H4' | 6:2G:91:ARG:HG3 | 1.82 | 0.62 |
| 35:2d:57:ARG:HB3 | 35:2d:206:PHE:HB2 | 1.79 | 0.62 |
| 48:2q:45:HIS:H | 48:2q:72:ARG:HA | 1.64 | 0.62 |
| 50:2s:19:VAL:O | 50:2s:23:ASN:ND2 | 2.32 | 0.62 |
| 39:1h:34:GLU:OE1 | 39:1h:37:ARG:NH1 | 2.33 | 0.62 |
| 20:2Y:28:LYS:HB3 | 20:2Y:38:ILE:HG22 | 1.82 | 0.62 |
| 38:2g:18:TYR:HB3 | 38:2g:59:LEU:HD22 | 1.81 | 0.62 |
| 46:2o:25:THR:HG21 | 46:2o:70:LEU:HB2 | 1.81 | 0.62 |
| 1:1A:286:C:H2' | 1:1A:287:C:H6 | 1.64 | 0.62 |
| 5:1F:185:ASP:HA | 5:1F:188:ARG:HD3 | 1.80 | 0.62 |
| 14:1S:61:ASN:HD22 | 14:1S:64:GLU:H | 1.46 | 0.62 |
| 32:1a:828:A:H2' | 32:1a:829:G:O4' | 1.99 | 0.62 |
| 32:1a:1237:C:O2' | 32:1a:1300:G:N2 | 2.26 | 0.62 |
| 57:1a:1835:V7A:NBD | 57:1a:1835:V7A:OBB | 2.30 | 0.62 |
| 33:1b:98:LEU:HD12 | 33:1b:101:MET:HE3 | 1.82 | 0.62 |
| 35:2d:112:VAL:H | 35:2d:116:GLN:NE2 | 1.98 | 0.62 |
| 35:2d:191:ARG:NH1 | 35:2d:191:ARG:O | 2.33 | 0.62 |
| 45:2n:21:TYR:HE1 | 45:2n:23:ARG:HD2 | 1.65 | 0.62 |
| 1:1A:2023:G:H5' | 1:1A:2617:C:H4' | 1.81 | 0.62 |
| 6:1G:150:ASP:N | 6:1G:150:ASP:OD1 | 2.33 | 0.62 |
| 32:1a:1299:A:O2' | 32:1a:1301:U:O4' | 2.17 | 0.62 |
| 57:2a:3210:V7A:NBD | 57:2a:3210:V7A:OBB | 2.30 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:2j:5:ARG:N | 41:2j:99:LYS:O | 2.32 | 0.62 |
| 18:1W:73:ALA:HB3 | 18:1W:106:ILE:HD12 | 1.80 | 0.62 |
| 1:2A:948:G:O6 | 59:2A:3945:HOH:O | 2.16 | 0.62 |
| 1:2A:1824:G:N3 | 3:2D:254:THR:OG1 | 2.33 | 0.62 |
| 32:2a:269:C:H2' | 32:2a:270:A:C8 | 2.35 | 0.62 |
| 1:1A:859:G:O2' | 1:1A:916:G:O6 | 2.16 | 0.62 |
| 1:1A:2155:G:H3' | 1:1A:2156:G:C8 | 2.35 | 0.62 |
| 16:1U:46:ALA:O | 16:1U:50:ARG:HG2 | 1.99 | 0.62 |
| 18:1W:11:ARG:HA | 18:1W:100:THR:HG22 | 1.81 | 0.62 |
| 33:2b:216:SER:O | 33:2b:220:ASP:N | 2.21 | 0.62 |
| 40:2i:50:LEU:HD13 | 40:2i:56:LEU:HA | 1.81 | 0.62 |
| 41:2j:34:VAL:HG12 | 41:2j:74:ILE:HG22 | 1.80 | 0.62 |
| 47:2p:53:VAL:HG13 | 47:2p:79:VAL:HG22 | 1.82 | 0.62 |
| 1:1A:668:G:H5' | 1:1A:669:G:OP2 | 2.00 | 0.61 |
| 1:1A:1003:G:O2' | 1:1A:1010:A:N1 | 2.31 | 0.61 |
| 32:1a:204:U:H4' | 32:1a:216:G:O5' | 2.00 | 0.61 |
| 34:1c:3:ASN:OD1 | 34:1c:3:ASN:N | 2.32 | 0.61 |
| 1:2A:581:C:H2' | 1:2A:582:G:H8 | 1.65 | 0.61 |
| 1:2A:674:G:O2' | 5:2F:74:ARG:HD3 | 2.00 | 0.61 |
| 5:2F:156:LEU:HD21 | 5:2F:163:VAL:HG12 | 1.82 | 0.61 |
| 32:2a:1002:G:C6 | 32:2a:1003:G:H8 | 2.17 | 0.61 |
| 33:2b:74:LYS:O | 33:2b:78:GLN:HG2 | 1.99 | 0.61 |
| 38:1g:78:ARG:HG2 | 38:1g:79:ARG:H | 1.64 | 0.61 |
| 47:1p:17:TYR:HB2 | 47:1p:39:TYR:HB3 | 1.83 | 0.61 |
| 2:2B:7:G:H21 | 14:2S:38:GLN:HE22 | 1.48 | 0.61 |
| 26:24:53:GLU:C | 26:24:55:ARG:H | 2.07 | 0.61 |
| 32:1a:1033:G:H2' | 32:1a:1034:G:H8 | 1.64 | 0.61 |
| 1:2A:574:C:N3 | 4:2E:145:LYS:NZ | 2.42 | 0.61 |
| 6:2G:63:ILE:HD11 | 6:2G:144:ILE:HG12 | 1.82 | 0.61 |
| 8:2I:1:MET:N | 8:2I:20:ASP:OD1 | 2.21 | 0.61 |
| 28:26:25:LYS:HE3 | 28:26:27:LYS:HB3 | 1.81 | 0.61 |
| 32:2a:1417:G:O6 | 59:2a:3304:HOH:O | 2.12 | 0.61 |
| 1:1A:271(M):G:N2 | 8:1I:50:ARG:HH12 | 1.99 | 0.61 |
| 1:1A:910:A:N3 | 1:1A:2264:C:O2' | 2.30 | 0.61 |
| 1:1A:1429:G:H2' | 1:1A:1430:C:C6 | 2.35 | 0.61 |
| 4:1E:70:ALA:O | 4:1E:72:VAL:N | 2.34 | 0.61 |
| 22:10:27:GLU:HB2 | 22:10:69:PHE:HD1 | 1.66 | 0.61 |
| 1:1A:2292:C:OP1 | 14:1S:17:ARG:NH2 | 2.33 | 0.61 |
| 3:1D:175:LEU:HD12 | 3:1D:185:VAL:HG21 | 1.81 | 0.61 |
| 32:1a:1505:G:O2' | 53:1v:13:A:O2' | 2.19 | 0.61 |
| 35:1d:108:LEU:HD21 | 35:1d:174:LEU:HD22 | 1.83 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:1i:17:VAL:HG21 | 40:1i:81:ILE:HG13 | 1.83 | 0.61 |
| 1:2A:854:G:H2' | 1:2A:855:G:H8 | 1.65 | 0.61 |
| 14:2S:50:SER:O | 14:2S:76:LYS:NZ | 2.33 | 0.61 |
| 1:1A:2224:G:H4' | 1:1A:2226:C:C2 | 2.35 | 0.61 |
| 1:2A:468:G:N7 | 29:27:39:ARG:NH2 | 2.48 | 0.61 |
| 1:2A:1324:G:O6 | 59:2A:3935:HOH:O | 2.13 | 0.61 |
| 14:2S:35:ILE:HD11 | 14:2S:101:LEU:HD12 | 1.82 | 0.61 |
| 32:2a:196:A:N3 | 32:2a:222:U:H1' | 2.16 | 0.61 |
| 32:2a:673:G:H2' | 32:2a:674:G:C8 | 2.35 | 0.61 |
| 32:2a:1074:G:O2' | 32:2a:1101:A:N1 | 2.32 | 0.61 |
| 39:2h:19:VAL:HG23 | 39:2h:21:LYS:HG3 | 1.82 | 0.61 |
| 40:2i:42:ARG:NH1 | 40:2i:75:ASP:OD1 | 2.34 | 0.61 |
| 44:2m:86:CYS:SG | 44:2m:87:TYR:N | 2.73 | 0.61 |
| 1:1A:242:G:O2' | 1:1A:254:G:O6 | 2.17 | 0.61 |
| 32:1a:1305:G:H22 | 32:1a:1331:G:H1' | 1.65 | 0.61 |
| 32:1a:1356:G:H2' | 32:1a:1357:A:H8 | 1.64 | 0.61 |
| 1:2A:2116:G:N2 | 1:2A:2162:G:OP1 | 2.33 | 0.61 |
| 6:2G:64:THR:HB | 6:2G:94:LEU:HD21 | 1.82 | 0.61 |
| 41:2j:11:PHE:HE1 | 41:2j:67:THR:HG22 | 1.66 | 0.61 |
| 50:2s:49:ILE:HG22 | 50:2s:62:ILE:HD11 | 1.82 | 0.61 |
| 1:1A:28:A:OP2 | 59:1A:4272:HOH:O | 2.16 | 0.61 |
| 1:1A:2469:A:O2' | 12:1Q:56:ARG:NH1 | 2.34 | 0.61 |
| 8:1I:95:LYS:H | 8:1I:95:LYS:HD3 | 1.66 | 0.61 |
| 32:1a:110:C:O2' | 47:1p:25:ARG:O | 2.19 | 0.61 |
| 33:1b:48:MET:HA | 33:1b:51:LEU:HD12 | 1.83 | 0.61 |
| 50:1s:22:LEU:HB3 | 50:1s:27:GLU:HB3 | 1.81 | 0.61 |
| 1:2A:947:G:O2' | 1:2A:984:A:N1 | 2.33 | 0.61 |
| 1:2A:1932:A:H2' | 1:2A:1933:G:O4' | 2.00 | 0.61 |
| 1:2A:2148:G:H2' | 1:2A:2149:G:C8 | 2.36 | 0.61 |
| 1:2A:2803:C:H2' | 1:2A:2804:C:C6 | 2.35 | 0.61 |
| 10:2O:73:ASP:HB2 | 15:2T:82:LEU:HD13 | 1.81 | 0.61 |
| 32:2a:6:G:H1 | 36:2e:98:THR:HG21 | 1.66 | 0.61 |
| 1:1A:1071:G:H1' | 1:1A:1089:G:H2' | 1.81 | 0.61 |
| 1:1A:2687:U:H2' | 1:1A:2688:U:O4' | 2.01 | 0.61 |
| 1:2A:1378:A:O2' | 1:2A:1380:G:N7 | 2.30 | 0.61 |
| 1:2A:1920:4OC:HM22 | 1:2A:1921:G:H5' | 1.82 | 0.61 |
| 30:28:4:MET:HE3 | 30:28:63:PRO:HG3 | 1.83 | 0.61 |
| 32:2a:405:U:O4 | 35:2d:2:GLY:N | 2.34 | 0.61 |
| 40:2i:26:VAL:HG22 | 40:2i:61:ALA:HB3 | 1.82 | 0.61 |
| 21:1Z:26:GLY:HA3 | 21:1Z:86:VAL:HG23 | 1.83 | 0.61 |
| 1:2A:1379:A:H4' | 1:2A:1380:G:OP2 | 2.00 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:2A:1991:U:H2' | 1:2A:1992:G:H5" | 1.83 | 0.61 |
| 1:2A:2446:G:N2 | 1:2A:2449:U:O2 | 2.32 | 0.61 |
| 6:2G:146:TYR:HB3 | 44:2m:11:ARG:HH22 | 1.66 | 0.61 |
| 32:2a:107:G:N7 | 51:2t:15:ARG:NH2 | 2.49 | 0.61 |
| 32:2a:1142:G:H3' | 32:2a:1143:G:H8 | 1.64 | 0.61 |
| 1:1A:1636:C:H2' | 1:1A:1637:A:C8 | 2.35 | 0.60 |
| 1:1A:2787:C:H1' | 4:1E:62:PRO:HG3 | 1.82 | 0.60 |
| 11:1P:59:LEU:HD21 | 30:18:10:ALA:HA | 1.82 | 0.60 |
| 15:1T:60:THR:HG22 | 15:1T:77:PRO:HA | 1.82 | 0.60 |
| 1:2A:30:G:O2' | 1:2A:1214:A:N3 | 2.30 | 0.60 |
| 1:2A:451:C:N4 | 1:2A:454:A:OP2 | 2.23 | 0.60 |
| 1:2A:1639:U:H2' | 1:2A:1640:C:H5" | 1.83 | 0.60 |
| 4:2E:77:ILE:HD13 | 4:2E:195:LEU:HD22 | 1.84 | 0.60 |
| 1:1A:2100:G:O6 | 1:1A:2189:U:O4 | 2.19 | 0.60 |
| 1:2A:2268:A:OP1 | 59:2A:3942:HOH:O | 2.16 | 0.60 |
| 7:2H:24:VAL:HG23 | 7:2H:35:VAL:HB | 1.83 | 0.60 |
| 32:2a:34:C:H2' | 32:2a:35:G:C8 | 2.36 | 0.60 |
| 51:2t:43:LEU:O | 51:2t:47:GLY:N | 2.26 | 0.60 |
| 1:1A:2125:G:N1 | 1:1A:2172:U:OP1 | 2.27 | 0.60 |
| 1:1A:2751:G:H4' | 7:1H:4:ILE:HD11 | 1.83 | 0.60 |
| 32:1a:557:G:OP1 | 59:1a:1912:HOH:O | 2.16 | 0.60 |
| 32:1a:1025:U:O2 | 32:1a:1036:G:O6 | 2.18 | 0.60 |
| 1:2A:455:C:N3 | 1:2A:472:A:H2' | 2.16 | 0.60 |
| 2:2B:55:U:O3' | 6:2G:27:ASN:ND2 | 2.34 | 0.60 |
| 23:21:64:ALA:HA | 23:21:67:ILE:HG13 | 1.83 | 0.60 |
| 35:2d:150:GLU:OE1 | 35:2d:151:LYS:N | 2.33 | 0.60 |
| 4:1E:77:ILE:HD13 | 4:1E:195:LEU:HD13 | 1.83 | 0.60 |
| 6:1G:15:VAL:HG22 | 6:1G:175:LEU:HB3 | 1.83 | 0.60 |
| 20:1Y:34:LYS:NZ | 59:1Y:301:HOH:O | 2.34 | 0.60 |
| 32:1a:300:A:O2' | 32:1a:564:C:N3 | 2.33 | 0.60 |
| 32:1a:1412:C:H2' | 32:1a:1413:A:C8 | 2.37 | 0.60 |
| 1:2A:1503:U:H2' | 1:2A:1504:C:C6 | 2.36 | 0.60 |
| 1:2A:2183:C:H2' | 1:2A:2184:G:H8 | 1.66 | 0.60 |
| 32:2a:600:C:H2' | 32:2a:601:C:C6 | 2.36 | 0.60 |
| 32:2a:922:G:H2' | 32:2a:923:A:C8 | 2.36 | 0.60 |
| 32:2a:1128:C:O2' | 32:2a:1147:C:N3 | 2.26 | 0.60 |
| 34:2c:122:GLU:O | 34:2c:125:GLU:HG2 | 2.01 | 0.60 |
| 1:1A:2544:G:H1' | 1:1A:2646:C:H4' | 1.81 | 0.60 |
| 32:1a:136:C:H42 | 32:1a:227:G:H1 | 1.50 | 0.60 |
| 32:1a:1226:C:H2' | 44:1m:103:THR:HB | 1.83 | 0.60 |
| 32:1a:1503:A:O2' | 53:1v:13:A:N1 | 2.34 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 48:1q:26:GLN:HG2 | 48:1q:37:LYS:HG2 | 1.83 | 0.60 |
| 8:2I:4:ILE:HD11 | 8:2I:44:LEU:HD23 | 1.84 | 0.60 |
| 32:2a:1518:MA6:N6 | 32:2a:1519:MA6:H103 | 2.16 | 0.60 |
| 1:1A:2165:G:H1 | 1:1A:2171:A:H2' | 1.67 | 0.60 |
| 19:1X:94:GLY:H | 19:1X:95:LEU:C | 2.09 | 0.60 |
| 32:1a:707:C:OP1 | 42:1k:85:ARG:NH1 | 2.35 | 0.60 |
| 1:2A:922:U:H2' | 1:2A:923:C:C6 | 2.36 | 0.60 |
| 1:2A:994:C:O2' | 1:2A:996:A:OP1 | 2.17 | 0.60 |
| 1:2A:1349:A:OP1 | 59:2A:3941:HOH:O | 2.15 | 0.60 |
| 32:2a:1089:G:H1 | 32:2a:1096:C:H42 | 1.49 | 0.60 |
| 35:2d:173:TRP:CD1 | 35:2d:189:PRO:HG3 | 2.36 | 0.60 |
| 1:1A:694:U:OP1 | 3:1D:59:LYS:NZ | 2.32 | 0.60 |
| 14:1S:84:GLN:HA | 14:1S:111:GLU:HB2 | 1.81 | 0.60 |
| 17:1V:6:LYS:HB2 | 17:1V:38:LEU:HD11 | 1.83 | 0.60 |
| 20:1Y:102:CYS:SG | 20:1Y:103:GLY:N | 2.75 | 0.60 |
| 26:14:60:GLN:HA | 26:14:62:ARG:HG2 | 1.84 | 0.60 |
| 36:1e:78:HIS:HD2 | 39:1h:104:ARG:HD2 | 1.64 | 0.60 |
| 43:1l:71:PRO:O | 43:1l:102:ARG:NH1 | 2.34 | 0.60 |
| 1:2A:212:G:H2' | 1:2A:213:A:O4' | 2.02 | 0.60 |
| 1:2A:740:U:H2' | 1:2A:741:G:C8 | 2.37 | 0.60 |
| 4:2E:2:LYS:HG3 | 4:2E:200:GLU:HB2 | 1.83 | 0.60 |
| 33:2b:80:ILE:HD13 | 33:2b:211:ILE:HB | 1.84 | 0.60 |
| 8:1I:109:ILE:HG13 | 8:1I:130:TYR:CZ | 2.37 | 0.60 |
| 39:1h:11:THR:HG22 | 39:1h:14:ARG:HH12 | 1.67 | 0.60 |
| 1:2A:900:A:O2' | 1:2A:901:A:OP1 | 2.18 | 0.60 |
| 4:2E:9:VAL:HB | 15:2T:3:ARG:HG2 | 1.84 | 0.60 |
| 13:2R:36:THR:HG22 | 13:2R:37:THR:H | 1.66 | 0.60 |
| 39:2h:11:THR:HG22 | 39:2h:14:ARG:HH12 | 1.67 | 0.60 |
| 1:1A:1617:C:OP2 | 59:1A:4273:HOH:O | 2.17 | 0.60 |
| 1:1A:2298:A:N6 | 1:1A:2318:G:O2' | 2.31 | 0.60 |
| 32:1a:427:U:OP1 | 35:1d:13:ARG:NH1 | 2.29 | 0.60 |
| 32:1a:1391:U:H2' | 32:1a:1392:G:C8 | 2.37 | 0.60 |
| 39:1h:121:ASP:OD2 | 39:1h:125:ARG:NH2 | 2.34 | 0.60 |
| 47:1p:74:LEU:HG | 47:1p:79:VAL:HG21 | 1.82 | 0.60 |
| 1:2A:249:C:O2 | 30:28:12:LYS:NZ | 2.30 | 0.60 |
| 1:2A:2751:G:H5' | 7:2H:2:SER:HA | 1.84 | 0.60 |
| 1:2A:2821:A:O2' | 1:2A:2826:A:N1 | 2.34 | 0.60 |
| 2:2B:75:G:H22 | 21:2Z:73:GLN:HE21 | 1.49 | 0.60 |
| 7:2H:20:ALA:HB3 | 7:2H:23:ARG:HB2 | 1.82 | 0.60 |
| 35:2d:74:GLN:NE2 | 35:2d:137:SER:OG | 2.34 | 0.60 |
| 41:2j:57:LYS:O | 41:2j:60:ARG:NE | 2.30 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1A:1174:A:H4' | 1:1A:1175:U:OP1 | 2.00 | 0.60 |
| 3:1D:4:LYS:HB3 | 3:1D:18:VAL:HG23 | 1.84 | 0.60 |
| 33:1b:82:ARG:NH1 | 33:1b:150:SER:OG | 2.35 | 0.60 |
| 1:2A:2680:C:OP2 | 4:2E:111:ARG:NH2 | 2.29 | 0.60 |
| 21:2Z:77:ASP:OD2 | 21:2Z:80:ARG:NH1 | 2.35 | 0.60 |
| 1:1A:1028:A:N6 | 1:1A:1125:G:H2' | 2.17 | 0.59 |
| 1:1A:2627:G:O2' | 1:1A:2781:A:N1 | 2.33 | 0.59 |
| 32:1a:863:U:O2' | 32:1a:865:A:N7 | 2.33 | 0.59 |
| 33:1b:74:LYS:NZ | 33:1b:205:ASP:O | 2.34 | 0.59 |
| 36:1e:78:HIS:CD2 | 39:1h:104:ARG:HD2 | 2.37 | 0.59 |
| 46:1o:25:THR:HG21 | 46:1o:70:LEU:HB2 | 1.84 | 0.59 |
| 52:1u:6:ARG:HG2 | 52:1u:15:ARG:HD2 | 1.83 | 0.59 |
| 1:2A:1159:U:H2' | 1:2A:1160:G:H8 | 1.67 | 0.59 |
| 1:2A:1278:A:OP1 | 13:2R:36:THR:HG23 | 2.01 | 0.59 |
| 1:2A:2884:U:O4 | 27:25:40:LYS:NZ | 2.32 | 0.59 |
| 12:2Q:111:GLU:OE2 | 12:2Q:133:ARG:NH2 | 2.35 | 0.59 |
| 20:2Y:83:THR:HG21 | 20:2Y:99:CYS:HB2 | 1.82 | 0.59 |
| 32:2a:514:C:H2' | 32:2a:515:G:H8 | 1.67 | 0.59 |
| 32:2a:769:G:H4' | 32:2a:1513:A:H4' | 1.83 | 0.59 |
| 32:2a:964:A:N3 | 32:2a:969:A:O2' | 2.31 | 0.59 |
| 1:1A:1817:G:OP1 | 3:1D:88:ARG:NH2 | 2.34 | 0.59 |
| 42:1k:29:ILE:HG23 | 42:1k:44:SER:HB3 | 1.84 | 0.59 |
| 1:2A:588:U:H1' | 5:2F:90:PHE:HB3 | 1.83 | 0.59 |
| 32:2a:45:U:H2' | 32:2a:46:G:C8 | 2.37 | 0.59 |
| 2:1B:86:G:H1 | 2:1B:91:C:H42 | 1.49 | 0.59 |
| 32:1a:1409:C:H2' | 32:1a:1410:G:C8 | 2.38 | 0.59 |
| 41:1j:11:PHE:HE1 | 41:1j:67:THR:HG22 | 1.66 | 0.59 |
| 1:2A:2104:G:N2 | 1:2A:2185:C:N3 | 2.47 | 0.59 |
| 1:2A:2116:G:H22 | 1:2A:2162:G:H5' | 1.66 | 0.59 |
| 6:2G:125:PHE:HB3 | 6:2G:166:ASP:CG | 2.28 | 0.59 |
| 32:2a:1134:G:C2 | 32:2a:1135:U:H1' | 2.37 | 0.59 |
| 34:2c:58:GLU:HB3 | 41:2j:92:THR:HG21 | 1.84 | 0.59 |
| 1:1A:1750:G:O2' | 1:1A:2860:A:N1 | 2.28 | 0.59 |
| 5:1F:167:ALA:HB1 | 5:1F:173:VAL:HG11 | 1.83 | 0.59 |
| 6:1G:121:ASN:O | 6:1G:131:TYR:OH | 2.19 | 0.59 |
| 1:2A:2134:A:H62 | 1:2A:2157:G:H4' | 1.68 | 0.59 |
| 1:2A:2646:C:OP2 | 1:2A:2732:G:O2' | 2.19 | 0.59 |
| 1:2A:2680:C:H5' | 4:2E:189:PRO:HA | 1.85 | 0.59 |
| 7:2H:143:GLN:HG3 | 7:2H:147:ASN:HD21 | 1.67 | 0.59 |
| 44:2m:4:ILE:HG23 | 44:2m:5:ALA:H | 1.67 | 0.59 |
| 1:1A:861:A:N3 | 2:1B:79:C:O2' | 2.33 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1A:2855:C:H2' | 1:1A:2856:C:C6 | 2.36 | 0.59 |
| 1:2A:637:A:OP1 | 11:2P:133:SER:OG | 2.15 | 0.59 |
| 1:2A:2090:G:N2 | 23:21:45:ASN:OD1 | 2.24 | 0.59 |
| 1:2A:2773:C:OP1 | 4:2E:166:THR:OG1 | 2.20 | 0.59 |
| 8:2I:93:THR:OG1 | 8:2I:94:ALA:N | 2.34 | 0.59 |
| 22:20:27:GLU:HG3 | 22:20:68:GLU:HA | 1.83 | 0.59 |
| 32:2a:1272:G:N2 | 32:2a:1273:G:N7 | 2.49 | 0.59 |
| 32:2a:1356:G:H2' | 32:2a:1357:A:C8 | 2.38 | 0.59 |
| 33:2b:9:GLU:HG3 | 33:2b:10:LEU:H | 1.66 | 0.59 |
| 38:2g:23:VAL:HG13 | 38:2g:43:PHE:CE2 | 2.38 | 0.59 |
| 1:1A:800:A:H8 | 1:1A:800:A:OP1 | 1.86 | 0.59 |
| 1:1A:1165:U:H2' | 1:1A:1166:C:C6 | 2.37 | 0.59 |
| 1:1A:1478:G:H2' | 1:1A:1479:G:H8 | 1.66 | 0.59 |
| 25:13:5:LYS:NZ | 25:13:34:GLU:OE2 | 2.34 | 0.59 |
| 32:1a:343:U:O2' | 32:1a:346:G:O6 | 2.13 | 0.59 |
| 32:1a:1034:G:N2 | 32:1a:1035:A:N3 | 2.51 | 0.59 |
| 1:2A:878:A:N6 | 1:2A:899:A:O2' | 2.35 | 0.59 |
| 32:2a:509:A:N3 | 32:2a:543:C:O2' | 2.35 | 0.59 |
| 32:2a:1250:A:H4' | 40:2i:68:GLY:N | 2.18 | 0.59 |
| 1:1A:2404:C:O3' | 11:1P:77:ARG:NH2 | 2.36 | 0.59 |
| 54:1x:8:4SU:O2 | 54:1x:21:A:C2 | 2.55 | 0.59 |
| 1:2A:195:A:H61 | 1:2A:198:C:H3' | 1.67 | 0.59 |
| 1:2A:568:U:H5' | 1:2A:945:A:N1 | 2.18 | 0.59 |
| 1:2A:2166:G:N7 | 1:2A:2168:G:N2 | 2.50 | 0.59 |
| 32:2a:783:C:OP2 | 59:2a:3308:HOH:O | 2.17 | 0.59 |
| 32:2a:1316:G:H22 | 32:2a:1319:A:H5" | 1.68 | 0.59 |
| 1:1A:2429:G:OP1 | 59:1A:4215:HOH:O | 2.16 | 0.59 |
| 1:1A:2564:A:C2 | 1:1A:2647:U:H4' | 2.38 | 0.59 |
| 1:2A:581:C:H2' | 1:2A:582:G:C8 | 2.37 | 0.59 |
| 1:2A:952:G:OP1 | 12:2Q:16:ARG:NH2 | 2.36 | 0.59 |
| 1:2A:1816:G:O6 | 3:2D:35:LYS:NZ | 2.35 | 0.59 |
| 1:1A:1007:C:H5" | 9:1N:35:ARG:HH11 | 1.68 | 0.59 |
| 1:1A:1266:G:O5' | 18:1W:15:ARG:NH2 | 2.36 | 0.59 |
| 5:1F:117:ARG:NH2 | 5:1F:189:THR:O | 2.32 | 0.59 |
| 7:1H:25:LYS:NZ | 7:1H:32:GLU:OE1 | 2.36 | 0.59 |
| 10:1O:64:ARG:HG2 | 10:1O:83:ALA:HB3 | 1.84 | 0.59 |
| 14:1S:61:ASN:HD22 | 14:1S:64:GLU:HG3 | 1.68 | 0.59 |
| 14:1S:83:LYS:HB3 | 14:1S:111:GLU:HG3 | 1.85 | 0.59 |
| 32:1a:398:C:H2' | 32:1a:399:G:C8 | 2.38 | 0.59 |
| 1:2A:1796:U:H2' | 1:2A:1797:C:C6 | 2.38 | 0.59 |
| 8:2I:69:LYS:O | 8:2I:73:GLU:HB3 | 2.03 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 42:2k:85:ARG:HA | 42:2k:112:THR:HG22 | 1.84 | 0.59 |
| 1:1A:587:C:OP2 | 11:1P:21:ARG:NH2 | 2.36 | 0.59 |
| 1:1A:1054:A:N6 | 1:1A:1105:U:N3 | 2.33 | 0.59 |
| 32:1a:53:A:OP2 | 59:1a:1913:HOH:O | 2.17 | 0.59 |
| 32:1a:445:G:H2' | 32:1a:446:G:C8 | 2.38 | 0.59 |
| 32:1a:1209:C:O2' | 32:1a:1214:C:N4 | 2.33 | 0.59 |
| 41:1j:35:SER:HB3 | 41:1j:73:ASP:HB2 | 1.84 | 0.59 |
| 1:2A:2577:A:OP1 | 59:2A:3944:HOH:O | 2.16 | 0.59 |
| 1:1A:2312:U:H5' | 6:1G:88:ILE:HD11 | 1.85 | 0.58 |
| 4:1E:18:ASP:OD2 | 15:1T:33:LYS:NZ | 2.22 | 0.58 |
| 32:1a:102:G:O2' | 32:1a:151:A:N3 | 2.34 | 0.58 |
| 32:1a:398:C:H2' | 32:1a:399:G:H8 | 1.68 | 0.58 |
| 1:2A:2533:A:OP1 | 1:2A:2665:A:O2' | 2.21 | 0.58 |
| 13:2R:56:LYS:NZ | 13:2R:90:ARG:O | 2.35 | 0.58 |
| 32:2a:951:G:N7 | 44:2m:102:ARG:NH2 | 2.51 | 0.58 |
| 1:1A:2518:A:OP2 | 59:1A:4276:HOH:O | 2.17 | 0.58 |
| 4:1E:111:ARG:O | 59:1E:402:HOH:O | 2.16 | 0.58 |
| 32:1a:976:G:H5' | 32:1a:1358:U:O2' | 2.03 | 0.58 |
| 33:1b:16:HIS:HB2 | 33:1b:204:ASN:CB | 2.31 | 0.58 |
| 38:1g:108:ALA:O | 38:1g:119:ARG:HD2 | 2.04 | 0.58 |
| 40:1i:128:ARG:NH2 | 54:1x:33:U:OP2 | 2.36 | 0.58 |
| 1:2A:2079:U:O3' | 23:21:35:THR:OG1 | 2.20 | 0.58 |
| 1:2A:2802:G:H2' | 1:2A:2803:C:O4' | 2.04 | 0.58 |
| 6:2G:97:ASP:HA | 6:2G:100:TRP:HD1 | 1.68 | 0.58 |
| 32:2a:692:U:O2' | 32:2a:694:A:N7 | 2.31 | 0.58 |
| 35:2d:119:GLN:HG3 | 35:2d:123:HIS:HD2 | 1.69 | 0.58 |
| 48:2q:6:LEU:HD23 | 48:2q:23:VAL:HG11 | 1.85 | 0.58 |
| 1:1A:8:A:H2' | 1:1A:9:U:H6 | 1.68 | 0.58 |
| 3:1D:147:LEU:HD13 | 3:1D:155:LEU:HD21 | 1.85 | 0.58 |
| 32:1a:401:C:O2' | 32:1a:621:A:N3 | 2.35 | 0.58 |
| 1:2A:445:C:OP1 | 16:2U:2:PRO:HA | 2.02 | 0.58 |
| 1:2A:1828:G:OP1 | 59:2A:3947:HOH:O | 2.17 | 0.58 |
| 1:2A:1889:A:H2' | 1:2A:1890:A:C8 | 2.37 | 0.58 |
| 1:2A:2821:A:H2' | 1:2A:2822:G:C8 | 2.38 | 0.58 |
| 32:2a:1327:C:H2' | 32:2a:1328:C:C6 | 2.38 | 0.58 |
| 36:2e:80:ILE:HG22 | 36:2e:91:LEU:HB2 | 1.84 | 0.58 |
| 1:1A:948:G:OP2 | 59:1A:4275:HOH:O | 2.17 | 0.58 |
| 1:1A:1093:G:H3' | 1:1A:1094:U:H5" | 1.85 | 0.58 |
| 1:1A:2111:C:N3 | 1:1A:2145:C:O2' | 2.34 | 0.58 |
| 1:1A:2255:G:OP2 | 59:1A:4277:HOH:O | 2.17 | 0.58 |
| 32:1a:976:G:N2 | 32:1a:1363:C:OP2 | 2.25 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 32:1a:1151:A:HO2' | 32:1a:1152:A:H8 | 1.50 | 0.58 |
| 32:1a:1337:G:OP2 | 59:1a:1911:HOH:O | 2.16 | 0.58 |
| 43:1l:56:ALA:HB2 | 43:1l:70:ILE:HD11 | 1.85 | 0.58 |
| 1:2A:1593:G:H2' | 1:2A:1594:G:C8 | 2.38 | 0.58 |
| 1:2A:1599:C:OP1 | 59:2A:3948:HOH:O | 2.17 | 0.58 |
| 1:2A:2723:C:OP2 | 4:2E:109:LYS:NZ | 2.35 | 0.58 |
| 2:2B:17:C:H2' | 2:2B:18:G:O4' | 2.03 | 0.58 |
| 4:2E:9:VAL:HG13 | 4:2E:25:VAL:O | 2.03 | 0.58 |
| 42:2k:29:ILE:HG23 | 42:2k:44:SER:HB3 | 1.85 | 0.58 |
| 1:1A:1292:U:H2' | 1:1A:1293:C:C6 | 2.39 | 0.58 |
| 1:1A:2090:G:O6 | 59:1A:4262:HOH:O | 2.14 | 0.58 |
| 6:1G:5:VAL:HG11 | 6:1G:101:ILE:HG12 | 1.85 | 0.58 |
| 7:1H:154:PRO:HB3 | 7:1H:163:TYR:CZ | 2.39 | 0.58 |
| 25:13:18:ASP:OD1 | 25:13:18:ASP:N | 2.33 | 0.58 |
| 32:1a:429:U:OP2 | 35:1d:36:ARG:NH2 | 2.36 | 0.58 |
| 32:1a:693:G:OP2 | 59:1a:1915:HOH:O | 2.17 | 0.58 |
| 32:1a:1442:G:H2' | 32:1a:1442:G:N3 | 2.18 | 0.58 |
| 1:2A:1316:U:H2' | 1:2A:1317:A:C8 | 2.37 | 0.58 |
| 5:2F:155:LEU:HD11 | 5:2F:176:LEU:HD12 | 1.86 | 0.58 |
| 7:2H:88:LEU:HD11 | 7:2H:165:ALA:HA | 1.86 | 0.58 |
| 19:2X:46:ALA:HB1 | 24:22:33:MET:HE1 | 1.85 | 0.58 |
| 1:1A:1246:A:N6 | 59:1A:4398:HOH:O | 2.34 | 0.58 |
| 4:1E:59:VAL:HG12 | 4:1E:64:LYS:HG3 | 1.84 | 0.58 |
| 32:1a:234:C:H5" | 48:1q:70:ARG:HH21 | 1.68 | 0.58 |
| 36:1e:78:HIS:CE1 | 36:1e:143:ARG:H | 2.21 | 0.58 |
| 36:1e:142:LEU:O | 36:1e:143:ARG:NH1 | 2.37 | 0.58 |
| 1:2A:576:U:O4 | 59:2A:3943:HOH:O | 2.16 | 0.58 |
| 16:2U:52:ARG:HA | 16:2U:55:ARG:HD2 | 1.85 | 0.58 |
| 32:2a:9:G:H2' | 32:2a:10:A:C8 | 2.38 | 0.58 |
| 32:2a:726:C:H2' | 32:2a:727:G:H8 | 1.67 | 0.58 |
| 34:2c:19:GLU:O | 34:2c:57:ILE:N | 2.34 | 0.58 |
| 1:1A:1053:C:H42 | 1:1A:1106:G:H1 | 1.51 | 0.58 |
| 1:1A:1864:U:OP1 | 1:1A:2410:G:O2' | 2.13 | 0.58 |
| 1:1A:2393:A:H2' | 1:1A:2394:C:H6 | 1.68 | 0.58 |
| 1:1A:2682:U:O2' | 15:1T:58:ASN:ND2 | 2.37 | 0.58 |
| 25:13:8:LEU:HG | 25:13:31:LEU:HD23 | 1.86 | 0.58 |
| 32:1a:800:G:O6 | 59:1a:1914:HOH:O | 2.17 | 0.58 |
| 38:1g:86:GLN:HB2 | 38:1g:148:ASN:ND2 | 2.19 | 0.58 |
| 14:2S:67:ARG:HG2 | 14:2S:71:ARG:HD2 | 1.85 | 0.58 |
| 15:2T:105:LEU:HD22 | 15:2T:109:GLU:HB3 | 1.86 | 0.58 |
| 26:24:24:THR:OG1 | 26:24:25:TYR:N | 2.21 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 32:2a:918:A:H2' | 32:2a:919:A:C8 | 2.38 | 0.58 |
| 36:2e:77:PRO:HD2 | 36:2e:142:LEU:HD22 | 1.85 | 0.58 |
| 37:2f:67:MET:HE1 | 37:2f:75:LEU:HD22 | 1.84 | 0.58 |
| 25:13:12:PRO:HB2 | 25:13:20:LYS:HG2 | 1.86 | 0.58 |
| 32:1a:1277:C:O2' | 32:1a:1279:A:H1' | 2.02 | 0.58 |
| 35:1d:12:CYS:CB | 58:1d:501:SF4:S2 | 2.89 | 0.58 |
| 1:2A:302:C:OP2 | 20:2Y:73:ARG:NH1 | 2.28 | 0.58 |
| 1:2A:1651:G:H2' | 1:2A:1652:A:O4' | 2.04 | 0.58 |
| 1:2A:2162:G:H4' | 1:2A:2172:U:C2' | 2.34 | 0.58 |
| 32:2a:1273:G:H3' | 32:2a:1274:G:C8 | 2.37 | 0.58 |
| 32:2a:1316:G:N7 | 50:2s:7:LYS:NZ | 2.52 | 0.58 |
| 35:2d:102:ASP:HB2 | 35:2d:118:ARG:HG2 | 1.86 | 0.58 |
| 4:1E:105:THR:HG1 | 4:1E:166:THR:HG1 | 1.51 | 0.58 |
| 8:1I:78:THR:O | 8:1I:104:GLN:NE2 | 2.33 | 0.58 |
| 32:1a:34:C:H2' | 32:1a:35:G:C8 | 2.39 | 0.58 |
| 1:2A:621:A:OP2 | 11:2P:108:LYS:NZ | 2.34 | 0.58 |
| 2:2B:75:G:H22 | 21:2Z:73:GLN:NE2 | 2.01 | 0.58 |
| 3:2D:17:THR:O | 3:2D:211:ARG:NH2 | 2.37 | 0.58 |
| 4:2E:105:THR:HG1 | 4:2E:199:ARG:HH21 | 1.50 | 0.58 |
| 20:2Y:86:ARG:HE | 20:2Y:100:ALA:HA | 1.68 | 0.58 |
| 32:2a:426:G:OP1 | 35:2d:38:TYR:OH | 2.17 | 0.58 |
| 32:2a:748:C:H4' | 32:2a:749:C:O5' | 2.03 | 0.58 |
| 1:1A:311:A:OP2 | 59:1A:4278:HOH:O | 2.17 | 0.58 |
| 1:1A:2135:A:H5' | 1:1A:2160:G:H4' | 1.84 | 0.58 |
| 21:1Z:69:THR:HG22 | 21:1Z:90:VAL:HA | 1.85 | 0.58 |
| 32:1a:1414:U:H3 | 32:1a:1486:G:H1 | 1.51 | 0.58 |
| 34:1c:34:LEU:HD21 | 34:1c:38:ARG:HE | 1.69 | 0.58 |
| 36:1e:33:VAL:HG21 | 36:1e:109:ILE:HA | 1.86 | 0.58 |
| 2:2B:9:G:OP2 | 14:2S:15:ARG:NH1 | 2.35 | 0.58 |
| 4:2E:105:THR:HG21 | 4:2E:164:ARG:CZ | 2.34 | 0.58 |
| 15:2T:127:ALA:C | 15:2T:129:ARG:H | 2.12 | 0.58 |
| 32:2a:1291:G:O2' | 40:2i:38:GLN:OE1 | 2.21 | 0.58 |
| 32:2a:1312:G:H5' | 50:2s:5:LEU:HD11 | 1.84 | 0.58 |
| 1:1A:729:G:C6 | 3:1D:208:LYS:HB2 | 2.39 | 0.57 |
| 21:1Z:3:TYR:CD2 | 21:1Z:51:ALA:HB2 | 2.39 | 0.57 |
| 32:1a:186:C:H2' | 32:1a:187:C:C6 | 2.38 | 0.57 |
| 32:1a:974:A:OP2 | 45:1n:29:ARG:NH1 | 2.37 | 0.57 |
| 33:1b:195:ASP:O | 39:1h:68:ARG:NH2 | 2.36 | 0.57 |
| 1:2A:760:G:H2' | 1:2A:761:A:O4' | 2.04 | 0.57 |
| 1:2A:2165:G:H2' | 1:2A:2166:G:O4' | 2.04 | 0.57 |
| 1:2A:2805:G:H2' | 1:2A:2807:G:C8 | 2.39 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 14:2S:35:ILE:HB | 14:2S:97:ARG:HH21 | 1.68 | 0.57 |
| 24:22:65:ASN:HD21 | 24:22:69:ARG:HD3 | 1.69 | 0.57 |
| 32:2a:309:G:H2' | 32:2a:310:G:H8 | 1.69 | 0.57 |
| 32:2a:1316:G:N2 | 32:2a:1319:A:OP2 | 2.37 | 0.57 |
| 34:2c:78:GLY:HA3 | 34:2c:83:ARG:H | 1.69 | 0.57 |
| 50:2s:64:GLU:CD | 50:2s:64:GLU:H | 2.11 | 0.57 |
| 1:1A:1642:G:N7 | 59:1A:4383:HOH:O | 2.32 | 0.57 |
| 26:14:50:VAL:HG21 | 44:1m:64:TRP:C | 2.29 | 0.57 |
| 28:16:13:CYS:SG | 28:16:47:THR:HG21 | 2.44 | 0.57 |
| 32:1a:195:A:H2' | 32:1a:196:A:C4 | 2.39 | 0.57 |
| 32:1a:453:A:O2' | 47:1p:68:ASP:O | 2.23 | 0.57 |
| 32:1a:503:C:OP2 | 43:1l:116:SER:OG | 2.16 | 0.57 |
| 32:1a:1192:C:O2 | 36:1e:25:ARG:NH2 | 2.37 | 0.57 |
| 32:1a:1456:G:O3' | 51:1t:39:LYS:NZ | 2.34 | 0.57 |
| 34:1c:11:ARG:NH2 | 34:1c:177:THR:O | 2.37 | 0.57 |
| 1:2A:2646:C:H2' | 1:2A:2647:U:O4' | 2.04 | 0.57 |
| 5:2F:25:PRO:HD2 | 5:2F:115:ALA:HB2 | 1.84 | 0.57 |
| 8:2I:89:TYR:CD2 | 8:2I:89:TYR:CE2 | 2.92 | 0.57 |
| 32:2a:998:G:H1 | 32:2a:1043:C:H42 | 1.50 | 0.57 |
| 33:2b:178:ARG:HH12 | 39:2h:68:ARG:HH22 | 1.50 | 0.57 |
| 35:2d:172:PRO:HB2 | 35:2d:187:ARG:HH21 | 1.69 | 0.57 |
| 50:2s:37:ARG:O | 50:2s:70:LYS:NZ | 2.29 | 0.57 |
| 1:1A:1239:G:H2' | 1:1A:1240:U:O4' | 2.04 | 0.57 |
| 1:1A:1419:A:O2' | 1:1A:1421:G:N7 | 2.36 | 0.57 |
| 14:1S:25:ARG:NH1 | 14:1S:42:ASP:OD1 | 2.37 | 0.57 |
| 14:1S:27:SER:HA | 14:1S:88:ASP:HB3 | 1.86 | 0.57 |
| 46:1o:64:ARG:HH12 | 46:1o:68:ARG:HH21 | 1.52 | 0.57 |
| 1:2A:646:A:H2' | 1:2A:647:G:O4' | 2.05 | 0.57 |
| 1:2A:698:C:O2' | 1:2A:734:A:N6 | 2.37 | 0.57 |
| 1:2A:1462:C:H4' | 1:2A:2703:C:H5' | 1.86 | 0.57 |
| 2:2B:24:G:H4' | 2:2B:25:A:C8 | 2.39 | 0.57 |
| 32:2a:1071:C:H2' | 32:2a:1072:G:H8 | 1.69 | 0.57 |
| 41:2j:37:PRO:HA | 41:2j:72:VAL:HG12 | 1.85 | 0.57 |
| 1:1A:2291:U:O2' | 1:1A:2374:C:O2 | 2.17 | 0.57 |
| 3:1D:61:LEU:O | 3:1D:63:ARG:NH1 | 2.37 | 0.57 |
| 32:1a:944:G:OP1 | 59:1a:1903:HOH:O | 2.17 | 0.57 |
| 32:1a:1074:G:O2' | 32:1a:1101:A:N1 | 2.30 | 0.57 |
| 1:2A:1499:C:H2' | 1:2A:1500:G:H8 | 1.69 | 0.57 |
| 1:2A:2285:C:OP2 | 28:26:6:ARG:NH1 | 2.38 | 0.57 |
| 1:2A:2513:G:N2 | 4:2E:143:ASN:OD1 | 2.37 | 0.57 |
| 32:2a:1305:G:N2 | 32:2a:1331:G:H1' | 2.20 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 36:2e:105:VAL:HG21 | 36:2e:128:PRO:HB3 | 1.85 | 0.57 |
| 1:1A:579:G:H2' | 1:1A:580:C:C6 | 2.39 | 0.57 |
| 1:1A:956:G:H2' | 1:1A:957:A:H2' | 1.84 | 0.57 |
| 1:1A:999:U:OP2 | 59:1A:4271:HOH:O | 2.17 | 0.57 |
| 1:1A:1664:A:OP1 | 59:1A:4274:HOH:O | 2.17 | 0.57 |
| 1:2A:1341:U:OP2 | 1:2A:1394:U:O2' | 2.19 | 0.57 |
| 1:2A:2031:A:N3 | 1:2A:2455:G:O2' | 2.31 | 0.57 |
| 2:2B:14:U:OP2 | 2:2B:70:C:O2' | 2.17 | 0.57 |
| 4:2E:201:THR:HG23 | 4:2E:203:LYS:H | 1.70 | 0.57 |
| 11:2P:96:THR:HG23 | 11:2P:99:LEU:HD12 | 1.85 | 0.57 |
| 18:2W:20:VAL:HG12 | 18:2W:39:THR:HG21 | 1.87 | 0.57 |
| 32:2a:108:G:N1 | 51:2t:15:ARG:HG2 | 2.20 | 0.57 |
| 32:2a:1230:C:H2' | 32:2a:1231:G:H8 | 1.70 | 0.57 |
| 32:2a:1240:U:C2 | 38:2g:32:ARG:HG3 | 2.39 | 0.57 |
| 35:2d:112:VAL:H | 35:2d:116:GLN:HE21 | 1.52 | 0.57 |
| 39:2h:11:THR:HG22 | 39:2h:14:ARG:NH1 | 2.19 | 0.57 |
| 42:2k:48:ILE:HD11 | 42:2k:64:ALA:HA | 1.85 | 0.57 |
| 5:1F:70:THR:HG23 | 5:1F:72:ARG:H | 1.70 | 0.57 |
| 32:1a:662:G:H2' | 32:1a:663:A:C8 | 2.39 | 0.57 |
| 33:1b:168:THR:OG1 | 33:1b:192:SER:HA | 2.04 | 0.57 |
| 1:2A:1786:A:H1' | 1:2A:1938:A:N6 | 2.20 | 0.57 |
| 1:2A:1798:U:H5' | 3:2D:259:THR:CG2 | 2.35 | 0.57 |
| 3:2D:108:PRO:HB3 | 3:2D:143:HIS:CE1 | 2.40 | 0.57 |
| 6:2G:11:TYR:CZ | 6:2G:16:ARG:HD3 | 2.40 | 0.57 |
| 32:2a:984:C:H2' | 32:2a:985:C:C6 | 2.40 | 0.57 |
| 41:2j:61:GLU:OE1 | 45:2n:49:HIS:NE2 | 2.35 | 0.57 |
| 1:1A:210:C:OP2 | 29:17:29:LYS:NZ | 2.30 | 0.57 |
| 1:1A:1357:U:H2' | 1:1A:1358:G:O4' | 2.05 | 0.57 |
| 1:1A:2036:C:OP1 | 59:1A:4280:HOH:O | 2.18 | 0.57 |
| 1:1A:2131:G:H5" | 1:1A:2132:U:H3' | 1.86 | 0.57 |
| 5:1F:107:LYS:HE2 | 5:1F:206:ILE:HA | 1.87 | 0.57 |
| 7:1H:56:SER:OG | 7:1H:57:ASP:N | 2.36 | 0.57 |
| 1:2A:1259:G:H2' | 1:2A:1260:G:C8 | 2.39 | 0.57 |
| 1:2A:2183:C:H2' | 1:2A:2184:G:C8 | 2.39 | 0.57 |
| 22:20:15:ASP:OD1 | 22:20:16:SER:N | 2.38 | 0.57 |
| 24:22:1:MET:H1 | 24:22:52:ASP:CG | 2.13 | 0.57 |
| 30:28:63:PRO:HG2 | 30:28:64:TYR:CE2 | 2.39 | 0.57 |
| 32:2a:985:C:H2' | 32:2a:986:A:C8 | 2.39 | 0.57 |
| 32:2a:1346:A:H5" | 40:2i:120:ARG:HH12 | 1.70 | 0.57 |
| 4:1E:7:VAL:HG23 | 4:1E:51:PHE:HE2 | 1.70 | 0.57 |
| 1:2A:1798:U:H5' | 3:2D:259:THR:HG22 | 1.85 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:2A:2314:C:H2' | 1:2A:2315:G:C8 | 2.40 | 0.57 |
| 7:2H:98:LEU:HD13 | 7:2H:125:VAL:HG23 | 1.86 | 0.57 |
| 21:2Z:138:GLU:H | 21:2Z:156:LYS:HE2 | 1.69 | 0.57 |
| 32:2a:1510:U:H2' | 32:2a:1511:G:C8 | 2.39 | 0.57 |
| 34:2c:140:ARG:HA | 34:2c:143:GLU:HB2 | 1.85 | 0.57 |
| 38:2g:59:LEU:HG | 38:2g:63:LYS:HE2 | 1.87 | 0.57 |
| 48:2q:66:SER:O | 48:2q:70:ARG:NH1 | 2.37 | 0.57 |
| 50:2s:36:ARG:HA | 50:2s:71:LEU:HD23 | 1.87 | 0.57 |
| 1:1A:1062:G:H1 | 1:1A:1077:A:N6 | 1.91 | 0.57 |
| 21:1Z:153:SER:HA | 21:1Z:167:PRO:HB3 | 1.86 | 0.57 |
| 1:2A:271(H):G:H2' | 1:2A:271(I):G:H8 | 1.70 | 0.57 |
| 10:1O:64:ARG:NH2 | 10:1O:99:PHE:O | 2.38 | 0.57 |
| 1:2A:1796:U:H2' | 1:2A:1797:C:H6 | 1.69 | 0.57 |
| 1:2A:2232:U:P | 23:21:40:ARG:HH12 | 2.27 | 0.57 |
| 1:2A:2822:G:OP2 | 59:2A:3908:HOH:O | 2.17 | 0.57 |
| 17:2V:43:GLU:OE1 | 17:2V:43:GLU:N | 2.38 | 0.57 |
| 21:2Z:124:ILE:HG22 | 21:2Z:126:VAL:HG23 | 1.85 | 0.57 |
| 23:21:56:GLN:HA | 23:21:56:GLN:HE21 | 1.70 | 0.57 |
| 32:2a:254:G:OP1 | 48:2q:66:SER:OG | 2.23 | 0.57 |
| 32:2a:382:A:H2' | 32:2a:383:A:C8 | 2.39 | 0.57 |
| 32:2a:1182:G:H4' | 32:2a:1183:A:H5" | 1.86 | 0.57 |
| 32:2a:1292:U:H4' | 40:2i:38:GLN:HE22 | 1.69 | 0.57 |
| 36:2e:76:ILE:HD12 | 36:2e:142:LEU:HD21 | 1.86 | 0.57 |
| 37:2f:79:LEU:HB3 | 37:2f:88:VAL:HG21 | 1.87 | 0.57 |
| 46:2o:11:VAL:HG21 | 46:2o:34:LEU:HD22 | 1.86 | 0.57 |
| 1:1A:1226:A:OP1 | 17:1V:84:LYS:NZ | 2.36 | 0.56 |
| 1:1A:1354:A:H2' | 1:1A:1355:G:O4' | 2.05 | 0.56 |
| 52:1u:3:LYS:HD3 | 52:1u:14:TRP:CD1 | 2.40 | 0.56 |
| 12:2Q:39:PRO:HD3 | 12:2Q:99:PRO:HG3 | 1.86 | 0.56 |
| 21:2Z:33:LEU:HD21 | 21:2Z:90:VAL:HG11 | 1.85 | 0.56 |
| 32:2a:164:U:H2' | 32:2a:165:C:C6 | 2.40 | 0.56 |
| 32:2a:1053:G:H4' | 32:2a:1054:C:H3' | 1.87 | 0.56 |
| 32:2a:1270:C:H2' | 32:2a:1271:G:C8 | 2.40 | 0.56 |
| 43:2l:53:ARG:HB3 | 43:2l:69:TYR:HE1 | 1.69 | 0.56 |
| 1:1A:279:C:N4 | 1:1A:361:G:H1 | 1.97 | 0.56 |
| 1:1A:336:C:O2' | 20:1Y:35:TYR:OH | 2.22 | 0.56 |
| 1:1A:793:A:OP2 | 1:1A:2071:A:O2' | 2.23 | 0.56 |
| 1:1A:1076:C:O2' | 1:1A:1077:A:N7 | 2.38 | 0.56 |
| 8:1I:5:LEU:H | 8:1I:5:LEU:HD12 | 1.71 | 0.56 |
| 34:1c:59:ARG:HG2 | 34:1c:64:VAL:HG23 | 1.87 | 0.56 |
| 38:1g:16:LEU:HD21 | 40:1i:45:ALA:HB2 | 1.87 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:1i:26:VAL:HG13 | 40:1i:61:ALA:HB3 | 1.87 | 0.56 |
| 47:1p:43:LYS:HA | 47:1p:48:TRP:HB3 | 1.87 | 0.56 |
| 49:1r:25:THR:HG21 | 49:1r:42:ARG:HH12 | 1.70 | 0.56 |
| 54:1x:10:G:N2 | 54:1x:26:G:H1' | 2.19 | 0.56 |
| 1:2A:893:C:H2' | 1:2A:894:C:C5 | 2.40 | 0.56 |
| 32:2a:726:C:H2' | 32:2a:727:G:C8 | 2.39 | 0.56 |
| 32:2a:1271:G:C2 | 32:2a:1272:G:N7 | 2.73 | 0.56 |
| 32:2a:1316:G:N2 | 32:2a:1318:A:H3' | 2.20 | 0.56 |
| 54:2x:40:C:H2' | 54:2x:41:C:C6 | 2.40 | 0.56 |
| 1:1A:279:C:N3 | 1:1A:361:G:N2 | 2.50 | 0.56 |
| 1:1A:475:U:H4' | 1:1A:510:C:H5' | 1.87 | 0.56 |
| 1:1A:673:C:H5" | 5:1F:81:PRO:HD2 | 1.87 | 0.56 |
| 1:1A:826:U:H4' | 11:1P:55:ARG:HB3 | 1.87 | 0.56 |
| 1:1A:1671:U:O4 | 59:1A:4214:HOH:O | 2.16 | 0.56 |
| 10:1O:64:ARG:HD3 | 10:1O:79:PHE:CD1 | 2.40 | 0.56 |
| 14:1S:31:SER:O | 14:1S:97:ARG:NH2 | 2.34 | 0.56 |
| 15:1T:127:ALA:C | 15:1T:129:ARG:H | 2.13 | 0.56 |
| 32:1a:193:C:H2' | 32:1a:194:C:H6 | 1.70 | 0.56 |
| 32:1a:1095:U:P | 32:1a:1108:G:H1 | 2.28 | 0.56 |
| 32:1a:1130:A:OP2 | 40:1i:62:TYR:OH | 2.12 | 0.56 |
| 46:1o:64:ARG:HH12 | 46:1o:68:ARG:NH2 | 2.03 | 0.56 |
| 49:1r:70:ILE:O | 49:1r:74:ARG:HG3 | 2.05 | 0.56 |
| 49:1r:70:ILE:HG22 | 49:1r:74:ARG:HD2 | 1.85 | 0.56 |
| 1:2A:247:G:H4' | 1:2A:386:G:C5 | 2.40 | 0.56 |
| 1:2A:2189:U:H2' | 1:2A:2190:G:H8 | 1.70 | 0.56 |
| 1:2A:2264:C:N4 | 22:20:15:ASP:OD2 | 2.36 | 0.56 |
| 8:2I:123:LEU:HD21 | 8:2I:146:ALA:HB2 | 1.87 | 0.56 |
| 31:29:14:CYS:HA | 31:29:27:CYS:HB2 | 1.85 | 0.56 |
| 32:2a:1052:U:O2' | 32:2a:1055:A:OP2 | 2.16 | 0.56 |
| 32:2a:1189:C:OP1 | 41:2j:51:ARG:NH2 | 2.36 | 0.56 |
| 40:2i:128:ARG:NH2 | 54:2x:33:U:OP2 | 2.38 | 0.56 |
| 49:2r:53:ARG:O | 49:2r:57:GLY:N | 2.38 | 0.56 |
| 32:1a:414:A:H2' | 32:1a:415:A:C8 | 2.41 | 0.56 |
| 32:1a:1015:A:H2' | 32:1a:1016:A:C8 | 2.40 | 0.56 |
| 37:1f:78:GLU:O | 37:1f:81:ILE:HG22 | 2.05 | 0.56 |
| 47:1p:49:LEU:HD21 | 47:1p:51:VAL:HG23 | 1.88 | 0.56 |
| 5:2F:12:LEU:HB2 | 5:2F:124:LEU:HD11 | 1.85 | 0.56 |
| 12:2Q:27:VAL:HG23 | 12:2Q:28:ALA:H | 1.70 | 0.56 |
| 32:2a:269:C:H2' | 32:2a:270:A:H8 | 1.70 | 0.56 |
| 33:2b:31:TYR:CZ | 33:2b:200:ILE:HD13 | 2.41 | 0.56 |
| 1:1A:613:G:N2 | 1:1A:614(C):A:O2' | 2.38 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1A:739:G:OP1 | 59:1A:4279:HOH:O | 2.17 | 0.56 |
| 1:1A:848:G:H2' | 1:1A:849:A:C8 | 2.41 | 0.56 |
| 1:1A:1171:G:OP2 | 1:1A:1174:A:N6 | 2.38 | 0.56 |
| 1:1A:2334:G:H5' | 14:1S:9:ARG:HG2 | 1.86 | 0.56 |
| 1:1A:2683:C:H2' | 1:1A:2684:U:H6 | 1.70 | 0.56 |
| 32:1a:1289:A:N1 | 32:1a:1371:G:O2' | 2.35 | 0.56 |
| 35:1d:178:VAL:C | 35:1d:180:GLY:H | 2.13 | 0.56 |
| 38:1g:89:MET:SD | 38:1g:155:ARG:HB2 | 2.45 | 0.56 |
| 1:2A:1426:G:O2' | 1:2A:1572:A:N6 | 2.36 | 0.56 |
| 1:2A:2375:G:O2' | 1:2A:2377:A:N7 | 2.26 | 0.56 |
| 8:2I:12:LEU:HD22 | 8:2I:19:VAL:HG21 | 1.87 | 0.56 |
| 32:2a:688:G:H2' | 32:2a:689:C:H6 | 1.70 | 0.56 |
| 32:2a:1275:A:H3' | 32:2a:1276:G:H8 | 1.69 | 0.56 |
| 33:2b:55:PHE:O | 33:2b:59:GLU:N | 2.33 | 0.56 |
| 39:2h:30:ARG:O | 39:2h:34:GLU:HG2 | 2.05 | 0.56 |
| 40:2i:14:VAL:HG23 | 40:2i:66:ARG:HG3 | 1.85 | 0.56 |
| 48:2q:24:GLU:HA | 48:2q:39:SER:HA | 1.87 | 0.56 |
| 21:1Z:93:ASP:HB2 | 21:1Z:131:ARG:HH22 | 1.69 | 0.56 |
| 32:1a:165:C:H2' | 32:1a:166:G:H8 | 1.69 | 0.56 |
| 32:1a:772:U:H2' | 32:1a:773:G:O4' | 2.04 | 0.56 |
| 38:1g:62:PHE:HA | 38:1g:124:LEU:HD22 | 1.86 | 0.56 |
| 1:2A:154(A):C:H42 | 1:2A:171:G:H1 | 1.53 | 0.56 |
| 1:2A:1266:G:O4' | 18:2W:15:ARG:NH2 | 2.38 | 0.56 |
| 12:2Q:135:ASP:OD2 | 21:2Z:49:ARG:NH2 | 2.38 | 0.56 |
| 32:2a:79:G:H1 | 32:2a:90:U:H3 | 1.54 | 0.56 |
| 32:2a:583:A:P | 46:2o:68:ARG:HH22 | 2.28 | 0.56 |
| 46:2o:36:ILE:HG23 | 46:2o:56:LEU:HD11 | 1.87 | 0.56 |
| 1:1A:624:C:O2' | 1:1A:657:U:OP1 | 2.22 | 0.56 |
| 9:1N:67:LEU:HD12 | 9:1N:87:LEU:HD13 | 1.87 | 0.56 |
| 32:1a:123:C:OP1 | 32:1a:311:C:O2' | 2.14 | 0.56 |
| 32:1a:136:C:O2' | 47:1p:65:GLN:NE2 | 2.38 | 0.56 |
| 33:1b:8:LYS:O | 33:1b:217:ARG:NH1 | 2.39 | 0.56 |
| 35:1d:109:GLY:HA3 | 35:1d:165:MET:HG3 | 1.88 | 0.56 |
| 38:1g:27:ILE:HD13 | 38:1g:40:ALA:HA | 1.86 | 0.56 |
| 32:2a:390:C:O3' | 47:2p:28:ARG:NH2 | 2.39 | 0.56 |
| 43:2l:10:LEU:HB3 | 48:2q:32:TYR:CE2 | 2.40 | 0.56 |
| 44:2m:96:LEU:HD23 | 44:2m:103:THR:HG21 | 1.87 | 0.56 |
| 1:1A:2022:U:O2' | 1:1A:2617:C:H5' | 2.06 | 0.56 |
| 1:1A:2136:C:N4 | 1:1A:2155:G:C6 | 2.74 | 0.56 |
| 6:1G:179:PRO:HG3 | 26:14:43:TYR:OH | 2.05 | 0.56 |
| 33:1b:16:HIS:CD2 | 33:1b:204:ASN:H | 2.23 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 37:1f:65:VAL:HG21 | 37:1f:67:MET:HE2 | 1.86 | 0.56 |
| 4:2E:36:ARG:NH1 | 4:2E:85:ASN:OD1 | 2.38 | 0.56 |
| 10:2O:68:GLU:OE1 | 10:2O:78:ARG:NH1 | 2.39 | 0.56 |
| 36:2e:126:ARG:HA | 36:2e:131:ILE:HD11 | 1.87 | 0.56 |
| 1:1A:2130:U:H2' | 1:1A:2158:A:N6 | 2.19 | 0.56 |
| 1:1A:2600:A:N6 | 59:1A:4323:HOH:O | 2.25 | 0.56 |
| 32:1a:100:C:H2' | 32:1a:101:A:C8 | 2.41 | 0.56 |
| 1:2A:143:G:H2' | 1:2A:143(A):C:C6 | 2.40 | 0.56 |
| 1:2A:1449:A:O2' | 1:2A:1529:G:N2 | 2.29 | 0.56 |
| 10:2O:34:THR:OG1 | 10:2O:35:VAL:N | 2.38 | 0.56 |
| 18:2W:88:ARG:NH1 | 18:2W:94:ASP:OD2 | 2.39 | 0.56 |
| 32:2a:736:C:H2' | 32:2a:737:A:C8 | 2.41 | 0.56 |
| 39:2h:64:LYS:HG2 | 39:2h:79:VAL:HG21 | 1.88 | 0.56 |
| 43:2l:86:ARG:NH1 | 59:2l:301:HOH:O | 2.38 | 0.56 |
| 1:1A:221:A:N1 | 1:1A:265:A:O2' | 2.36 | 0.56 |
| 1:1A:363(A):A:H2' | 1:1A:363(B):G:C8 | 2.41 | 0.56 |
| 1:1A:489:G:N7 | 18:1W:49:LYS:NZ | 2.54 | 0.56 |
| 1:1A:1385:G:O2' | 1:1A:1396:U:O2 | 2.18 | 0.56 |
| 1:1A:1490:A:O2' | 3:1D:99:ASP:OD1 | 2.23 | 0.56 |
| 1:1A:2576:G:OP1 | 59:1A:4281:HOH:O | 2.18 | 0.56 |
| 10:1O:64:ARG:HB2 | 10:1O:79:PHE:CG | 2.41 | 0.56 |
| 32:1a:194:C:H2' | 32:1a:195:A:H5" | 1.88 | 0.56 |
| 32:1a:539:A:H2' | 32:1a:540:G:H8 | 1.70 | 0.56 |
| 32:1a:967:5MC:H4' | 40:1i:125:TYR:HE1 | 1.71 | 0.56 |
| 40:1i:24:GLY:HA3 | 40:1i:57:GLY:HA2 | 1.88 | 0.56 |
| 1:2A:27:G:N2 | 1:2A:512:G:H1' | 2.20 | 0.56 |
| 1:2A:428:A:OP1 | 59:2A:3950:HOH:O | 2.18 | 0.56 |
| 3:2D:37:LEU:HD13 | 3:2D:62:TYR:HB2 | 1.86 | 0.56 |
| 14:2S:27:SER:HA | 14:2S:88:ASP:HB3 | 1.88 | 0.56 |
| 19:2X:53:LYS:HB3 | 19:2X:82:GLN:HB3 | 1.88 | 0.56 |
| 33:2b:31:TYR:CE2 | 33:2b:194:PRO:HB3 | 2.40 | 0.56 |
| 1:1A:2537:U:H2' | 1:1A:2538:C:C6 | 2.42 | 0.55 |
| 1:1A:2701:C:H2' | 1:1A:2702:U:H2' | 1.89 | 0.55 |
| 32:1a:542:G:OP1 | 35:1d:10:ARG:NH2 | 2.30 | 0.55 |
| 33:1b:155:LEU:HD11 | 33:1b:159:PRO:HG3 | 1.89 | 0.55 |
| 34:1c:36:ASP:N | 34:1c:36:ASP:OD1 | 2.37 | 0.55 |
| 38:1g:69:VAL:HG22 | 38:1g:135:VAL:HG22 | 1.87 | 0.55 |
| 40:1i:11:LYS:H | 40:1i:104:ARG:HH21 | 1.53 | 0.55 |
| 1:2A:1568:G:H5" | 3:2D:61:LEU:HD13 | 1.88 | 0.55 |
| 1:2A:2273:A:H2' | 1:2A:2274:A:C8 | 2.42 | 0.55 |
| 32:2a:861:G:HO2' | 32:2a:874:G:HO2' | 1.49 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 32:2a:1060:C:H2' | 32:2a:1061:G:H8 | 1.70 | 0.55 |
| 32:2a:1346:A:N6 | 32:2a:1375:A:OP2 | 2.29 | 0.55 |
| 41:2j:20:ALA:O | 41:2j:24:VAL:N | 2.38 | 0.55 |
| 1:1A:2136:C:N4 | 1:1A:2155:G:H1 | 2.03 | 0.55 |
| 23:11:60:PHE:HE1 | 23:11:95:LEU:HD21 | 1.71 | 0.55 |
| 35:1d:31:CYS:SG | 35:1d:33:MET:N | 2.79 | 0.55 |
| 42:1k:27:ASN:OD1 | 42:1k:28:THR:N | 2.38 | 0.55 |
| 1:2A:1183:G:H5" | 25:23:30:ARG:NH2 | 2.21 | 0.55 |
| 1:2A:1899:G:H2' | 1:2A:1899:G:N3 | 2.20 | 0.55 |
| 1:2A:2529:G:O6 | 31:29:31:LYS:NZ | 2.38 | 0.55 |
| 1:2A:2657:A:N6 | 1:2A:2664:G:O2' | 2.40 | 0.55 |
| 8:2I:108:THR:HG22 | 8:2I:109:ILE:H | 1.70 | 0.55 |
| 40:2i:3:GLN:HE21 | 40:2i:20:ARG:HE | 1.54 | 0.55 |
| 8:1I:3:VAL:HA | 8:1I:38:LEU:HA | 1.89 | 0.55 |
| 21:1Z:40:ASP:HB3 | 21:1Z:43:GLU:HB2 | 1.88 | 0.55 |
| 26:14:46:GLN:O | 26:14:46:GLN:HG2 | 2.07 | 0.55 |
| 32:1a:1005:A:H1' | 32:1a:1036:G:O6 | 2.06 | 0.55 |
| 1:2A:55:G:H2' | 1:2A:56:A:H8 | 1.72 | 0.55 |
| 1:2A:307:G:N2 | 1:2A:310:A:O5' | 2.40 | 0.55 |
| 1:2A:857:C:H4' | 22:20:23:VAL:HG21 | 1.87 | 0.55 |
| 2:2B:115:G:H2' | 2:2B:116:G:O4' | 2.06 | 0.55 |
| 5:2F:143:ALA:HB1 | 5:2F:148:LEU:HB2 | 1.87 | 0.55 |
| 7:2H:3:ARG:NH1 | 7:2H:4:ILE:H | 2.05 | 0.55 |
| 7:2H:9:ILE:HB | 7:2H:50:VAL:HG13 | 1.87 | 0.55 |
| 32:2a:17:U:H2' | 32:2a:18:C:C6 | 2.42 | 0.55 |
| 32:2a:1346:A:N1 | 32:2a:1374:A:H5" | 2.21 | 0.55 |
| 34:2c:131:ARG:HH21 | 36:2e:50:GLU:HG3 | 1.70 | 0.55 |
| 1:1A:1213:A:N3 | 1:1A:1238:G:O2' | 2.36 | 0.55 |
| 1:1A:1482:G:N2 | 1:1A:1507:A:H1' | 2.22 | 0.55 |
| 1:1A:2286:A:H4' | 1:1A:2287:A:O4' | 2.06 | 0.55 |
| 12:1Q:10:ARG:NH2 | 12:1Q:90:VAL:H | 2.05 | 0.55 |
| 32:1a:1074:G:O2' | 33:1b:103:THR:OG1 | 2.22 | 0.55 |
| 38:1g:67:GLU:OE1 | 38:1g:70:LYS:NZ | 2.30 | 0.55 |
| 1:2A:784:A:C6 | 3:2D:229:VAL:HG11 | 2.41 | 0.55 |
| 1:2A:2522:U:O2' | 1:2A:2647:U:OP1 | 2.24 | 0.55 |
| 32:2a:1029:C:C2 | 32:2a:1032:G:N2 | 2.75 | 0.55 |
| 32:2a:1176:A:H2' | 32:2a:1177:G:C8 | 2.42 | 0.55 |
| 34:2c:58:GLU:HB2 | 34:2c:65:ALA:HB3 | 1.87 | 0.55 |
| 1:1A:588:U:H2' | 1:1A:589:C:C6 | 2.41 | 0.55 |
| 1:1A:2136:C:N3 | 1:1A:2155:G:C2 | 2.74 | 0.55 |
| 1:1A:2319:G:H22 | 14:1S:3:ARG:HD3 | 1.71 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:1D:108:PRO:HB3 | 3:1D:143:HIS:CE1 | 2.42 | 0.55 |
| 7:1H:92:ILE:HD12 | 7:1H:92:ILE:H | 1.72 | 0.55 |
| 18:1W:19:LEU:HB3 | 27:15:25:LEU:HG | 1.88 | 0.55 |
| 33:1b:22:LYS:HG2 | 33:1b:40:HIS:HE1 | 1.72 | 0.55 |
| 1:2A:83:G:N2 | 1:2A:103:A:OP2 | 2.39 | 0.55 |
| 1:2A:746:A:HO2' | 1:2A:2611:U:HO2' | 1.52 | 0.55 |
| 32:2a:815:A:N7 | 32:2a:1509:C:O2' | 2.37 | 0.55 |
| 32:2a:864:A:H5' | 36:2e:86:ALA:HB2 | 1.87 | 0.55 |
| 32:2a:1485:U:H2' | 32:2a:1486:G:C8 | 2.41 | 0.55 |
| 36:2e:57:LYS:HG2 | 36:2e:61:TYR:HE2 | 1.71 | 0.55 |
| 1:1A:223:A:N1 | 1:1A:407:G:O2' | 2.39 | 0.55 |
| 1:1A:1598:C:H2' | 1:1A:1599:C:H6 | 1.72 | 0.55 |
| 1:1A:1815:A:OP1 | 59:1A:4285:HOH:O | 2.18 | 0.55 |
| 1:1A:2072:G:N2 | 59:1A:4441:HOH:O | 2.39 | 0.55 |
| 5:1F:34:TRP:HA | 11:1P:6:LEU:HD13 | 1.89 | 0.55 |
| 5:1F:140:LEU:HD11 | 5:1F:170:LEU:HD21 | 1.89 | 0.55 |
| 16:1U:10:ARG:NH2 | 59:1U:301:HOH:O | 2.40 | 0.55 |
| 32:1a:1298:C:H2' | 38:1g:114:ARG:NH2 | 2.22 | 0.55 |
| 32:1a:1409:C:H2' | 32:1a:1410:G:H8 | 1.71 | 0.55 |
| 33:1b:24:TRP:CZ3 | 33:1b:26:PRO:HA | 2.41 | 0.55 |
| 33:1b:167:PRO:HG2 | 33:1b:192:SER:HB3 | 1.88 | 0.55 |
| 1:2A:1266:G:O2' | 1:2A:2012:G:O6 | 2.25 | 0.55 |
| 1:2A:2134:A:N6 | 1:2A:2157:G:H4' | 2.21 | 0.55 |
| 2:2B:19:G:H2' | 2:2B:20:C:O4' | 2.07 | 0.55 |
| 14:2S:15:ARG:O | 14:2S:19:LYS:HG2 | 2.06 | 0.55 |
| 25:23:10:LYS:HB3 | 25:23:53:LEU:HA | 1.88 | 0.55 |
| 30:28:6:THR:HG23 | 30:28:64:TYR:HD2 | 1.71 | 0.55 |
| 32:2a:15:G:O4' | 36:2e:24:ARG:NH2 | 2.39 | 0.55 |
| 40:2i:85:LEU:HB3 | 40:2i:92:TYR:CD2 | 2.42 | 0.55 |
| 42:2k:82:VAL:HB | 42:2k:108:ILE:HG12 | 1.88 | 0.55 |
| 1:1A:819:A:OP2 | 1:1A:1187:G:N2 | 2.33 | 0.55 |
| 1:1A:882:G:H1 | 1:1A:894:C:H42 | 1.55 | 0.55 |
| 1:1A:2364:C:H2' | 1:1A:2365:G:O4' | 2.06 | 0.55 |
| 5:1F:164:ARG:HD2 | 5:1F:175:THR:HG23 | 1.89 | 0.55 |
| 41:1j:49:VAL:HB | 45:1n:41:ARG:HG3 | 1.88 | 0.55 |
| 1:2A:1019:U:H3 | 1:2A:1142(A):A:H62 | 1.54 | 0.55 |
| 2:2B:11:C:H3' | 2:2B:12:C:C6 | 2.42 | 0.55 |
| 3:2D:148:GLU:HB2 | 3:2D:151:LYS:HD2 | 1.88 | 0.55 |
| 30:28:56:GLU:HA | 30:28:59:LYS:HE3 | 1.87 | 0.55 |
| 32:2a:56:U:H2' | 32:2a:57:G:H8 | 1.69 | 0.55 |
| 32:2a:619:U:N3 | 35:2d:134:ASP:OD1 | 2.39 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 32:2a:728:A:H2' | 32:2a:729:A:C8 | 2.42 | 0.55 |
| 32:2a:974:A:OP2 | 45:2n:29:ARG:NH1 | 2.40 | 0.55 |
| 32:2a:1404:5MC:O2 | 32:2a:1519:MA6:O2' | 2.21 | 0.55 |
| 48:2q:45:HIS:NE2 | 48:2q:47:PRO:HG3 | 2.22 | 0.55 |
| 1:1A:1466:G:H2' | 1:1A:1547:C:H41 | 1.72 | 0.55 |
| 1:1A:1899:G:N3 | 1:1A:1899:G:H2' | 2.20 | 0.55 |
| 28:16:18:ARG:HD2 | 28:16:42:TRP:CG | 2.42 | 0.55 |
| 32:1a:973:G:OP1 | 41:1j:57:LYS:NZ | 2.31 | 0.55 |
| 1:2A:954:G:H5" | 12:2Q:13:GLN:HB3 | 1.89 | 0.55 |
| 1:2A:1186:G:C2 | 1:2A:1187:G:H1' | 2.41 | 0.55 |
| 1:2A:1419:A:H5' | 1:2A:1579:A:H61 | 1.71 | 0.55 |
| 1:2A:2101:G:O6 | 1:2A:2188:C:N3 | 2.39 | 0.55 |
| 7:2H:159:GLU:HG3 | 7:2H:169:VAL:HG11 | 1.88 | 0.55 |
| 12:2Q:111:GLU:O | 12:2Q:115:MET:HG2 | 2.07 | 0.55 |
| 17:2V:56:SER:H | 17:2V:100:ARG:HB2 | 1.72 | 0.55 |
| 26:24:62:ARG:HA | 26:24:62:ARG:CZ | 2.36 | 0.55 |
| 39:2h:20:TYR:HA | 39:2h:65:TYR:CZ | 2.42 | 0.55 |
| 48:2q:84:LEU:O | 48:2q:87:LYS:HG3 | 2.06 | 0.55 |
| 1:1A:1047:G:H2' | 1:1A:1110:G:N2 | 2.22 | 0.55 |
| 6:1G:11:TYR:HA | 6:1G:15:VAL:HB | 1.88 | 0.55 |
| 1:2A:910:A:C5 | 12:2Q:13:GLN:HG3 | 2.42 | 0.55 |
| 1:2A:1477:A:H2' | 1:2A:1478:G:O4' | 2.07 | 0.55 |
| 1:2A:2689:U:OP2 | 1:2A:2719:G:N2 | 2.34 | 0.55 |
| 3:2D:145:VAL:HG13 | 3:2D:191:ALA:HB2 | 1.87 | 0.55 |
| 15:2T:54:ARG:HA | 15:2T:59:THR:HG23 | 1.88 | 0.55 |
| 32:2a:707:C:H2' | 32:2a:708:C:C6 | 2.41 | 0.55 |
| 36:2e:32:VAL:HG11 | 36:2e:59:GLY:HA2 | 1.89 | 0.55 |
| 1:1A:1031:G:N3 | 31:19:36:GLN:NE2 | 2.50 | 0.55 |
| 1:1A:1991:U:H2' | 1:1A:1992:G:H5" | 1.88 | 0.55 |
| 32:1a:977:A:H2' | 32:1a:978:A:H5" | 1.89 | 0.55 |
| 32:1a:1068:G:H8 | 32:1a:1068:G:OP2 | 1.89 | 0.55 |
| 47:1p:4:ILE:HG13 | 47:1p:64:ALA:HB1 | 1.89 | 0.55 |
| 1:2A:2334:G:H5' | 14:2S:9:ARG:HG2 | 1.89 | 0.55 |
| 15:2T:51:ARG:HG2 | 15:2T:62:THR:HB | 1.89 | 0.55 |
| 32:2a:131:C:H2' | 32:2a:132:C:C6 | 2.42 | 0.55 |
| 32:2a:922:G:H4' | 36:2e:20:GLN:HA | 1.88 | 0.55 |
| 32:2a:1084:G:H5' | 32:2a:1102:A:OP2 | 2.06 | 0.55 |
| 32:2a:1136:U:OP2 | 32:2a:1137:C:N4 | 2.40 | 0.55 |
| 38:2g:153:HIS:HE1 | 42:2k:57:THR:HB | 1.72 | 0.55 |
| 1:1A:1416:G:N2 | 1:1A:1582:C:O2 | 2.20 | 0.54 |
| 5:1F:34:TRP:CE3 | 5:1F:35:GLU:HG2 | 2.42 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 32:1a:328:C:H4' | 32:1a:329:A:H5' | 1.88 | 0.54 |
| 32:1a:601:C:H2' | 32:1a:602:A:H8 | 1.73 | 0.54 |
| 37:1f:35:ALA:HA | 37:1f:67:MET:HB3 | 1.90 | 0.54 |
| 1:2A:1946:U:H2' | 1:2A:1947:C:C6 | 2.42 | 0.54 |
| 1:2A:2108:C:H2' | 1:2A:2109:U:C6 | 2.42 | 0.54 |
| 1:2A:2164:C:H5" | 1:2A:2165:G:C8 | 2.42 | 0.54 |
| 1:2A:2467:C:H4' | 12:2Q:123:HIS:CD2 | 2.42 | 0.54 |
| 1:2A:2683:C:O2 | 10:2O:70:LYS:NZ | 2.26 | 0.54 |
| 32:2a:147:G:H2' | 32:2a:148:G:H8 | 1.72 | 0.54 |
| 37:2f:46:ARG:HH22 | 49:2r:37:VAL:HG11 | 1.72 | 0.54 |
| 1:1A:1060:U:H3 | 1:1A:1062:G:H1' | 1.71 | 0.54 |
| 1:1A:2134:A:H61 | 1:1A:2157:G:H4' | 1.72 | 0.54 |
| 4:1E:1:MET:O | 4:1E:84:PHE:HB2 | 2.06 | 0.54 |
| 10:1O:75:SER:OG | 15:1T:74:ARG:NH1 | 2.39 | 0.54 |
| 15:1T:91:ARG:HB2 | 15:1T:121:ILE:HG13 | 1.88 | 0.54 |
| 32:1a:950:U:H2' | 32:1a:951:G:H8 | 1.72 | 0.54 |
| 32:1a:958:A:N3 | 32:1a:985:C:O2' | 2.32 | 0.54 |
| 32:1a:1027:C:C4 | 32:1a:1034:G:N1 | 2.76 | 0.54 |
| 35:1d:76:ARG:NH2 | 35:1d:80:GLU:OE2 | 2.35 | 0.54 |
| 37:1f:43:LEU:HD22 | 37:1f:46:ARG:HH21 | 1.72 | 0.54 |
| 1:2A:7:G:H2' | 1:2A:8:A:C8 | 2.42 | 0.54 |
| 1:2A:658:C:H2' | 1:2A:659:C:C6 | 2.43 | 0.54 |
| 1:2A:2648:C:H2' | 1:2A:2649:U:H6 | 1.72 | 0.54 |
| 4:2E:109:LYS:O | 4:2E:111:ARG:NH1 | 2.40 | 0.54 |
| 18:2W:15:ARG:NH1 | 59:2W:301:HOH:O | 2.40 | 0.54 |
| 32:2a:646:U:H2' | 32:2a:647:C:C6 | 2.42 | 0.54 |
| 32:2a:1138:G:C6 | 32:2a:1140:C:H1' | 2.42 | 0.54 |
| 32:2a:1202:G:N2 | 45:2n:46:GLU:OE2 | 2.35 | 0.54 |
| 32:2a:1263:C:C4 | 32:2a:1272:G:O6 | 2.61 | 0.54 |
| 5:1F:156:LEU:HD21 | 5:1F:163:VAL:HG12 | 1.89 | 0.54 |
| 32:1a:96:U:H2' | 32:1a:97:G:C8 | 2.42 | 0.54 |
| 32:1a:237:C:OP2 | 48:1q:40:LYS:NZ | 2.39 | 0.54 |
| 32:1a:373:A:H2' | 32:1a:374:A:H8 | 1.72 | 0.54 |
| 32:1a:539:A:H2' | 32:1a:540:G:C8 | 2.42 | 0.54 |
| 32:1a:677:U:H3 | 32:1a:713:G:H22 | 1.54 | 0.54 |
| 35:1d:81:GLU:CD | 35:1d:139:ARG:HH22 | 2.16 | 0.54 |
| 1:2A:2848:G:O6 | 59:2A:3952:HOH:O | 2.18 | 0.54 |
| 11:2P:50:ARG:HD3 | 30:28:7:HIS:CD2 | 2.42 | 0.54 |
| 18:2W:12:ILE:HD13 | 18:2W:17:VAL:HG13 | 1.89 | 0.54 |
| 1:1A:135:G:N7 | 59:1A:4394:HOH:O | 2.33 | 0.54 |
| 1:1A:1047:G:HO2' | 1:1A:1048:A:H8 | 1.55 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1A:1063:G:H2' | 1:1A:1064:C:C6 | 2.43 | 0.54 |
| 5:1F:135:LYS:HB2 | 5:1F:138:GLU:CD | 2.32 | 0.54 |
| 6:1G:117:PHE:HZ | 6:1G:179:PRO:HG2 | 1.72 | 0.54 |
| 18:1W:65:LEU:HD12 | 18:1W:68:ARG:HE | 1.71 | 0.54 |
| 32:1a:472:A:H2' | 32:1a:473:G:O4' | 2.08 | 0.54 |
| 32:1a:950:U:H2' | 32:1a:951:G:C8 | 2.43 | 0.54 |
| 32:1a:1148:U:H2' | 32:1a:1149:C:O4' | 2.07 | 0.54 |
| 1:2A:2022:U:O2' | 1:2A:2616:C:O2' | 2.15 | 0.54 |
| 3:2D:108:PRO:HD2 | 3:2D:111:LEU:HD22 | 1.88 | 0.54 |
| 14:2S:26:LEU:N | 14:2S:86:ALA:O | 2.36 | 0.54 |
| 32:2a:515:G:H2' | 32:2a:516:PSU:C6 | 2.42 | 0.54 |
| 32:2a:953:G:H5' | 32:2a:965:A:N6 | 2.21 | 0.54 |
| 38:2g:23:VAL:HG13 | 38:2g:43:PHE:HE2 | 1.72 | 0.54 |
| 1:1A:1815:A:P | 3:1D:54:ARG:HH22 | 2.30 | 0.54 |
| 1:1A:1936:A:OP1 | 1:1A:1937:A:H5' | 2.06 | 0.54 |
| 15:1T:51:ARG:HG3 | 15:1T:98:LYS:HD2 | 1.90 | 0.54 |
| 32:1a:197:A:C6 | 32:1a:221:C:H4' | 2.43 | 0.54 |
| 32:1a:266:G:H5" | 32:1a:268:C:H41 | 1.72 | 0.54 |
| 32:1a:1346:A:OP1 | 40:1i:120:ARG:NH1 | 2.28 | 0.54 |
| 33:1b:21:ARG:HB3 | 33:1b:39:ILE:HA | 1.89 | 0.54 |
| 1:2A:639:U:H2' | 1:2A:640:C:C6 | 2.42 | 0.54 |
| 1:2A:652(D):C:H42 | 1:2A:652(U):G:H1 | 1.55 | 0.54 |
| 1:2A:686:G:N2 | 1:2A:788:A:H61 | 2.05 | 0.54 |
| 1:2A:821:A:H2' | 1:2A:946:G:H5" | 1.88 | 0.54 |
| 1:2A:1021:A:H62 | 1:2A:1141:U:H3 | 1.55 | 0.54 |
| 1:2A:1713:U:H2' | 1:2A:1714:G:C8 | 2.41 | 0.54 |
| 1:2A:2022:U:O2' | 1:2A:2617:C:H5' | 2.07 | 0.54 |
| 1:2A:2408:U:H2' | 1:2A:2409:G:C8 | 2.43 | 0.54 |
| 1:2A:2638:G:P | 4:2E:82:ARG:HH22 | 2.31 | 0.54 |
| 12:2Q:85:LYS:HD3 | 22:20:7:LEU:HD22 | 1.89 | 0.54 |
| 19:2X:50:LYS:HB3 | 19:2X:84:ALA:HB2 | 1.90 | 0.54 |
| 31:29:2:LYS:NZ | 31:29:31:LYS:O | 2.41 | 0.54 |
| 32:2a:603:U:H2' | 32:2a:604:G:H8 | 1.71 | 0.54 |
| 45:2n:48:ALA:HB2 | 45:2n:53:LEU:HD12 | 1.90 | 0.54 |
| 1:1A:213:A:OP2 | 59:1A:4282:HOH:O | 2.18 | 0.54 |
| 1:1A:1902:C:H5' | 3:1D:246:PRO:HD3 | 1.88 | 0.54 |
| 11:1P:70:GLN:N | 11:1P:70:GLN:OE1 | 2.41 | 0.54 |
| 12:1Q:27:VAL:O | 12:1Q:67:ARG:NH1 | 2.41 | 0.54 |
| 32:1a:108:G:N1 | 51:1t:15:ARG:HG2 | 2.23 | 0.54 |
| 32:1a:262:A:H2' | 32:1a:263:A:C8 | 2.42 | 0.54 |
| 1:2A:2319:G:N2 | 14:2S:3:ARG:HD2 | 2.23 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 32:2a:1029:C:C4 | 32:2a:1032:G:N1 | 2.76 | 0.54 |
| 1:1A:1044:G:H1' | 1:1A:1048:A:H1' | 1.90 | 0.54 |
| 32:1a:630:G:H2' | 32:1a:631:G:H8 | 1.73 | 0.54 |
| 33:1b:33:TYR:HB2 | 33:1b:43:ASP:HB2 | 1.90 | 0.54 |
| 40:1i:17:VAL:HA | 40:1i:63:ILE:HG23 | 1.89 | 0.54 |
| 1:2A:2680:C:H1' | 4:2E:187:ALA:HB1 | 1.88 | 0.54 |
| 12:2Q:75:THR:HG21 | 12:2Q:87:LYS:HE2 | 1.90 | 0.54 |
| 16:2U:17:ILE:HG13 | 16:2U:32:PHE:HE1 | 1.72 | 0.54 |
| 21:2Z:33:LEU:HD11 | 21:2Z:90:VAL:HG21 | 1.90 | 0.54 |
| 36:2e:139:LEU:HA | 36:2e:142:LEU:HD12 | 1.89 | 0.54 |
| 1:1A:783:A:O2' | 1:1A:785:G:OP1 | 2.25 | 0.54 |
| 1:1A:1179:C:H2' | 1:1A:1180:C:H6 | 1.73 | 0.54 |
| 1:1A:2031:A:C6 | 1:1A:2498:C:H1' | 2.43 | 0.54 |
| 20:1Y:20:TYR:CE2 | 20:1Y:43:ASN:HA | 2.43 | 0.54 |
| 32:1a:129:U:H5' | 48:1q:3:LYS:HZ1 | 1.73 | 0.54 |
| 32:1a:1052:U:OP2 | 59:1a:1916:HOH:O | 2.18 | 0.54 |
| 51:1t:33:ILE:O | 51:1t:37:SER:OG | 2.24 | 0.54 |
| 1:2A:125:G:C6 | 29:27:10:ARG:HG3 | 2.42 | 0.54 |
| 1:2A:1456:G:OP2 | 59:2A:3953:HOH:O | 2.19 | 0.54 |
| 1:2A:2055:C:N3 | 59:2A:4025:HOH:O | 2.33 | 0.54 |
| 1:2A:2127:G:C6 | 1:2A:2161:C:N4 | 2.76 | 0.54 |
| 5:2F:103:LYS:HA | 5:2F:106:ARG:HD3 | 1.90 | 0.54 |
| 11:2P:38:GLN:HB3 | 11:2P:45:LEU:HD23 | 1.90 | 0.54 |
| 22:20:53:MET:HG2 | 22:20:57:PHE:HA | 1.90 | 0.54 |
| 32:2a:1396:A:H2 | 36:2e:19:MET:HG3 | 1.73 | 0.54 |
| 32:2a:1465:C:H2' | 32:2a:1466:C:O4' | 2.08 | 0.54 |
| 39:2h:12:ARG:HD2 | 39:2h:26:VAL:HG12 | 1.90 | 0.54 |
| 1:1A:2377:A:H2' | 1:1A:2378:A:C8 | 2.43 | 0.54 |
| 1:2A:2857:G:N2 | 1:2A:2860:A:OP2 | 2.40 | 0.54 |
| 21:2Z:28:MET:HE1 | 21:2Z:61:LEU:HD21 | 1.89 | 0.54 |
| 21:2Z:47:VAL:HA | 21:2Z:50:GLN:HE22 | 1.73 | 0.54 |
| 21:2Z:52:SER:HB3 | 21:2Z:54:HIS:ND1 | 2.22 | 0.54 |
| 32:2a:1329:A:H5' | 44:2m:29:ARG:HE | 1.72 | 0.54 |
| 33:2b:27:LYS:HB2 | 33:2b:194:PRO:HD2 | 1.89 | 0.54 |
| 35:2d:36:ARG:HD2 | 35:2d:38:TYR:HE2 | 1.73 | 0.54 |
| 54:2x:61:C:H2' | 54:2x:62:C:H6 | 1.73 | 0.54 |
| 1:1A:1091:G:C6 | 1:1A:1101:U:C2 | 2.96 | 0.54 |
| 1:1A:1759:A:H1' | 1:1A:2711:A:C2 | 2.43 | 0.54 |
| 8:1I:38:LEU:HG | 8:1I:40:THR:HG22 | 1.89 | 0.54 |
| 1:2A:84:A:H5" | 20:2Y:8:LYS:HE3 | 1.88 | 0.54 |
| 1:2A:140:G:H1' | 1:2A:141:A:H2 | 1.73 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:2A:774:A:H2' | 1:2A:774:A:N3 | 2.23 | 0.54 |
| 1:2A:1259:G:H2' | 1:2A:1260:G:H8 | 1.72 | 0.54 |
| 1:2A:1662:C:O2' | 1:2A:2687:U:OP1 | 2.25 | 0.54 |
| 13:2R:2:ARG:NH1 | 13:2R:5:LYS:O | 2.41 | 0.54 |
| 26:24:62:ARG:HA | 26:24:62:ARG:NH1 | 2.23 | 0.54 |
| 32:2a:1240:U:N3 | 38:2g:30:ILE:O | 2.29 | 0.54 |
| 32:2a:1301:U:O2' | 32:2a:1302:U:H5' | 2.08 | 0.54 |
| 1:1A:1055:G:H1 | 1:1A:1104:C:H42 | 1.57 | 0.53 |
| 1:1A:1266:G:O2' | 1:1A:2012:G:O6 | 2.24 | 0.53 |
| 1:1A:2462:U:H1' | 1:1A:2491:U:O4 | 2.08 | 0.53 |
| 14:1S:28:VAL:HG11 | 14:1S:98:VAL:HG13 | 1.90 | 0.53 |
| 32:1a:406:G:N2 | 35:1d:119:GLN:HE22 | 2.05 | 0.53 |
| 48:1q:14:LYS:HD3 | 48:1q:14:LYS:H | 1.73 | 0.53 |
| 1:2A:1803:A:O2' | 3:2D:259:THR:HG21 | 2.08 | 0.53 |
| 1:2A:2010:G:H5" | 18:2W:42:ARG:HB2 | 1.90 | 0.53 |
| 1:2A:2801(A):A:H5' | 1:2A:2802:G:H8 | 1.73 | 0.53 |
| 5:2F:117:ARG:NH2 | 5:2F:189:THR:O | 2.38 | 0.53 |
| 32:2a:1095:U:OP1 | 32:2a:1108:G:N1 | 2.39 | 0.53 |
| 37:2f:30:LEU:HD23 | 37:2f:75:LEU:HD11 | 1.89 | 0.53 |
| 1:1A:825:C:O2' | 11:1P:55:ARG:HD3 | 2.08 | 0.53 |
| 1:1A:1876:A:H2' | 1:1A:1877:A:C8 | 2.42 | 0.53 |
| 32:1a:685:G:N2 | 32:1a:704:A:OP2 | 2.40 | 0.53 |
| 32:1a:1308:U:OP1 | 44:1m:98:VAL:N | 2.39 | 0.53 |
| 1:2A:1113:U:H2' | 1:2A:1114:G:C8 | 2.43 | 0.53 |
| 1:2A:1187:G:H5' | 17:2V:81:TYR:CE1 | 2.44 | 0.53 |
| 1:2A:2110:G:H3' | 1:2A:2111:C:H5' | 1.90 | 0.53 |
| 1:2A:2495:G:H5" | 12:2Q:82:ARG:HG2 | 1.90 | 0.53 |
| 33:2b:219:VAL:HA | 33:2b:222:ILE:HG12 | 1.90 | 0.53 |
| 34:2c:20:SER:OG | 34:2c:36:ASP:OD2 | 2.21 | 0.53 |
| 1:1A:207:A:H2' | 1:1A:208:C:O4' | 2.07 | 0.53 |
| 1:1A:963:U:OP1 | 59:1A:4287:HOH:O | 2.19 | 0.53 |
| 1:1A:993:G:OP1 | 16:1U:50:ARG:NH2 | 2.41 | 0.53 |
| 1:1A:2305:A:H5" | 6:1G:134:GLY:HA3 | 1.90 | 0.53 |
| 12:1Q:17:LEU:HD22 | 12:1Q:96:VAL:HG13 | 1.90 | 0.53 |
| 32:1a:406:G:H21 | 35:1d:119:GLN:HE22 | 1.55 | 0.53 |
| 32:1a:695:A:OP2 | 42:1k:53:SER:N | 2.38 | 0.53 |
| 32:1a:1127:G:H5' | 32:1a:1280:A:O2' | 2.08 | 0.53 |
| 50:1s:51:VAL:HB | 50:1s:75:ALA:HB2 | 1.91 | 0.53 |
| 1:2A:72:U:OP1 | 59:2A:3955:HOH:O | 2.19 | 0.53 |
| 1:2A:251:A:C5 | 1:2A:252:G:H1' | 2.43 | 0.53 |
| 1:2A:1015:G:H2' | 1:2A:1016:G:H8 | 1.72 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1A:245:G:O6 | 30:18:8:LYS:NZ | 2.34 | 0.53 |
| 22:10:40:GLN:OE1 | 22:10:44:ARG:N | 2.40 | 0.53 |
| 32:1a:1067:A:N1 | 32:1a:1108:G:O2' | 2.39 | 0.53 |
| 1:2A:1446:C:H42 | 1:2A:1465:G:H1 | 1.54 | 0.53 |
| 1:2A:1836:C:H2' | 1:2A:1837:C:H6 | 1.73 | 0.53 |
| 6:2G:15:VAL:HB | 6:2G:175:LEU:HD23 | 1.90 | 0.53 |
| 6:2G:43:LEU:O | 6:2G:45:GLU:N | 2.34 | 0.53 |
| 14:2S:14:VAL:O | 14:2S:18:ILE:HG12 | 2.08 | 0.53 |
| 32:2a:495:A:H1' | 32:2a:496:A:H5" | 1.90 | 0.53 |
| 32:2a:952:U:H2' | 32:2a:953:G:C8 | 2.43 | 0.53 |
| 32:2a:1226:C:H4' | 50:2s:80:TYR:CZ | 2.43 | 0.53 |
| 32:2a:1239:A:H4' | 32:2a:1240:U:H5' | 1.90 | 0.53 |
| 1:1A:994:C:OP1 | 16:1U:53:ARG:NH2 | 2.41 | 0.53 |
| 1:1A:1058:G:H1 | 1:1A:1080:C:N4 | 2.04 | 0.53 |
| 1:1A:1069:A:H4' | 1:1A:1070:A:H8 | 1.73 | 0.53 |
| 1:1A:1301:A:O2' | 1:1A:1302:A:H3' | 2.08 | 0.53 |
| 1:1A:1339:G:H5" | 19:1X:16:LYS:HD3 | 1.91 | 0.53 |
| 1:1A:1504:C:H2' | 1:1A:1505:C:C6 | 2.42 | 0.53 |
| 5:1F:132:VAL:HA | 5:1F:138:GLU:HB3 | 1.91 | 0.53 |
| 5:1F:155:LEU:HB2 | 5:1F:189:THR:HG21 | 1.90 | 0.53 |
| 17:1V:52:VAL:HG22 | 17:1V:55:ALA:HB3 | 1.91 | 0.53 |
| 32:1a:160:A:H1' | 32:1a:344:A:N7 | 2.24 | 0.53 |
| 32:1a:473:G:H2' | 32:1a:474:G:C8 | 2.44 | 0.53 |
| 57:1a:1835:V7A:OAZ | 57:1a:1835:V7A:OAY | 2.25 | 0.53 |
| 37:1f:48:LEU:HB2 | 37:1f:56:PRO:O | 2.07 | 0.53 |
| 40:1i:4:TYR:HB2 | 40:1i:19:LEU:HB2 | 1.89 | 0.53 |
| 1:2A:84:A:N1 | 1:2A:98:G:O2' | 2.37 | 0.53 |
| 1:2A:390:A:N6 | 59:2A:4074:HOH:O | 2.41 | 0.53 |
| 1:2A:458:G:O2' | 1:2A:469:G:O6 | 2.26 | 0.53 |
| 1:2A:849:A:H2 | 25:23:24:LYS:HB3 | 1.73 | 0.53 |
| 1:2A:2503:2MA:O2' | 1:2A:2505:G:OP2 | 2.18 | 0.53 |
| 6:2G:44:GLY:C | 6:2G:46:ALA:H | 2.16 | 0.53 |
| 7:2H:43:VAL:HG13 | 7:2H:52:VAL:HG22 | 1.89 | 0.53 |
| 14:2S:38:GLN:HE21 | 14:2S:47:THR:HG1 | 1.49 | 0.53 |
| 32:2a:514:C:H2' | 32:2a:515:G:C8 | 2.43 | 0.53 |
| 32:2a:840:C:H4' | 32:2a:841:U:OP1 | 2.08 | 0.53 |
| 32:2a:1137:C:H5" | 32:2a:1138:G:OP1 | 2.08 | 0.53 |
| 32:2a:1288:A:H2' | 32:2a:1289:A:C8 | 2.43 | 0.53 |
| 38:2g:42:ILE:HG21 | 38:2g:116:ALA:HB3 | 1.88 | 0.53 |
| 1:1A:7:G:H2' | 1:1A:8:A:C8 | 2.43 | 0.53 |
| 1:1A:526:A:OP1 | 59:1A:4260:HOH:O | 2.18 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1A:747:U:O2 | 1:1A:2014:A:H1' | 2.07 | 0.53 |
| 1:1A:2075:U:OP2 | 1:1A:2238:G:O2' | 2.19 | 0.53 |
| 7:1H:43:VAL:HG22 | 7:1H:52:VAL:HG22 | 1.91 | 0.53 |
| 37:1f:69:GLU:H | 37:1f:69:GLU:CD | 2.16 | 0.53 |
| 1:2A:322:A:OP2 | 5:2F:169:ASN:HB2 | 2.09 | 0.53 |
| 1:2A:2163:C:H5' | 1:2A:2172:U:C5' | 2.37 | 0.53 |
| 1:2A:2413:G:H21 | 11:2P:70:GLN:HE22 | 1.55 | 0.53 |
| 17:2V:6:LYS:HB2 | 17:2V:38:LEU:HD11 | 1.91 | 0.53 |
| 1:1A:183:C:N4 | 1:1A:213:A:H61 | 2.06 | 0.53 |
| 1:1A:1188:U:C2' | 1:1A:1189:A:H5' | 2.38 | 0.53 |
| 5:1F:195:ASP:HB3 | 5:1F:198:ALA:H | 1.72 | 0.53 |
| 40:1i:17:VAL:HG11 | 40:1i:80:GLY:C | 2.34 | 0.53 |
| 1:2A:2105:C:H2' | 1:2A:2106:G:C8 | 2.44 | 0.53 |
| 1:2A:2849:U:H4' | 1:2A:2868:A:C2 | 2.44 | 0.53 |
| 2:2B:105:A:H5' | 2:2B:106:G:OP2 | 2.09 | 0.53 |
| 6:2G:54:GLU:HA | 6:2G:57:ALA:HB3 | 1.91 | 0.53 |
| 21:2Z:31:ARG:NH1 | 21:2Z:94:GLU:HG2 | 2.23 | 0.53 |
| 32:2a:973:G:H3' | 32:2a:974:A:H5" | 1.91 | 0.53 |
| 32:2a:1267:C:O2 | 52:2u:20:LYS:NZ | 2.38 | 0.53 |
| 1:1A:409:C:OP1 | 59:1A:4221:HOH:O | 2.18 | 0.53 |
| 1:1A:536:A:H2' | 1:1A:537:C:C6 | 2.44 | 0.53 |
| 1:1A:1153:C:OP1 | 16:1U:92:ARG:NH2 | 2.37 | 0.53 |
| 1:1A:1512:U:H2' | 1:1A:1513:C:C6 | 2.43 | 0.53 |
| 1:1A:2689:U:OP2 | 1:1A:2719:G:N2 | 2.37 | 0.53 |
| 5:1F:70:THR:CG2 | 5:1F:72:ARG:H | 2.22 | 0.53 |
| 18:1W:39:THR:O | 18:1W:41:LYS:N | 2.42 | 0.53 |
| 38:1g:91:VAL:HG13 | 38:1g:95:ARG:HD3 | 1.91 | 0.53 |
| 1:2A:271(R):G:OP1 | 23:21:76:ARG:NE | 2.41 | 0.53 |
| 1:2A:1316:U:H2' | 1:2A:1317:A:H8 | 1.72 | 0.53 |
| 1:2A:2315:G:H2' | 1:2A:2316:C:C6 | 2.44 | 0.53 |
| 15:2T:102:ILE:HA | 15:2T:105:LEU:HD12 | 1.90 | 0.53 |
| 32:2a:533:A:O2' | 32:2a:535:A:OP2 | 2.17 | 0.53 |
| 42:2k:81:ASP:OD1 | 42:2k:106:LYS:HB2 | 2.09 | 0.53 |
| 44:2m:108:ARG:HD2 | 44:2m:114:ARG:HG2 | 1.90 | 0.53 |
| 47:2p:28:ARG:NH1 | 47:2p:29:ASP:OD1 | 2.42 | 0.53 |
| 54:2x:18:G:O2' | 54:2x:19:G:H5' | 2.09 | 0.53 |
| 1:1A:1957:C:H2' | 1:1A:1958:C:C6 | 2.44 | 0.53 |
| 2:1B:66:A:N6 | 2:1B:109:C:H5' | 2.23 | 0.53 |
| 18:1W:68:ARG:HB2 | 18:1W:109:GLU:HG2 | 1.91 | 0.53 |
| 32:1a:946:A:H2' | 32:1a:947:G:C8 | 2.44 | 0.53 |
| 32:1a:1129:C:OP1 | 40:1i:66:ARG:NH1 | 2.42 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 33:1b:93:VAL:HG21 | 33:1b:97:TRP:HD1 | 1.72 | 0.53 |
| 1:2A:2630:G:H2' | 1:2A:2631:G:C8 | 2.44 | 0.53 |
| 10:2O:68:GLU:CD | 10:2O:68:GLU:H | 2.17 | 0.53 |
| 28:26:6:ARG:NH1 | 28:26:26:ASN:HB2 | 2.23 | 0.53 |
| 32:2a:691:G:H2' | 32:2a:692:U:C6 | 2.44 | 0.53 |
| 32:2a:1148:U:O4' | 40:2i:16:ARG:HD2 | 2.07 | 0.53 |
| 32:2a:1224:G:OP1 | 59:2a:3309:HOH:O | 2.19 | 0.53 |
| 32:2a:1245:A:N6 | 32:2a:1292:U:H3 | 2.07 | 0.53 |
| 40:2i:85:LEU:HB3 | 40:2i:92:TYR:HD2 | 1.73 | 0.53 |
| 1:1A:2331:G:O2' | 1:1A:2336:A:N1 | 2.26 | 0.53 |
| 1:1A:2430:A:N3 | 1:1A:2430:A:H2' | 2.23 | 0.53 |
| 2:1B:8:U:O3' | 14:1S:25:ARG:NH2 | 2.41 | 0.53 |
| 2:1B:86:G:H1 | 2:1B:91:C:N4 | 2.07 | 0.53 |
| 3:1D:232:PRO:HB3 | 3:1D:244:ARG:CZ | 2.39 | 0.53 |
| 32:1a:688:G:H2' | 32:1a:689:C:H6 | 1.73 | 0.53 |
| 40:1i:9:ARG:HG2 | 40:1i:14:VAL:HG23 | 1.91 | 0.53 |
| 40:1i:53:VAL:O | 40:1i:55:ALA:N | 2.41 | 0.53 |
| 1:2A:784:A:N6 | 3:2D:229:VAL:HG11 | 2.24 | 0.53 |
| 1:2A:2378:A:H4' | 14:2S:23:ARG:NH1 | 2.24 | 0.53 |
| 1:2A:2705:A:OP2 | 59:2A:3949:HOH:O | 2.18 | 0.53 |
| 2:2B:81:G:OP2 | 59:2B:303:HOH:O | 2.19 | 0.53 |
| 3:2D:85:ASP:OD2 | 3:2D:88:ARG:NH1 | 2.36 | 0.53 |
| 32:2a:1179:A:H2' | 32:2a:1180:A:O4' | 2.09 | 0.53 |
| 32:2a:1269:A:N3 | 32:2a:1326:C:H1' | 2.24 | 0.53 |
| 1:1A:639:U:H2' | 1:1A:640:C:C6 | 2.44 | 0.52 |
| 7:1H:154:PRO:HB3 | 7:1H:163:TYR:CE1 | 2.44 | 0.52 |
| 32:1a:656:C:O2' | 46:1o:28:GLN:NE2 | 2.36 | 0.52 |
| 32:1a:1002:G:H3' | 32:1a:1003:G:C4' | 2.37 | 0.52 |
| 32:1a:1095:U:H5" | 32:1a:1109:C:O2 | 2.09 | 0.52 |
| 36:1e:11:ILE:HD11 | 36:1e:33:VAL:HB | 1.91 | 0.52 |
| 37:1f:99:ALA:O | 49:1r:28:GLU:HA | 2.09 | 0.52 |
| 1:2A:900:A:H3' | 1:2A:901:A:H8 | 1.74 | 0.52 |
| 1:2A:1567:A:OP2 | 3:2D:84:TYR:OH | 2.24 | 0.52 |
| 2:2B:5:C:OP1 | 2:2B:61:G:O2' | 2.22 | 0.52 |
| 32:2a:500:G:H2' | 32:2a:501:C:C6 | 2.44 | 0.52 |
| 32:2a:545:C:OP1 | 35:2d:61:LYS:NZ | 2.41 | 0.52 |
| 32:2a:951:G:N3 | 32:2a:970:C:O2' | 2.41 | 0.52 |
| 32:2a:1316:G:N2 | 32:2a:1319:A:H5" | 2.24 | 0.52 |
| 36:2e:105:VAL:HB | 36:2e:106:PRO:HD3 | 1.90 | 0.52 |
| 38:2g:89:MET:SD | 38:2g:155:ARG:HB2 | 2.49 | 0.52 |
| 51:2t:9:ASN:O | 51:2t:10:LEU:HB2 | 2.08 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1A:305:U:H2' | 1:1A:306:U:C6 | 2.44 | 0.52 |
| 1:1A:573:G:O2' | 1:1A:574:C:H3' | 2.09 | 0.52 |
| 1:1A:1588:C:H2' | 1:1A:1589:C:H6 | 1.74 | 0.52 |
| 1:1A:1913:A:H61 | 32:1a:1493:A:H2' | 1.74 | 0.52 |
| 1:1A:2153:G:H2' | 1:1A:2154:G:C8 | 2.40 | 0.52 |
| 1:1A:2567:G:H2' | 1:1A:2568:C:C6 | 2.44 | 0.52 |
| 12:1Q:85:LYS:HG2 | 22:10:7:LEU:HB3 | 1.90 | 0.52 |
| 32:1a:1106:G:H5" | 34:1c:172:ARG:HG2 | 1.91 | 0.52 |
| 32:1a:1108:G:H5' | 34:1c:176:HIS:CD2 | 2.43 | 0.52 |
| 32:1a:1513:A:H2' | 32:1a:1514:C:C6 | 2.44 | 0.52 |
| 1:2A:370:G:OP1 | 1:2A:403:U:N3 | 2.31 | 0.52 |
| 1:2A:524:U:H2' | 1:2A:525:U:C6 | 2.44 | 0.52 |
| 1:2A:746:A:H2' | 1:2A:2612:C:H5" | 1.91 | 0.52 |
| 1:2A:793:A:OP2 | 1:2A:2071:A:O2' | 2.26 | 0.52 |
| 1:2A:1942:5MC:HM52 | 1:2A:1943:U:C2 | 2.44 | 0.52 |
| 1:2A:2065:C:H2' | 1:2A:2066:C:C6 | 2.45 | 0.52 |
| 1:2A:2131:G:H4' | 1:2A:2132:U:H5' | 1.91 | 0.52 |
| 2:2B:41:U:H5 | 6:2G:70:VAL:H | 1.58 | 0.52 |
| 8:2I:87:LYS:O | 8:2I:123:LEU:HD13 | 2.09 | 0.52 |
| 25:23:11:SER:HA | 25:23:31:LEU:HD11 | 1.90 | 0.52 |
| 32:2a:91:C:H2' | 32:2a:92:C:H6 | 1.74 | 0.52 |
| 32:2a:677:U:O2 | 32:2a:777:A:O2' | 2.26 | 0.52 |
| 32:2a:1106:G:H2' | 32:2a:1107:C:C6 | 2.44 | 0.52 |
| 32:2a:1442:G:H2' | 32:2a:1442:G:N3 | 2.25 | 0.52 |
| 38:2g:153:HIS:CE1 | 42:2k:58:PRO:HD2 | 2.44 | 0.52 |
| 1:1A:448:U:H5' | 59:1A:4351:HOH:O | 2.09 | 0.52 |
| 1:1A:652(C):G:N2 | 1:1A:653:A:H1' | 2.24 | 0.52 |
| 2:1B:43:C:OP1 | 26:14:6:HIS:NE2 | 2.38 | 0.52 |
| 9:1N:13:TRP:CE2 | 9:1N:133:GLN:HG2 | 2.44 | 0.52 |
| 33:1b:207:ALA:O | 33:1b:210:SER:N | 2.42 | 0.52 |
| 41:1j:62:HIS:HB3 | 45:1n:59:ALA:HB3 | 1.91 | 0.52 |
| 42:1k:99:GLN:HG2 | 42:1k:105:VAL:HG21 | 1.92 | 0.52 |
| 47:1p:13:HIS:O | 47:1p:42:ARG:NH2 | 2.42 | 0.52 |
| 48:1q:24:GLU:HA | 48:1q:39:SER:HA | 1.91 | 0.52 |
| 1:2A:1990:C:H2' | 1:2A:1991:U:O4' | 2.10 | 0.52 |
| 1:2A:2679:A:H4' | 4:2E:165:VAL:HG11 | 1.91 | 0.52 |
| 1:2A:2684:U:H1' | 10:2O:70:LYS:HD2 | 1.90 | 0.52 |
| 3:2D:89:SER:HB2 | 3:2D:201:HIS:CD2 | 2.44 | 0.52 |
| 32:2a:984:C:H2' | 32:2a:985:C:H6 | 1.75 | 0.52 |
| 32:2a:1030(A):G:N2 | 32:2a:1030(C):G:H3' | 2.23 | 0.52 |
| 32:2a:1286:A:C8 | 32:2a:1287:A:H4' | 2.44 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 44:2m:15:VAL:O | 44:2m:19:LEU:HG | 2.09 | 0.52 |
| 1:1A:142:A:OP2 | 1:1A:142(A):C:N4 | 2.40 | 0.52 |
| 1:1A:1783:A:H5' | 1:1A:2608:G:H4' | 1.92 | 0.52 |
| 1:1A:2151:G:H2' | 1:1A:2152:G:C8 | 2.44 | 0.52 |
| 1:1A:2875:C:O2' | 15:1T:2:ASN:OD1 | 2.23 | 0.52 |
| 59:1A:4709:HOH:O | 54:1x:76:A:H1' | 2.08 | 0.52 |
| 3:1D:67:PHE:HB3 | 3:1D:153:ALA:H | 1.74 | 0.52 |
| 11:1P:89:ALA:O | 11:1P:121:LYS:NZ | 2.43 | 0.52 |
| 32:1a:17:U:H2' | 32:1a:18:C:C6 | 2.44 | 0.52 |
| 32:1a:44:G:C2 | 32:1a:45:U:H1' | 2.44 | 0.52 |
| 32:1a:141:A:H4' | 32:1a:182:U:H1' | 1.91 | 0.52 |
| 34:1c:58:GLU:HB3 | 41:1j:92:THR:HG21 | 1.92 | 0.52 |
| 1:2A:263:C:H2' | 1:2A:264:C:O4' | 2.10 | 0.52 |
| 1:2A:1141:U:OP2 | 9:2N:63:THR:OG1 | 2.26 | 0.52 |
| 1:2A:2126:A:H61 | 1:2A:2162:G:HO2' | 1.52 | 0.52 |
| 1:2A:2127:G:N2 | 1:2A:2161:C:C2 | 2.78 | 0.52 |
| 23:21:73:LEU:HB3 | 23:21:94:LEU:HD22 | 1.92 | 0.52 |
| 24:22:22:GLU:OE2 | 24:22:68:ARG:NH2 | 2.43 | 0.52 |
| 32:2a:7:G:H5' | 32:2a:298:A:O4' | 2.10 | 0.52 |
| 32:2a:524:G:H2' | 32:2a:525:C:C6 | 2.45 | 0.52 |
| 32:2a:560:U:H4' | 32:2a:561:U:O5' | 2.08 | 0.52 |
| 32:2a:1146:A:H2' | 32:2a:1147:C:O4' | 2.10 | 0.52 |
| 32:2a:1348:U:H2' | 32:2a:1349:A:H8 | 1.73 | 0.52 |
| 43:2l:40:VAL:HG21 | 43:2l:78:GLN:HA | 1.92 | 0.52 |
| 1:1A:272:G:N7 | 1:1A:421:U:H2' | 2.25 | 0.52 |
| 1:1A:528:A:O2' | 1:1A:529:A:H5' | 2.09 | 0.52 |
| 1:1A:1582:C:O2' | 1:1A:1586:A:N3 | 2.42 | 0.52 |
| 1:1A:2319:G:N2 | 14:1S:3:ARG:HA | 2.25 | 0.52 |
| 32:1a:831:U:H2' | 32:1a:832:C:C6 | 2.44 | 0.52 |
| 1:2A:330:A:H2 | 1:2A:1210:A:HO2' | 1.58 | 0.52 |
| 1:2A:403:U:H4' | 1:2A:404:C:H5' | 1.92 | 0.52 |
| 1:2A:2299:G:N1 | 1:2A:2318:G:N7 | 2.58 | 0.52 |
| 1:2A:2870:C:H2' | 1:2A:2871:C:O4' | 2.09 | 0.52 |
| 5:2F:126:VAL:HG21 | 5:2F:129:PHE:CZ | 2.44 | 0.52 |
| 8:2I:86:THR:C | 8:2I:123:LEU:HB2 | 2.35 | 0.52 |
| 17:2V:62:LEU:HD12 | 17:2V:93:GLU:HG2 | 1.91 | 0.52 |
| 31:29:22:ARG:HB2 | 31:29:24:TYR:HE2 | 1.74 | 0.52 |
| 32:2a:792:A:H4' | 32:2a:793:U:H5" | 1.92 | 0.52 |
| 32:2a:952:U:H2' | 32:2a:953:G:H8 | 1.74 | 0.52 |
| 32:2a:1272:G:N2 | 32:2a:1273:G:C5 | 2.78 | 0.52 |
| 32:2a:1369:C:OP2 | 40:2i:112:LYS:N | 2.34 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:2i:50:LEU:HD12 | 40:2i:51:ARG:HD3 | 1.91 | 0.52 |
| 1:1A:1186:G:H2' | 1:1A:1187:G:O4' | 2.10 | 0.52 |
| 3:1D:26:LYS:NZ | 3:1D:30:GLU:OE1 | 2.39 | 0.52 |
| 7:1H:105:LEU:HD11 | 7:1H:148:ILE:HG23 | 1.91 | 0.52 |
| 32:1a:221:C:H2' | 32:1a:222:U:H6 | 1.74 | 0.52 |
| 32:1a:258:G:H2' | 32:1a:259:G:H8 | 1.74 | 0.52 |
| 32:1a:476:G:H2' | 32:1a:477:A:C8 | 2.44 | 0.52 |
| 46:1o:56:LEU:O | 46:1o:60:VAL:HG23 | 2.09 | 0.52 |
| 1:2A:1149:G:H2' | 1:2A:1150:C:C6 | 2.45 | 0.52 |
| 1:2A:2313:C:H2' | 1:2A:2314:C:C6 | 2.43 | 0.52 |
| 1:2A:2805:G:H2' | 1:2A:2807:G:H8 | 1.74 | 0.52 |
| 1:1A:1779:U:H2' | 59:1A:4404:HOH:O | 2.09 | 0.52 |
| 1:1A:1798:U:H5' | 3:1D:259:THR:HG22 | 1.92 | 0.52 |
| 9:1N:121:LYS:HD3 | 9:1N:130:HIS:CE1 | 2.44 | 0.52 |
| 12:1Q:34:LEU:HD11 | 12:1Q:129:THR:HB | 1.92 | 0.52 |
| 32:1a:128:G:H4' | 48:1q:3:LYS:HG2 | 1.92 | 0.52 |
| 32:1a:1118:C:OP1 | 40:1i:9:ARG:HD2 | 2.10 | 0.52 |
| 32:1a:1367:C:H5' | 41:1j:60:ARG:NH1 | 2.25 | 0.52 |
| 40:1i:55:ALA:HA | 40:1i:58:HIS:CD2 | 2.44 | 0.52 |
| 1:2A:800:A:H8 | 1:2A:800:A:OP1 | 1.92 | 0.52 |
| 1:2A:1166:C:H2' | 1:2A:1167:U:C6 | 2.44 | 0.52 |
| 1:2A:1342:A:OP1 | 19:2X:36:LYS:NZ | 2.30 | 0.52 |
| 6:2G:106:LEU:HA | 6:2G:110:ALA:HB3 | 1.91 | 0.52 |
| 6:2G:120:LEU:HD23 | 6:2G:179:PRO:HD2 | 1.92 | 0.52 |
| 9:2N:42:TRP:HA | 9:2N:48:MET:SD | 2.50 | 0.52 |
| 32:2a:538:G:H5" | 43:2l:114:LYS:HB2 | 1.91 | 0.52 |
| 32:2a:988:G:H2' | 32:2a:989:C:O4' | 2.09 | 0.52 |
| 32:2a:1015:A:H1' | 32:2a:1219:U:H5' | 1.92 | 0.52 |
| 35:2d:189:PRO:HB2 | 35:2d:194:LEU:HD11 | 1.90 | 0.52 |
| 1:1A:1062:G:H5" | 1:1A:1070:A:H1' | 1.92 | 0.52 |
| 15:1T:1:MET:HE2 | 15:1T:3:ARG:HG2 | 1.92 | 0.52 |
| 32:1a:266:G:H2' | 32:1a:266:G:N3 | 2.24 | 0.52 |
| 32:1a:458:C:H2' | 32:1a:460:G:O4' | 2.10 | 0.52 |
| 32:1a:714:G:H2' | 32:1a:715:A:C8 | 2.45 | 0.52 |
| 36:1e:6:PHE:HB2 | 36:1e:34:VAL:HG22 | 1.92 | 0.52 |
| 5:2F:110:LEU:HD21 | 5:2F:181:LEU:HD23 | 1.91 | 0.52 |
| 13:2R:92:GLY:HA2 | 13:2R:94:TYR:CZ | 2.45 | 0.52 |
| 24:22:65:ASN:OD1 | 24:22:69:ARG:NH1 | 2.42 | 0.52 |
| 32:2a:107:G:H2' | 32:2a:108:G:O4' | 2.09 | 0.52 |
| 32:2a:1235:U:O2' | 32:2a:1305:G:O5' | 2.28 | 0.52 |
| 38:2g:151:TYR:OH | 42:2k:54:ARG:NH1 | 2.41 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 39:2h:85:ARG:HH11 | 39:2h:134:ILE:HG23 | 1.75 | 0.52 |
| 52:2u:6:ARG:HG2 | 52:2u:15:ARG:HD2 | 1.92 | 0.52 |
| 1:1A:29:U:H2' | 1:1A:30:G:C8 | 2.45 | 0.52 |
| 1:1A:320:A:OP1 | 5:1F:135:LYS:NZ | 2.41 | 0.52 |
| 1:1A:593:G:H4' | 30:18:4:MET:HE2 | 1.92 | 0.52 |
| 1:1A:1174:A:H1' | 1:1A:1175:U:H5" | 1.92 | 0.52 |
| 1:1A:1807:G:O6 | 59:1A:4283:HOH:O | 2.18 | 0.52 |
| 13:1R:97:VAL:HG22 | 13:1R:114:VAL:HG13 | 1.91 | 0.52 |
| 14:1S:15:ARG:NE | 14:1S:88:ASP:OD2 | 2.27 | 0.52 |
| 20:1Y:99:CYS:HB2 | 20:1Y:106:LEU:HD21 | 1.92 | 0.52 |
| 32:1a:40:C:H2' | 32:1a:41:G:C8 | 2.45 | 0.52 |
| 32:1a:1458:G:OP1 | 51:1t:35:THR:OG1 | 2.27 | 0.52 |
| 38:1g:16:LEU:HD22 | 40:1i:42:ARG:HA | 1.90 | 0.52 |
| 39:1h:41:ARG:NH2 | 39:1h:123:GLU:OE2 | 2.43 | 0.52 |
| 42:1k:48:ILE:HD12 | 42:1k:63:LEU:HB2 | 1.92 | 0.52 |
| 47:1p:1:MET:HG3 | 47:1p:3:LYS:HG3 | 1.92 | 0.52 |
| 1:2A:625:G:N7 | 11:2P:107:LYS:NZ | 2.55 | 0.52 |
| 1:2A:724:U:H2' | 1:2A:725:G:O4' | 2.10 | 0.52 |
| 1:2A:1275:A:N1 | 1:2A:1295:C:O2' | 2.38 | 0.52 |
| 1:2A:2567:G:H2' | 1:2A:2568:C:C6 | 2.45 | 0.52 |
| 1:2A:2698:U:O4 | 59:2A:3954:HOH:O | 2.19 | 0.52 |
| 1:2A:2734:A:H2' | 1:2A:2735:G:O4' | 2.10 | 0.52 |
| 2:2B:9:G:OP1 | 14:2S:25:ARG:NH1 | 2.26 | 0.52 |
| 8:2I:61:ARG:HH11 | 8:2I:61:ARG:H | 1.58 | 0.52 |
| 8:2I:128:LEU:C | 8:2I:139:GLN:HB3 | 2.34 | 0.52 |
| 18:2W:11:ARG:HH21 | 18:2W:98:LYS:HD3 | 1.74 | 0.52 |
| 32:2a:532:A:N1 | 34:2c:156:ARG:NH1 | 2.53 | 0.52 |
| 33:2b:111:ARG:HH11 | 33:2b:111:ARG:HA | 1.74 | 0.52 |
| 1:1A:1833:U:O2' | 1:1A:1969:A:N1 | 2.38 | 0.52 |
| 4:1E:179:GLU:HG3 | 15:1T:9:LEU:HD21 | 1.92 | 0.52 |
| 32:1a:1177:G:OP2 | 40:1i:97:LYS:NZ | 2.39 | 0.52 |
| 36:1e:110:LEU:HD13 | 36:1e:118:ILE:HG21 | 1.90 | 0.52 |
| 54:1x:23:C:H2' | 54:1x:24:U:C6 | 2.45 | 0.52 |
| 1:2A:863:A:H2' | 1:2A:864:G:C8 | 2.45 | 0.52 |
| 1:2A:2889:C:H2' | 1:2A:2891:G:O4' | 2.09 | 0.52 |
| 6:2G:107:LEU:HD23 | 6:2G:111:LEU:HD12 | 1.91 | 0.52 |
| 10:2O:2:ILE:HD12 | 10:2O:6:THR:HG21 | 1.92 | 0.52 |
| 10:2O:98:VAL:HG21 | 10:2O:114:ILE:HG23 | 1.92 | 0.52 |
| 20:2Y:13:VAL:HB | 20:2Y:72:VAL:HG22 | 1.91 | 0.52 |
| 32:2a:1051:C:H2' | 32:2a:1052:U:C6 | 2.45 | 0.52 |
| 37:2f:3:ARG:HB3 | 37:2f:93:SER:HB2 | 1.92 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:2i:9:ARG:HG2 | 40:2i:14:VAL:HG12 | 1.92 | 0.52 |
| 1:1A:1783:A:N7 | 59:1A:4404:HOH:O | 2.35 | 0.51 |
| 4:1E:8:LYS:HG2 | 4:1E:192:ASN:HA | 1.92 | 0.51 |
| 12:1Q:67:ARG:O | 12:1Q:101:ARG:NH2 | 2.39 | 0.51 |
| 22:10:18:ALA:HB3 | 22:10:20:ARG:NH1 | 2.26 | 0.51 |
| 32:1a:1239:A:H62 | 32:1a:1299:A:N6 | 2.08 | 0.51 |
| 35:1d:205:GLU:OE2 | 36:1e:107:ARG:NH1 | 2.43 | 0.51 |
| 37:1f:79:LEU:O | 37:1f:85:VAL:HG11 | 2.10 | 0.51 |
| 40:1i:111:ARG:O | 40:1i:113:LYS:NZ | 2.43 | 0.51 |
| 43:1l:11:VAL:HG13 | 48:1q:29:HIS:HD2 | 1.75 | 0.51 |
| 1:2A:190:A:OP2 | 23:21:39:LYS:HE3 | 2.10 | 0.51 |
| 1:2A:705:A:C2 | 1:2A:727:A:H1' | 2.44 | 0.51 |
| 4:2E:18:ASP:HB3 | 15:2T:82:LEU:HD21 | 1.92 | 0.51 |
| 32:2a:1071:C:H2' | 32:2a:1072:G:C8 | 2.43 | 0.51 |
| 32:2a:1324:A:O4' | 32:2a:1362:C:H4' | 2.11 | 0.51 |
| 40:2i:8:GLY:HA2 | 40:2i:79:LEU:HD23 | 1.91 | 0.51 |
| 40:2i:71:SER:HA | 40:2i:74:ILE:HD12 | 1.92 | 0.51 |
| 42:2k:86:GLY:H | 42:2k:112:THR:HG22 | 1.75 | 0.51 |
| 43:2l:70:ILE:HG12 | 43:2l:100:ILE:HD12 | 1.91 | 0.51 |
| 50:2s:49:ILE:HD13 | 50:2s:71:LEU:HD11 | 1.92 | 0.51 |
| 1:1A:1178:C:H2' | 1:1A:1179:C:C6 | 2.44 | 0.51 |
| 1:1A:2533:A:H2' | 1:1A:2534:A:O4' | 2.10 | 0.51 |
| 5:1F:22:ALA:HB1 | 5:1F:24:LEU:HD13 | 1.92 | 0.51 |
| 12:1Q:38:GLU:HA | 12:1Q:99:PRO:HG3 | 1.92 | 0.51 |
| 32:1a:191:G:N2 | 51:1t:102:GLY:O | 2.37 | 0.51 |
| 32:1a:971:G:N2 | 32:1a:1363(A):A:OP2 | 2.36 | 0.51 |
| 32:1a:972:C:O2' | 41:1j:55:LYS:O | 2.23 | 0.51 |
| 32:1a:1095:U:OP2 | 32:1a:1108:G:N1 | 2.37 | 0.51 |
| 51:1t:47:GLY:HA2 | 51:1t:48:LYS:C | 2.35 | 0.51 |
| 53:1v:14:A:H3' | 53:1v:15:A:H8 | 1.75 | 0.51 |
| 1:2A:205:G:N2 | 1:2A:206:U:O4 | 2.33 | 0.51 |
| 1:2A:1028:A:N6 | 1:2A:1125:G:H2' | 2.24 | 0.51 |
| 1:2A:2320:A:N3 | 1:2A:2320:A:H2' | 2.25 | 0.51 |
| 4:2E:52:LEU:O | 4:2E:76:ARG:N | 2.36 | 0.51 |
| 10:2O:63:VAL:HG11 | 10:2O:85:VAL:HG23 | 1.92 | 0.51 |
| 32:2a:841:U:H6 | 32:2a:841:U:P | 2.33 | 0.51 |
| 39:2h:51:VAL:HG11 | 39:2h:60:ARG:HH12 | 1.75 | 0.51 |
| 44:2m:80:ARG:HH21 | 50:2s:69:HIS:CE1 | 2.29 | 0.51 |
| 45:2n:32:SER:O | 45:2n:40:CYS:HA | 2.10 | 0.51 |
| 1:1A:600:G:N2 | 1:1A:605:C:O3' | 2.43 | 0.51 |
| 1:1A:1793:C:H2' | 1:1A:1794:U:C6 | 2.45 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:1R:12:ARG:O | 13:1R:17:ARG:NH1 | 2.44 | 0.51 |
| 32:1a:376:G:H5" | 47:1p:5:ARG:HB3 | 1.92 | 0.51 |
| 32:1a:958:A:N6 | 32:1a:959:A:N1 | 2.58 | 0.51 |
| 32:1a:966:M2G:HM13 | 32:1a:967:5MC:H1' | 1.93 | 0.51 |
| 32:1a:1221:G:OP1 | 32:1a:1320:C:N4 | 2.42 | 0.51 |
| 32:1a:1375:A:H4' | 38:1g:29:LYS:HD3 | 1.92 | 0.51 |
| 1:2A:606:U:H4' | 1:2A:658:C:H4' | 1.93 | 0.51 |
| 1:2A:1923:U:H2' | 1:2A:1924:C:C6 | 2.46 | 0.51 |
| 1:2A:2198:A:OP1 | 8:2I:33:ARG:NH2 | 2.44 | 0.51 |
| 1:2A:2360:A:H2' | 1:2A:2361:A:O4' | 2.09 | 0.51 |
| 4:2E:101:ARG:CZ | 4:2E:171:GLU:HB2 | 2.39 | 0.51 |
| 8:2I:54:GLN:O | 8:2I:58:LEU:N | 2.43 | 0.51 |
| 16:2U:10:ARG:NH1 | 59:2U:301:HOH:O | 2.42 | 0.51 |
| 19:2X:5:TYR:CZ | 24:22:30:ARG:HB2 | 2.45 | 0.51 |
| 32:2a:926:G:H22 | 53:2v:15:A:H3' | 1.75 | 0.51 |
| 34:2c:180:ALA:HB1 | 34:2c:203:PHE:HE1 | 1.76 | 0.51 |
| 38:2g:114:ARG:O | 38:2g:119:ARG:NH1 | 2.44 | 0.51 |
| 1:1A:647:G:N3 | 1:1A:2350:C:O2' | 2.44 | 0.51 |
| 1:1A:2602:A:OP1 | 59:1x:201:HOH:O | 2.19 | 0.51 |
| 22:10:46:LYS:HB2 | 22:10:78:TYR:CE1 | 2.46 | 0.51 |
| 32:1a:69:G:H2' | 32:1a:70:G:H8 | 1.75 | 0.51 |
| 32:1a:540:G:H2' | 32:1a:541:G:O4' | 2.09 | 0.51 |
| 32:1a:815:A:N7 | 32:1a:1509:C:O2' | 2.35 | 0.51 |
| 1:2A:479:A:N3 | 1:2A:481:G:H5" | 2.26 | 0.51 |
| 1:2A:2032:G:OP2 | 1:2A:2454:G:O2' | 2.26 | 0.51 |
| 1:2A:2595:G:N7 | 59:2A:4020:HOH:O | 2.33 | 0.51 |
| 4:2E:50:GLY:HA3 | 4:2E:75:VAL:HG21 | 1.93 | 0.51 |
| 5:2F:150:GLY:HA2 | 5:2F:172:TRP:CD2 | 2.45 | 0.51 |
| 5:2F:184:TYR:O | 5:2F:188:ARG:HG3 | 2.10 | 0.51 |
| 6:2G:170:ARG:NH2 | 6:2G:182:LYS:O | 2.44 | 0.51 |
| 32:2a:64:G:H4' | 32:2a:65:U:H3' | 1.91 | 0.51 |
| 32:2a:539:A:OP2 | 43:2l:115:LYS:HE2 | 2.10 | 0.51 |
| 32:2a:1166:G:N2 | 32:2a:1170:A:OP2 | 2.43 | 0.51 |
| 32:2a:1329:A:H5" | 44:2m:26:GLY:H | 1.75 | 0.51 |
| 33:2b:81:VAL:O | 33:2b:85:ALA:N | 2.43 | 0.51 |
| 50:2s:38:SER:HB2 | 50:2s:71:LEU:HD22 | 1.92 | 0.51 |
| 54:2x:43:A:H2' | 54:2x:44:A:C8 | 2.46 | 0.51 |
| 1:1A:1686:C:H2' | 1:1A:1687:G:O4' | 2.11 | 0.51 |
| 1:1A:2029:G:H2' | 1:1A:2031:A:OP1 | 2.10 | 0.51 |
| 4:1E:116:VAL:HG21 | 4:1E:138:PRO:HB3 | 1.92 | 0.51 |
| 32:1a:1035:A:C4 | 32:1a:1036:G:N2 | 2.79 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 32:1a:1150:U:H4' | 41:1j:41:PRO:HG3 | 1.92 | 0.51 |
| 35:1d:18:LYS:HB2 | 58:1d:501:SF4:S1 | 2.50 | 0.51 |
| 40:1i:29:ASN:OD1 | 40:1i:64:THR:HA | 2.10 | 0.51 |
| 1:2A:1223:G:O6 | 17:2V:69:LYS:NZ | 2.44 | 0.51 |
| 1:2A:2152:G:H2' | 1:2A:2153:G:O4' | 2.11 | 0.51 |
| 32:2a:537:G:H2' | 32:2a:538:G:H8 | 1.74 | 0.51 |
| 36:2e:84:PHE:O | 36:2e:86:ALA:N | 2.42 | 0.51 |
| 44:2m:3:ARG:HB3 | 44:2m:9:ILE:H | 1.76 | 0.51 |
| 44:2m:89:GLY:C | 44:2m:91:ARG:H | 2.19 | 0.51 |
| 1:1A:10:G:N2 | 1:1A:2802:G:OP1 | 2.32 | 0.51 |
| 1:1A:190:A:OP2 | 23:11:39:LYS:HE3 | 2.11 | 0.51 |
| 1:1A:476:G:H4' | 1:1A:502:A:N1 | 2.26 | 0.51 |
| 1:1A:628:G:H2' | 1:1A:629:G:C8 | 2.46 | 0.51 |
| 1:1A:1786:A:H1' | 1:1A:1938:A:N6 | 2.26 | 0.51 |
| 1:1A:2161:C:O2' | 1:1A:2162:G:H5" | 2.11 | 0.51 |
| 1:1A:2887:U:H2' | 1:1A:2888:C:C6 | 2.45 | 0.51 |
| 6:1G:16:ARG:O | 6:1G:20:ILE:HG13 | 2.11 | 0.51 |
| 6:1G:124:SER:HB2 | 6:1G:131:TYR:CE1 | 2.45 | 0.51 |
| 8:1I:126:TYR:HB2 | 8:1I:142:VAL:HG23 | 1.91 | 0.51 |
| 18:1W:2:GLU:OE2 | 18:1W:72:LYS:NZ | 2.31 | 0.51 |
| 32:1a:408:A:OP1 | 35:1d:113:SER:OG | 2.24 | 0.51 |
| 32:1a:794:A:OP2 | 59:1a:1917:HOH:O | 2.19 | 0.51 |
| 32:1a:1104:G:H4' | 33:1b:111:ARG:NH2 | 2.25 | 0.51 |
| 32:1a:1438:G:H2' | 32:1a:1439:C:C6 | 2.46 | 0.51 |
| 33:1b:71:VAL:HB | 33:1b:164:VAL:HA | 1.91 | 0.51 |
| 34:1c:71:ALA:HA | 34:1c:106:VAL:HG21 | 1.92 | 0.51 |
| 54:1x:8:4SU:O5' | 54:1x:8:4SU:H6 | 2.09 | 0.51 |
| 1:2A:1495:A:H2' | 1:2A:1496:A:C8 | 2.46 | 0.51 |
| 8:2I:127:VAL:HA | 8:2I:140:LEU:O | 2.11 | 0.51 |
| 32:2a:1517:G:H3' | 32:2a:1518:MA6:H8 | 1.92 | 0.51 |
| 1:1A:64:A:C5 | 19:1X:66:LEU:HD13 | 2.45 | 0.51 |
| 1:1A:606:U:H4' | 1:1A:658:C:H4' | 1.92 | 0.51 |
| 1:1A:1790:C:H5" | 1:1A:1791:A:OP1 | 2.10 | 0.51 |
| 1:1A:2353:G:H2' | 1:1A:2354:G:O4' | 2.11 | 0.51 |
| 15:1T:73:GLU:OE2 | 15:1T:103:ARG:NE | 2.28 | 0.51 |
| 19:1X:53:LYS:HB3 | 19:1X:82:GLN:HB3 | 1.93 | 0.51 |
| 32:1a:384:G:H2' | 32:1a:385:C:C6 | 2.45 | 0.51 |
| 32:1a:403:C:H4' | 35:1d:122:ARG:HE | 1.76 | 0.51 |
| 32:1a:565:U:H3' | 32:1a:566:G:H2' | 1.92 | 0.51 |
| 32:1a:1144:G:N2 | 32:1a:1146:A:H62 | 2.08 | 0.51 |
| 33:1b:68:ILE:HG12 | 33:1b:161:ALA:HB3 | 1.93 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 47:1p:48:TRP:CD1 | 47:1p:48:TRP:H | 2.28 | 0.51 |
| 1:2A:1405:U:H2' | 1:2A:1406:U:C6 | 2.45 | 0.51 |
| 1:2A:1638:C:H5" | 1:2A:2710:C:O2' | 2.10 | 0.51 |
| 21:2Z:4:ARG:NH2 | 21:2Z:66:SER:OG | 2.44 | 0.51 |
| 22:20:11:ARG:O | 22:20:14:ARG:NH2 | 2.40 | 0.51 |
| 24:22:13:ALA:HB1 | 24:22:21:LEU:HD21 | 1.93 | 0.51 |
| 36:2e:82:VAL:HG11 | 36:2e:137:GLU:HG3 | 1.91 | 0.51 |
| 38:2g:149:ARG:NE | 42:2k:59:TYR:OH | 2.44 | 0.51 |
| 1:1A:1843:C:H5' | 3:1D:253:GLN:OE1 | 2.11 | 0.51 |
| 1:1A:1858:G:N2 | 1:1A:1883:G:H2' | 2.26 | 0.51 |
| 1:1A:2134:A:H61 | 1:1A:2157:G:C4' | 2.23 | 0.51 |
| 32:1a:256:U:H2' | 32:1a:257:G:C8 | 2.46 | 0.51 |
| 32:1a:715:A:H2' | 32:1a:716:A:C8 | 2.45 | 0.51 |
| 32:1a:1192:C:OP2 | 34:1c:4:LYS:NZ | 2.34 | 0.51 |
| 32:1a:1347:G:N2 | 32:1a:1373:G:H2' | 2.25 | 0.51 |
| 40:1i:5:TYR:HD1 | 40:1i:17:VAL:O | 1.93 | 0.51 |
| 40:1i:7:THR:H | 40:1i:83:ARG:HD3 | 1.76 | 0.51 |
| 1:2A:1204:A:H2 | 1:2A:1241:A:N6 | 2.07 | 0.51 |
| 1:2A:1514:U:H2' | 1:2A:1515:G:H8 | 1.75 | 0.51 |
| 1:2A:1709:U:H2' | 1:2A:1710:C:C6 | 2.46 | 0.51 |
| 1:2A:2376:A:H3' | 1:2A:2377:A:H8 | 1.76 | 0.51 |
| 2:2B:14:U:O3' | 2:2B:108:U:O2' | 2.24 | 0.51 |
| 5:2F:24:LEU:HD21 | 5:2F:114:VAL:HG12 | 1.93 | 0.51 |
| 5:2F:165:ARG:HG2 | 5:2F:168:ARG:NH2 | 2.26 | 0.51 |
| 36:2e:78:HIS:CE1 | 36:2e:142:LEU:HD23 | 2.45 | 0.51 |
| 51:2t:100:ILE:HG22 | 51:2t:101:GLY:H | 1.75 | 0.51 |
| 52:2u:5:ASP:O | 52:2u:11:GLY:HA3 | 2.10 | 0.51 |
| 1:1A:675:A:H5" | 59:1A:4932:HOH:O | 2.10 | 0.51 |
| 1:1A:2505:G:O6 | 1:1A:2576:G:H2' | 2.10 | 0.51 |
| 2:1B:78:A:C2 | 2:1B:100:A:C4 | 2.98 | 0.51 |
| 32:1a:19:C:H2' | 32:1a:20:U:C6 | 2.45 | 0.51 |
| 32:1a:509:A:H3' | 59:1a:1998:HOH:O | 2.10 | 0.51 |
| 32:1a:848:C:H2' | 32:1a:849:C:H6 | 1.76 | 0.51 |
| 32:1a:1015:A:O3' | 45:1n:15:LYS:NZ | 2.44 | 0.51 |
| 42:1k:79:SER:HA | 42:1k:104:GLN:HB3 | 1.93 | 0.51 |
| 1:2A:414:C:H2' | 1:2A:415:A:C8 | 2.46 | 0.51 |
| 1:2A:587:C:P | 11:2P:21:ARG:HH22 | 2.34 | 0.51 |
| 1:2A:862:G:O2' | 2:2B:78:A:N3 | 2.44 | 0.51 |
| 1:2A:1266:G:O5' | 18:2W:15:ARG:NH2 | 2.43 | 0.51 |
| 1:2A:2148:G:H2' | 1:2A:2149:G:H8 | 1.73 | 0.51 |
| 6:2G:15:VAL:HB | 6:2G:175:LEU:HB3 | 1.92 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 8:2I:73:GLU:OE1 | 8:2I:74:ASN:ND2 | 2.39 | 0.51 |
| 12:2Q:45:GLN:OE1 | 12:2Q:45:GLN:N | 2.37 | 0.51 |
| 15:2T:73:GLU:OE2 | 15:2T:103:ARG:NE | 2.35 | 0.51 |
| 20:2Y:13:VAL:HG12 | 20:2Y:74:PRO:HA | 1.93 | 0.51 |
| 32:2a:1062:U:H2' | 32:2a:1063:C:C6 | 2.45 | 0.51 |
| 32:2a:1427:U:H2' | 32:2a:1428:A:C8 | 2.45 | 0.51 |
| 40:2i:9:ARG:O | 40:2i:104:ARG:HG3 | 2.10 | 0.51 |
| 43:2l:77:LEU:HD21 | 43:2l:107:ALA:HB2 | 1.93 | 0.51 |
| 1:1A:36:G:N3 | 1:1A:450:G:O2' | 2.44 | 0.51 |
| 1:1A:58:G:O2' | 1:1A:73:A:N1 | 2.41 | 0.51 |
| 1:1A:637:A:H5" | 11:1P:117:GLU:HG2 | 1.93 | 0.51 |
| 1:1A:792:G:N3 | 1:1A:2072:G:O2' | 2.35 | 0.51 |
| 1:1A:1364:G:N7 | 23:11:3:LYS:HD2 | 2.25 | 0.51 |
| 1:1A:1657:C:H4' | 4:1E:133:LYS:HB3 | 1.91 | 0.51 |
| 1:1A:2839:G:H5' | 13:1R:46:GLY:CA | 2.40 | 0.51 |
| 1:1A:2848:G:C8 | 15:1T:97:ALA:HB2 | 2.45 | 0.51 |
| 10:1O:75:SER:OG | 10:1O:76:ALA:N | 2.44 | 0.51 |
| 12:1Q:8:LYS:HB3 | 12:1Q:9:TYR:CD2 | 2.45 | 0.51 |
| 31:19:16:VAL:HG22 | 31:19:25:VAL:HG22 | 1.92 | 0.51 |
| 32:1a:189(K):U:H2' | 32:1a:189(L):G:C8 | 2.46 | 0.51 |
| 32:1a:1030(D):A:H62 | 32:1a:1031:G:H21 | 1.59 | 0.51 |
| 32:1a:1031:G:H2' | 32:1a:1032:G:C8 | 2.46 | 0.51 |
| 33:1b:69:LEU:HB2 | 33:1b:159:PRO:HG2 | 1.92 | 0.51 |
| 35:1d:10:ARG:HB2 | 35:1d:40:PRO:HG3 | 1.92 | 0.51 |
| 37:1f:99:ALA:HB1 | 49:1r:23:LYS:HE2 | 1.93 | 0.51 |
| 1:2A:386:G:O2' | 59:2A:3946:HOH:O | 2.17 | 0.51 |
| 1:2A:992:C:O2' | 17:2V:87:HIS:ND1 | 2.37 | 0.51 |
| 1:2A:1653:G:H3' | 13:2R:2:ARG:HD3 | 1.93 | 0.51 |
| 1:2A:1697:G:OP2 | 1:2A:1698:A:O2' | 2.21 | 0.51 |
| 1:2A:1997:G:OP2 | 59:2A:3956:HOH:O | 2.19 | 0.51 |
| 7:2H:58:GLU:OE2 | 7:2H:61:HIS:N | 2.40 | 0.51 |
| 21:2Z:50:GLN:OE1 | 21:2Z:50:GLN:N | 2.41 | 0.51 |
| 32:2a:537:G:H5" | 43:2l:113:ARG:NH1 | 2.26 | 0.51 |
| 32:2a:1010:G:N1 | 32:2a:1020:U:H1' | 2.26 | 0.51 |
| 33:2b:212:GLN:HE21 | 33:2b:235:SER:HA | 1.76 | 0.51 |
| 36:2e:83:GLU:HG2 | 36:2e:88:LYS:HD2 | 1.92 | 0.51 |
| 50:2s:28:LYS:HB2 | 50:2s:29:ARG:CA | 2.30 | 0.51 |
| 1:1A:296:C:H2' | 1:1A:297:C:H6 | 1.76 | 0.50 |
| 1:1A:881:G:C2 | 1:1A:882:G:H1' | 2.46 | 0.50 |
| 1:1A:1105:U:H2' | 1:1A:1106:G:H8 | 1.73 | 0.50 |
| 1:1A:1893:C:OP1 | 59:1A:4286:HOH:O | 2.19 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 11:1P:130:PHE:HB2 | 11:1P:135:LEU:HG | 1.93 | 0.50 |
| 30:18:33:ASN:HA | 30:18:36:LYS:HD2 | 1.93 | 0.50 |
| 30:18:62:LEU:HB3 | 30:18:65:GLU:HG3 | 1.93 | 0.50 |
| 32:1a:6:G:H4' | 32:1a:298:A:H4' | 1.93 | 0.50 |
| 32:1a:324:G:N2 | 32:1a:327:A:OP2 | 2.44 | 0.50 |
| 32:1a:715:A:OP1 | 32:1a:805:C:O2' | 2.24 | 0.50 |
| 32:1a:1273:G:H3' | 32:1a:1274:G:H8 | 1.74 | 0.50 |
| 35:1d:189:PRO:HB3 | 35:1d:193:ASP:HB2 | 1.92 | 0.50 |
| 1:2A:144:C:H5' | 19:2X:2:LYS:HG2 | 1.93 | 0.50 |
| 1:2A:184:C:H2' | 1:2A:185:U:C6 | 2.45 | 0.50 |
| 1:2A:254:G:N7 | 30:28:5:LYS:HE2 | 2.27 | 0.50 |
| 1:2A:297:C:H2' | 1:2A:298:G:O4' | 2.11 | 0.50 |
| 1:2A:1550:C:H2' | 1:2A:1551:C:C6 | 2.46 | 0.50 |
| 1:2A:2537:U:H2' | 1:2A:2538:C:C6 | 2.45 | 0.50 |
| 8:2I:66:GLU:OE2 | 8:2I:69:LYS:HD3 | 2.11 | 0.50 |
| 8:2I:93:THR:C | 8:2I:97:ILE:HG12 | 2.35 | 0.50 |
| 32:2a:129(A):G:C6 | 32:2a:189(E):U:H4' | 2.45 | 0.50 |
| 40:2i:28:VAL:HG22 | 40:2i:63:ILE:HB | 1.93 | 0.50 |
| 1:1A:983:A:O3' | 59:1A:4290:HOH:O | 2.19 | 0.50 |
| 1:1A:1466:G:H2' | 1:1A:1547:C:N4 | 2.26 | 0.50 |
| 1:1A:2529:G:H5" | 1:1A:2530:A:H5" | 1.94 | 0.50 |
| 10:1O:115:VAL:HG13 | 10:1O:121:VAL:HG21 | 1.92 | 0.50 |
| 32:1a:374:A:C6 | 32:1a:375:U:C4 | 2.99 | 0.50 |
| 32:1a:392:G:H2' | 32:1a:393:A:H8 | 1.76 | 0.50 |
| 32:1a:684:A:N6 | 59:1a:1956:HOH:O | 2.43 | 0.50 |
| 1:2A:265:A:H1' | 1:2A:266:G:O4' | 2.12 | 0.50 |
| 1:2A:327:G:N2 | 20:2Y:70:SER:OG | 2.44 | 0.50 |
| 1:2A:764:A:N1 | 1:2A:1789:A:O2' | 2.43 | 0.50 |
| 1:2A:807:U:P | 11:2P:36:LYS:HD3 | 2.52 | 0.50 |
| 1:2A:947:G:H2' | 1:2A:948:G:C8 | 2.46 | 0.50 |
| 1:2A:958:U:H5" | 12:2Q:14:ARG:HD3 | 1.93 | 0.50 |
| 1:2A:1529:G:O6 | 1:2A:1530:C:N4 | 2.45 | 0.50 |
| 1:2A:1537:G:H2' | 1:2A:1538:G:H8 | 1.76 | 0.50 |
| 2:2B:30:C:H2' | 2:2B:31:C:H5' | 1.94 | 0.50 |
| 11:2P:63:PRO:HG2 | 30:28:25:MET:HB2 | 1.92 | 0.50 |
| 32:2a:20:U:H2' | 32:2a:21:G:O4' | 2.12 | 0.50 |
| 33:2b:212:GLN:NE2 | 33:2b:234:PRO:O | 2.44 | 0.50 |
| 38:2g:79:ARG:H | 38:2g:79:ARG:HD3 | 1.76 | 0.50 |
| 1:1A:125:G:H5" | 29:17:19:ARG:HD3 | 1.92 | 0.50 |
| 1:1A:1195:G:O2' | 1:1A:1226:A:N1 | 2.41 | 0.50 |
| 1:1A:1430:C:H2' | 1:1A:1431:U:C6 | 2.46 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1A:2408:U:H2' | 1:1A:2409:G:C8 | 2.46 | 0.50 |
| 1:1A:2841:C:H2' | 1:1A:2842:G:H8 | 1.75 | 0.50 |
| 7:1H:157:TYR:CE1 | 7:1H:172:LYS:HG3 | 2.47 | 0.50 |
| 25:13:6:VAL:HG12 | 25:13:54:VAL:HG21 | 1.93 | 0.50 |
| 32:1a:769:G:H4' | 32:1a:1513:A:H4' | 1.93 | 0.50 |
| 32:1a:1047:G:H5" | 45:1n:4:LYS:CD | 2.40 | 0.50 |
| 32:1a:1073:U:O2 | 33:1b:104:ASN:ND2 | 2.41 | 0.50 |
| 32:1a:1157:A:H5' | 32:1a:1158:C:C6 | 2.46 | 0.50 |
| 1:2A:118:A:N3 | 1:2A:178:G:H1' | 2.26 | 0.50 |
| 1:2A:585:G:O2' | 1:2A:1254:A:N6 | 2.40 | 0.50 |
| 1:2A:829:A:N7 | 1:2A:2248:C:H5' | 2.26 | 0.50 |
| 1:2A:847:U:H5' | 1:2A:848:G:OP2 | 2.10 | 0.50 |
| 1:2A:1478:G:O2' | 1:2A:1558:A:N1 | 2.39 | 0.50 |
| 1:2A:1769:G:O2' | 1:2A:1958:C:OP1 | 2.24 | 0.50 |
| 1:2A:2127:G:C2 | 1:2A:2161:C:N3 | 2.79 | 0.50 |
| 1:2A:2134:A:H1' | 1:2A:2158:A:C6 | 2.46 | 0.50 |
| 32:2a:975:A:N1 | 41:2j:48:THR:HB | 2.26 | 0.50 |
| 32:2a:1105:A:H2' | 32:2a:1106:G:H8 | 1.77 | 0.50 |
| 47:2p:8:ARG:HB3 | 47:2p:28:ARG:NH1 | 2.27 | 0.50 |
| 48:2q:62:SER:OG | 48:2q:72:ARG:HG2 | 2.11 | 0.50 |
| 1:1A:323:G:H1' | 1:1A:1205:U:O2 | 2.12 | 0.50 |
| 1:1A:729:G:H2' | 1:1A:1775:U:H1' | 1.93 | 0.50 |
| 1:1A:1040:C:H2' | 1:1A:1041:C:O4' | 2.12 | 0.50 |
| 1:1A:1053:C:N4 | 1:1A:1106:G:H1 | 2.09 | 0.50 |
| 1:1A:1793:C:H2' | 1:1A:1794:U:H6 | 1.75 | 0.50 |
| 6:1G:137:GLU:HB2 | 6:1G:140:ILE:HD13 | 1.93 | 0.50 |
| 32:1a:119:A:H4' | 32:1a:120:A:C8 | 2.45 | 0.50 |
| 32:1a:255:G:H2' | 32:1a:256:U:C6 | 2.47 | 0.50 |
| 32:1a:345:C:H5' | 32:1a:346:G:C5 | 2.46 | 0.50 |
| 33:1b:19:HIS:CE1 | 33:1b:206:ASP:HB2 | 2.46 | 0.50 |
| 1:2A:240:G:O6 | 59:2A:3951:HOH:O | 2.18 | 0.50 |
| 1:2A:323:G:H1' | 1:2A:1205:U:O2 | 2.12 | 0.50 |
| 33:2b:175:ARG:O | 33:2b:179:LYS:HG2 | 2.12 | 0.50 |
| 34:2c:22:TRP:HA | 41:2j:93:GLY:HA2 | 1.92 | 0.50 |
| 1:1A:179:G:N7 | 59:1A:4407:HOH:O | 2.35 | 0.50 |
| 1:1A:722:A:H2' | 1:1A:723:G:C8 | 2.47 | 0.50 |
| 1:1A:787:U:H5" | 1:1A:788:A:H5' | 1.93 | 0.50 |
| 1:1A:1823:G:OP1 | 3:1D:54:ARG:NH1 | 2.44 | 0.50 |
| 1:1A:2774:C:H2' | 1:1A:2775:A:O4' | 2.11 | 0.50 |
| 4:1E:147:PRO:HB2 | 4:1E:149:ARG:HG2 | 1.92 | 0.50 |
| 6:1G:139:LEU:HA | 6:1G:144:ILE:HB | 1.92 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:1R:72:ASP:O | 13:1R:76:VAL:HG13 | 2.12 | 0.50 |
| 18:1W:56:ALA:O | 18:1W:60:ASN:HB2 | 2.12 | 0.50 |
| 23:11:2:SER:N | 59:11:201:HOH:O | 2.44 | 0.50 |
| 32:1a:153:C:N4 | 32:1a:169:C:H42 | 2.10 | 0.50 |
| 32:1a:176:C:H2' | 32:1a:177:C:H6 | 1.77 | 0.50 |
| 32:1a:457:C:H2' | 32:1a:458:C:C6 | 2.46 | 0.50 |
| 32:1a:659:U:H2' | 32:1a:660:G:C8 | 2.46 | 0.50 |
| 35:1d:103:ASN:O | 35:1d:107:ARG:HG2 | 2.10 | 0.50 |
| 42:1k:95:ILE:O | 42:1k:99:GLN:HG3 | 2.12 | 0.50 |
| 44:1m:67:GLU:HG3 | 44:1m:71:ARG:HH22 | 1.75 | 0.50 |
| 1:2A:55:G:O2' | 1:2A:127:A:N1 | 2.37 | 0.50 |
| 1:2A:239:U:H2' | 1:2A:240:G:O4' | 2.12 | 0.50 |
| 1:2A:859:G:N2 | 1:2A:917:A:OP2 | 2.37 | 0.50 |
| 1:2A:1448:G:H4' | 1:2A:1542:A:OP1 | 2.11 | 0.50 |
| 1:2A:2820:A:OP2 | 13:2R:2:ARG:NH2 | 2.44 | 0.50 |
| 3:2D:9:TYR:HD1 | 3:2D:10:THR:HG23 | 1.75 | 0.50 |
| 8:2I:3:VAL:HG12 | 8:2I:38:LEU:HA | 1.93 | 0.50 |
| 32:2a:1323:G:H2' | 32:2a:1324:A:C8 | 2.46 | 0.50 |
| 32:2a:1376:U:H2' | 32:2a:1377:A:C8 | 2.46 | 0.50 |
| 50:2s:12:ASP:OD2 | 50:2s:37:ARG:NH1 | 2.44 | 0.50 |
| 51:2t:60:GLU:HG3 | 51:2t:81:LYS:HD2 | 1.94 | 0.50 |
| 1:1A:9:U:H3 | 1:1A:2629:A:H2 | 1.57 | 0.50 |
| 1:1A:83:G:OP1 | 20:1Y:95:LYS:NZ | 2.43 | 0.50 |
| 5:1F:39:TRP:O | 5:1F:43:LYS:HG2 | 2.12 | 0.50 |
| 32:1a:601:C:H2' | 32:1a:602:A:C8 | 2.46 | 0.50 |
| 32:1a:874:G:H21 | 39:1h:15:ASN:HD21 | 1.59 | 0.50 |
| 32:1a:953:G:H2' | 32:1a:954:G:O4' | 2.12 | 0.50 |
| 32:1a:1240:U:C2 | 38:1g:32:ARG:HG3 | 2.47 | 0.50 |
| 32:1a:1320:C:O2 | 50:1s:36:ARG:NH2 | 2.45 | 0.50 |
| 1:2A:142:A:HO2' | 1:2A:1407:C:HO2' | 1.54 | 0.50 |
| 1:2A:504:U:H5' | 1:2A:506:G:OP2 | 2.12 | 0.50 |
| 1:2A:887:A:H4' | 1:2A:888:C:H5 | 1.76 | 0.50 |
| 1:2A:900:A:H3' | 1:2A:901:A:C8 | 2.47 | 0.50 |
| 1:2A:2206:G:H3' | 1:2A:2207:G:H8 | 1.70 | 0.50 |
| 1:2A:2391:G:O6 | 1:2A:2425:A:H8 | 1.95 | 0.50 |
| 1:2A:2584:U:H2' | 1:2A:2585:U:H2' | 1.92 | 0.50 |
| 7:2H:10:PRO:O | 7:2H:12:PRO:HD3 | 2.10 | 0.50 |
| 9:2N:96:GLU:CD | 9:2N:96:GLU:H | 2.19 | 0.50 |
| 11:2P:63:PRO:HB2 | 30:28:30:ARG:HH21 | 1.77 | 0.50 |
| 16:2U:107:ALA:O | 16:2U:111:GLU:HG2 | 2.12 | 0.50 |
| 32:2a:583:A:OP1 | 46:2o:68:ARG:NH2 | 2.44 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 32:2a:982:U:N3 | 32:2a:1223:C:N3 | 2.59 | 0.50 |
| 32:2a:1004:A:H5" | 32:2a:1024:G:H22 | 1.77 | 0.50 |
| 33:2b:95:GLN:HB2 | 33:2b:148:TYR:CD1 | 2.46 | 0.50 |
| 1:1A:1025:G:C4 | 1:1A:1135:C:H1' | 2.46 | 0.50 |
| 1:1A:1751:C:HO2' | 1:1A:2861:G:HO2' | 1.59 | 0.50 |
| 1:1A:1795:C:H2' | 1:1A:1796:U:O4' | 2.11 | 0.50 |
| 2:1B:1:U:O2' | 2:1B:2:C:OP1 | 2.27 | 0.50 |
| 14:1S:46:VAL:HG12 | 14:1S:48:LEU:HD12 | 1.92 | 0.50 |
| 15:1T:74:ARG:HG2 | 15:1T:76:PHE:CZ | 2.46 | 0.50 |
| 19:1X:49:VAL:HG11 | 19:1X:89:ILE:HG12 | 1.94 | 0.50 |
| 25:13:37:LEU:HB3 | 25:13:43:ILE:HD13 | 1.94 | 0.50 |
| 34:1c:152:ILE:HB | 34:1c:199:LYS:HB2 | 1.94 | 0.50 |
| 37:1f:55:ASP:HB2 | 37:1f:86:ARG:HH12 | 1.76 | 0.50 |
| 1:2A:286:C:H2' | 1:2A:287:C:H6 | 1.76 | 0.50 |
| 1:2A:1657:C:H2' | 1:2A:1658:C:C6 | 2.46 | 0.50 |
| 1:2A:2206:G:OP1 | 3:2D:68:LYS:NZ | 2.45 | 0.50 |
| 1:2A:2648:C:H2' | 1:2A:2649:U:C6 | 2.47 | 0.50 |
| 3:2D:9:TYR:CD1 | 3:2D:10:THR:HG23 | 2.47 | 0.50 |
| 14:2S:62:LYS:HB3 | 14:2S:97:ARG:HD2 | 1.93 | 0.50 |
| 32:2a:187:C:H2' | 32:2a:188:C:H6 | 1.76 | 0.50 |
| 32:2a:261:U:OP2 | 51:2t:79:ARG:NH2 | 2.45 | 0.50 |
| 32:2a:677:U:H3 | 32:2a:713:G:N2 | 2.09 | 0.50 |
| 32:2a:1011:G:N2 | 32:2a:1018:C:N3 | 2.58 | 0.50 |
| 36:2e:145:LYS:HA | 36:2e:148:VAL:HG22 | 1.93 | 0.50 |
| 39:2h:20:TYR:HA | 39:2h:65:TYR:CE1 | 2.46 | 0.50 |
| 44:2m:3:ARG:HB3 | 44:2m:8:GLU:HA | 1.93 | 0.50 |
| 46:2o:24:SER:O | 46:2o:28:GLN:HG3 | 2.12 | 0.50 |
| 48:2q:95:TYR:HA | 48:2q:98:LEU:HD12 | 1.93 | 0.50 |
| 1:1A:70:G:H5" | 1:1A:112:U:O2 | 2.12 | 0.50 |
| 1:1A:753:C:H2' | 1:1A:754:C:H6 | 1.76 | 0.50 |
| 1:1A:910:A:N1 | 1:1A:2277:G:H1' | 2.26 | 0.50 |
| 1:1A:1010:A:N3 | 1:1A:1153:C:H1' | 2.26 | 0.50 |
| 1:1A:1230:C:H2' | 1:1A:1231:G:C8 | 2.46 | 0.50 |
| 21:1Z:136:PHE:O | 21:1Z:137:ILE:HG13 | 2.12 | 0.50 |
| 21:1Z:154:ASP:OD1 | 21:1Z:154:ASP:N | 2.45 | 0.50 |
| 32:1a:66:G:C2 | 32:1a:104:G:H1' | 2.47 | 0.50 |
| 32:1a:599:C:H4' | 39:1h:130:GLY:C | 2.36 | 0.50 |
| 32:1a:1111:A:N1 | 34:1c:177:THR:OG1 | 2.39 | 0.50 |
| 33:1b:52:GLU:O | 33:1b:56:ARG:HB3 | 2.12 | 0.50 |
| 48:1q:66:SER:OG | 48:1q:67:LYS:N | 2.43 | 0.50 |
| 1:2A:224:G:N7 | 1:2A:420:C:H4' | 2.27 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:2A:459:U:H5” | 29:27:40:TRP:CD2 | 2.47 | 0.50 |
| 1:2A:718:A:H3’ | 1:2A:719:C:H6 | 1.77 | 0.50 |
| 1:2A:2347:C:H4’ | 1:2A:2347:C:OP1 | 2.12 | 0.50 |
| 1:2A:2651:C:H2’ | 1:2A:2652:C:H6 | 1.76 | 0.50 |
| 2:2B:98:G:H3’ | 2:2B:99:G:H8 | 1.76 | 0.50 |
| 32:2a:457:C:H2’ | 32:2a:458:C:H6 | 1.77 | 0.50 |
| 33:2b:128:GLU:C | 33:2b:130:ARG:H | 2.20 | 0.50 |
| 34:2c:122:GLU:O | 34:2c:126:ARG:HG3 | 2.11 | 0.50 |
| 48:2q:3:LYS:HD2 | 48:2q:60:ILE:HD11 | 1.93 | 0.50 |
| 1:1A:8:A:H2’ | 1:1A:9:U:C6 | 2.45 | 0.50 |
| 1:1A:598:G:H2’ | 1:1A:599:G:O4’ | 2.12 | 0.50 |
| 1:1A:674:G:H1’ | 5:1F:74:ARG:HD3 | 1.93 | 0.50 |
| 1:1A:2337:G:OP1 | 59:1A:4288:HOH:O | 2.19 | 0.50 |
| 14:1S:106:ARG:O | 14:1S:109:GLY:N | 2.44 | 0.50 |
| 15:1T:112:ARG:HG3 | 15:1T:115:ARG:HH21 | 1.76 | 0.50 |
| 30:18:39:LYS:O | 30:18:43:GLN:HG3 | 2.11 | 0.50 |
| 32:1a:1027:C:C4 | 32:1a:1034:G:C2 | 3.00 | 0.50 |
| 33:1b:166:ASP:HB3 | 33:1b:169:LYS:HB3 | 1.93 | 0.50 |
| 51:1t:90:GLN:HA | 51:1t:93:GLU:HG2 | 1.93 | 0.50 |
| 1:2A:616:G:H5’ | 5:2F:205:ARG:HD3 | 1.94 | 0.50 |
| 1:2A:2305:A:H1’ | 6:2G:136:ARG:HB3 | 1.94 | 0.50 |
| 1:2A:2412:A:H2’ | 1:2A:2413:G:O4’ | 2.11 | 0.50 |
| 2:2B:7:G:N2 | 14:2S:38:GLN:HE22 | 2.10 | 0.50 |
| 9:2N:73:THR:HA | 9:2N:83:LYS:O | 2.12 | 0.50 |
| 21:2Z:146:ILE:HA | 21:2Z:174:VAL:HG12 | 1.93 | 0.50 |
| 28:26:23:THR:OG1 | 28:26:24:GLU:N | 2.44 | 0.50 |
| 32:2a:952:U:H4’ | 32:2a:964:A:N1 | 2.26 | 0.50 |
| 32:2a:1070:U:H2’ | 32:2a:1071:C:C6 | 2.46 | 0.50 |
| 32:2a:1240:U:OP2 | 38:2g:115:ARG:HA | 2.12 | 0.50 |
| 32:2a:1411:C:H2’ | 32:2a:1412:C:C6 | 2.47 | 0.50 |
| 33:2b:7:VAL:HG22 | 33:2b:8:LYS:H | 1.77 | 0.50 |
| 33:2b:178:ARG:NH1 | 39:2h:68:ARG:HH22 | 2.10 | 0.50 |
| 39:2h:10:LEU:HD12 | 39:2h:85:ARG:HG2 | 1.92 | 0.50 |
| 42:2k:34:ASP:OD1 | 42:2k:38:ASN:N | 2.44 | 0.50 |
| 1:1A:1314:C:OP1 | 59:1A:4243:HOH:O | 2.19 | 0.49 |
| 1:1A:1668:A:O2’ | 1:1A:1674:G:N7 | 2.41 | 0.49 |
| 26:14:41:PRO:HA | 26:14:47:GLN:HB3 | 1.94 | 0.49 |
| 33:1b:77:ALA:HA | 33:1b:80:ILE:HD13 | 1.92 | 0.49 |
| 39:1h:19:VAL:HG23 | 39:1h:21:LYS:HG3 | 1.94 | 0.49 |
| 1:2A:657:U:H2’ | 1:2A:658:C:C6 | 2.47 | 0.49 |
| 1:2A:1660:C:H2’ | 1:2A:1661:G:H8 | 1.77 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 15:2T:24:PRO:HA | 15:2T:49:VAL:HG23 | 1.92 | 0.49 |
| 21:2Z:3:TYR:O | 21:2Z:57:ILE:HA | 2.12 | 0.49 |
| 21:2Z:92:SER:O | 21:2Z:130:PRO:HG3 | 2.12 | 0.49 |
| 32:2a:201:C:H42 | 32:2a:216:G:H1 | 1.60 | 0.49 |
| 32:2a:1333:A:H2' | 32:2a:1334:G:O4' | 2.12 | 0.49 |
| 1:1A:234:C:H2' | 1:1A:235:U:C6 | 2.47 | 0.49 |
| 1:1A:1070:A:N7 | 1:1A:1096:A:O2' | 2.35 | 0.49 |
| 1:1A:1432:C:H2' | 1:1A:1433:U:O4' | 2.12 | 0.49 |
| 1:1A:1478:G:H2' | 1:1A:1479:G:C8 | 2.47 | 0.49 |
| 6:1G:43:LEU:HD22 | 6:1G:153:ARG:HD2 | 1.92 | 0.49 |
| 32:1a:580:U:H2' | 32:1a:581:G:O4' | 2.12 | 0.49 |
| 32:1a:629:G:H2' | 32:1a:630:G:O4' | 2.11 | 0.49 |
| 32:1a:1095:U:OP1 | 32:1a:1108:G:N2 | 2.45 | 0.49 |
| 32:1a:1333:A:H2' | 32:1a:1334:G:O4' | 2.12 | 0.49 |
| 1:2A:907:U:O2' | 12:2Q:101:ARG:NH2 | 2.34 | 0.49 |
| 1:2A:1003:G:O2' | 1:2A:1010:A:N1 | 2.37 | 0.49 |
| 1:2A:1247:A:OP1 | 5:2F:95:ARG:NH2 | 2.44 | 0.49 |
| 1:2A:1889:A:N1 | 1:2A:2234:G:H1' | 2.27 | 0.49 |
| 1:2A:2118:U:OP1 | 1:2A:2149:G:H5' | 2.12 | 0.49 |
| 1:2A:2127:G:N1 | 1:2A:2161:C:C4 | 2.80 | 0.49 |
| 1:2A:2136:C:N3 | 1:2A:2155:G:N2 | 2.53 | 0.49 |
| 7:2H:113:VAL:HG11 | 7:2H:151:ILE:HD13 | 1.93 | 0.49 |
| 35:2d:8:VAL:HG21 | 35:2d:21:LEU:HB2 | 1.94 | 0.49 |
| 41:2j:27:ALA:HB2 | 41:2j:85:LEU:HD21 | 1.94 | 0.49 |
| 48:2q:19:VAL:HG23 | 48:2q:44:ALA:HB3 | 1.93 | 0.49 |
| 1:1A:2635:C:O2' | 4:1E:80:GLU:OE2 | 2.29 | 0.49 |
| 3:1D:223:GLY:HA2 | 3:1D:226:MET:HE3 | 1.94 | 0.49 |
| 6:1G:80:PHE:HB2 | 6:1G:82:LEU:HB2 | 1.92 | 0.49 |
| 24:12:1:MET:H1 | 24:12:52:ASP:CG | 2.21 | 0.49 |
| 32:1a:401:C:H2' | 32:1a:402:G:C8 | 2.47 | 0.49 |
| 32:1a:520:A:N1 | 32:1a:536:C:H1' | 2.27 | 0.49 |
| 32:1a:691:G:H2' | 32:1a:692:U:C6 | 2.47 | 0.49 |
| 32:1a:1352:C:H2' | 32:1a:1353:G:C8 | 2.48 | 0.49 |
| 49:1r:59:SER:OG | 49:1r:60:ALA:N | 2.45 | 0.49 |
| 1:2A:409:C:H2' | 1:2A:410:G:C8 | 2.47 | 0.49 |
| 1:2A:749:C:OP2 | 59:2A:3959:HOH:O | 2.20 | 0.49 |
| 1:2A:1803:A:H4' | 3:2D:259:THR:HG23 | 1.93 | 0.49 |
| 5:2F:63:LYS:HG3 | 5:2F:76:GLY:HA2 | 1.94 | 0.49 |
| 9:2N:43:THR:HG22 | 9:2N:44:PRO:HD2 | 1.94 | 0.49 |
| 32:2a:123:C:OP1 | 32:2a:311:C:O2' | 2.25 | 0.49 |
| 32:2a:876:G:H1' | 39:2h:11:THR:HG21 | 1.93 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 32:2a:923:A:N6 | 32:2a:1392:G:O6 | 2.45 | 0.49 |
| 32:2a:1056:U:N3 | 32:2a:1205:U:O2 | 2.44 | 0.49 |
| 43:2l:8:ASN:O | 43:2l:12:ARG:HG3 | 2.12 | 0.49 |
| 1:1A:30:G:H2' | 1:1A:31:C:O4' | 2.12 | 0.49 |
| 1:1A:2478:A:OP2 | 31:19:2:LYS:NZ | 2.30 | 0.49 |
| 1:1A:2612:C:OP2 | 27:15:2:ALA:N | 2.45 | 0.49 |
| 1:1A:2773:C:H2' | 1:1A:2774:C:H6 | 1.76 | 0.49 |
| 3:1D:125:ILE:HB | 37:1f:81:ILE:HD11 | 1.94 | 0.49 |
| 6:1G:18:GLU:OE2 | 6:1G:21:ARG:NH1 | 2.45 | 0.49 |
| 32:1a:353:A:H5' | 32:1a:353:A:H8 | 1.77 | 0.49 |
| 38:1g:46:ALA:O | 38:1g:50:ILE:HG12 | 2.13 | 0.49 |
| 41:1j:6:ILE:HA | 41:1j:98:ILE:HA | 1.93 | 0.49 |
| 44:1m:23:TYR:CE2 | 44:1m:71:ARG:HG3 | 2.47 | 0.49 |
| 51:1t:36:LEU:HD13 | 51:1t:58:LYS:HG3 | 1.93 | 0.49 |
| 1:2A:1401:G:H2' | 1:2A:1402:C:O4' | 2.12 | 0.49 |
| 4:2E:134:ILE:HA | 4:2E:137:HIS:CD2 | 2.47 | 0.49 |
| 5:2F:197:ASP:HA | 5:2F:200:GLU:HB3 | 1.95 | 0.49 |
| 7:2H:24:VAL:HG21 | 7:2H:72:ILE:HG12 | 1.94 | 0.49 |
| 32:2a:1068:G:H8 | 32:2a:1068:G:OP2 | 1.94 | 0.49 |
| 32:2a:1142:G:H3' | 32:2a:1143:G:C8 | 2.46 | 0.49 |
| 32:2a:1218:C:H2' | 32:2a:1219:U:C6 | 2.47 | 0.49 |
| 32:2a:1286:A:H2 | 52:2u:18:TYR:OH | 1.95 | 0.49 |
| 32:2a:1512:U:H2' | 32:2a:1513:A:C8 | 2.48 | 0.49 |
| 33:2b:29:ALA:HA | 33:2b:32:ILE:HD12 | 1.94 | 0.49 |
| 33:2b:135:GLN:O | 33:2b:139:LYS:HB2 | 2.12 | 0.49 |
| 38:2g:70:LYS:HG2 | 38:2g:100:ALA:HB2 | 1.95 | 0.49 |
| 1:1A:292:C:C2 | 1:1A:349:G:C2 | 3.01 | 0.49 |
| 1:1A:784:A:O4' | 3:1D:227:ASN:ND2 | 2.45 | 0.49 |
| 1:1A:1045:A:H1' | 1:1A:1047:G:N3 | 2.27 | 0.49 |
| 1:1A:1153:C:H2' | 1:1A:1154:G:O4' | 2.12 | 0.49 |
| 2:1B:29:A:O2' | 2:1B:58:A:N1 | 2.38 | 0.49 |
| 4:1E:59:VAL:HG21 | 4:1E:74:PRO:HB3 | 1.94 | 0.49 |
| 6:1G:37:VAL:HG21 | 6:1G:103:LEU:HD11 | 1.95 | 0.49 |
| 25:13:26:LEU:O | 25:13:35:ARG:HD3 | 2.13 | 0.49 |
| 32:1a:202:U:O2' | 32:1a:203:U:O5' | 2.22 | 0.49 |
| 1:2A:492:A:H2' | 1:2A:493:G:O4' | 2.12 | 0.49 |
| 1:2A:1813:G:H1' | 3:2D:50:THR:OG1 | 2.12 | 0.49 |
| 1:2A:1999:C:H4' | 1:2A:2723:C:O2 | 2.12 | 0.49 |
| 1:2A:2144:U:O2' | 1:2A:2147:G:O6 | 2.31 | 0.49 |
| 1:2A:2318:G:H21 | 14:2S:3:ARG:NE | 2.09 | 0.49 |
| 6:2G:172:LEU:O | 6:2G:176:LEU:N | 2.39 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 11:2P:90:ARG:HH12 | 11:2P:105:LEU:HD11 | 1.76 | 0.49 |
| 32:2a:108:G:C6 | 51:2t:15:ARG:HG2 | 2.47 | 0.49 |
| 32:2a:409:G:C2 | 32:2a:410:G:H1' | 2.47 | 0.49 |
| 32:2a:1142:G:H2' | 32:2a:1143:G:O4' | 2.12 | 0.49 |
| 32:2a:1381:U:H1' | 38:2g:79:ARG:NE | 2.25 | 0.49 |
| 48:2q:45:HIS:HB2 | 48:2q:65:ILE:HD13 | 1.95 | 0.49 |
| 50:2s:11:VAL:C | 50:2s:13:ASP:H | 2.19 | 0.49 |
| 1:1A:1065:U:H5" | 1:1A:1066:U:OP2 | 2.12 | 0.49 |
| 1:1A:1798:U:H5' | 3:1D:259:THR:CG2 | 2.43 | 0.49 |
| 32:1a:165:C:H2' | 32:1a:166:G:C8 | 2.46 | 0.49 |
| 32:1a:407:G:H2' | 32:1a:408:A:C8 | 2.48 | 0.49 |
| 32:1a:542:G:P | 35:1d:10:ARG:HH22 | 2.33 | 0.49 |
| 32:1a:978:A:O2' | 32:1a:1322:C:N3 | 2.40 | 0.49 |
| 32:1a:1058:G:OP1 | 34:1c:199:LYS:NZ | 2.45 | 0.49 |
| 32:1a:1070:U:H2' | 32:1a:1071:C:C6 | 2.45 | 0.49 |
| 41:1j:40:LEU:HB2 | 41:1j:69:ASN:HB2 | 1.95 | 0.49 |
| 1:2A:342:G:H2' | 1:2A:343:C:H6 | 1.76 | 0.49 |
| 1:2A:494:G:O6 | 59:2A:3958:HOH:O | 2.20 | 0.49 |
| 1:2A:571:A:N6 | 1:2A:2499:C:O3' | 2.46 | 0.49 |
| 1:2A:839:U:H1' | 1:2A:1191:G:H1' | 1.93 | 0.49 |
| 1:2A:2291:U:O2' | 1:2A:2374:C:O2 | 2.28 | 0.49 |
| 1:2A:2552:2MU:H6 | 1:2A:2552:2MU:O5' | 2.11 | 0.49 |
| 2:2B:64:C:H2' | 2:2B:65:C:C6 | 2.48 | 0.49 |
| 2:2B:106:G:OP1 | 21:2Z:31:ARG:HG2 | 2.12 | 0.49 |
| 4:2E:26:ILE:HD11 | 4:2E:188:VAL:HG21 | 1.93 | 0.49 |
| 24:22:64:LEU:O | 24:22:68:ARG:HG3 | 2.12 | 0.49 |
| 32:2a:97:G:H2' | 32:2a:98:G:O4' | 2.12 | 0.49 |
| 32:2a:663:A:H5" | 49:2r:61:LYS:HE3 | 1.95 | 0.49 |
| 32:2a:1095:U:P | 32:2a:1108:G:H1 | 2.36 | 0.49 |
| 32:2a:1367:C:P | 40:2i:112:LYS:HZ1 | 2.36 | 0.49 |
| 33:2b:90:MET:HA | 33:2b:90:MET:HE2 | 1.94 | 0.49 |
| 34:2c:37:GLN:NE2 | 45:2n:52:GLN:OE1 | 2.33 | 0.49 |
| 39:2h:121:ASP:OD1 | 39:2h:121:ASP:N | 2.45 | 0.49 |
| 1:1A:459:U:H5" | 29:17:40:TRP:CD2 | 2.48 | 0.49 |
| 1:1A:971:C:H2' | 1:1A:972:G:O4' | 2.12 | 0.49 |
| 1:1A:1932:A:H2' | 1:1A:1933:G:O4' | 2.12 | 0.49 |
| 1:1A:2441:C:OP2 | 1:1A:2586:C:O2' | 2.30 | 0.49 |
| 11:1P:39:LYS:HB2 | 11:1P:45:LEU:HD21 | 1.94 | 0.49 |
| 14:1S:61:ASN:ND2 | 14:1S:64:GLU:H | 2.09 | 0.49 |
| 14:1S:93:LYS:O | 14:1S:95:HIS:N | 2.45 | 0.49 |
| 32:1a:1525:G:OP1 | 42:1k:120:ARG:NH2 | 2.46 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 38:1g:26:PHE:CE2 | 38:1g:30:ILE:HD11 | 2.48 | 0.49 |
| 41:1j:11:PHE:CE1 | 41:1j:67:THR:HG22 | 2.47 | 0.49 |
| 1:2A:648:G:O2' | 1:2A:2351:G:OP1 | 2.24 | 0.49 |
| 1:2A:984:A:H5" | 1:2A:985:C:H5 | 1.76 | 0.49 |
| 1:2A:2155:G:C5 | 1:2A:2156:G:H1' | 2.48 | 0.49 |
| 1:2A:2689:U:P | 1:2A:2719:G:H22 | 2.36 | 0.49 |
| 4:2E:27:LEU:HD22 | 15:2T:1:MET:HE1 | 1.94 | 0.49 |
| 6:2G:114:ILE:HG12 | 6:2G:140:ILE:HG12 | 1.94 | 0.49 |
| 7:2H:113:VAL:HG11 | 7:2H:151:ILE:HG21 | 1.94 | 0.49 |
| 8:2I:114:LEU:O | 8:2I:116:LEU:N | 2.45 | 0.49 |
| 10:2O:36:GLY:HA2 | 10:2O:106:LEU:HD23 | 1.93 | 0.49 |
| 13:2R:51:LEU:HD22 | 13:2R:66:VAL:HG13 | 1.94 | 0.49 |
| 15:2T:83:ILE:HD13 | 15:2T:86:ILE:HD11 | 1.94 | 0.49 |
| 33:2b:162:ILE:HG13 | 33:2b:184:VAL:HA | 1.95 | 0.49 |
| 34:2c:109:PRO:HB3 | 34:2c:115:LEU:HD23 | 1.95 | 0.49 |
| 34:2c:138:VAL:O | 34:2c:170:GLN:NE2 | 2.45 | 0.49 |
| 54:2x:61:C:H2' | 54:2x:62:C:C6 | 2.48 | 0.49 |
| 1:1A:888:C:O2 | 44:1m:83:ASP:HA | 2.13 | 0.49 |
| 1:1A:2467:C:H4' | 12:1Q:123:HIS:CD2 | 2.48 | 0.49 |
| 1:1A:2801(A):A:H1' | 1:1A:2895:U:H1' | 1.94 | 0.49 |
| 2:1B:24:G:N7 | 2:1B:56:G:H2' | 2.28 | 0.49 |
| 12:1Q:81:VAL:HB | 22:10:7:LEU:HG | 1.95 | 0.49 |
| 29:17:21:ARG:NH1 | 59:17:201:HOH:O | 2.44 | 0.49 |
| 32:1a:19:C:H2' | 32:1a:20:U:H6 | 1.78 | 0.49 |
| 32:1a:189(C):C:H2' | 32:1a:189(D):C:O4' | 2.13 | 0.49 |
| 32:1a:222:U:H2' | 32:1a:223:U:C6 | 2.48 | 0.49 |
| 32:1a:236:G:H5" | 48:1q:42:TYR:OH | 2.13 | 0.49 |
| 32:1a:1320:C:H2' | 32:1a:1321:C:O4' | 2.13 | 0.49 |
| 32:1a:1504:G:OP1 | 32:1a:1507:A:H4' | 2.13 | 0.49 |
| 53:1v:16:A:H2' | 53:1v:17:U:O4' | 2.13 | 0.49 |
| 54:1x:50:U:H2' | 54:1x:51:C:C6 | 2.48 | 0.49 |
| 1:2A:27:G:O2' | 1:2A:28:A:OP2 | 2.30 | 0.49 |
| 1:2A:30:G:H2' | 1:2A:31:C:C6 | 2.48 | 0.49 |
| 1:2A:154(A):C:N4 | 1:2A:171:G:H1 | 2.11 | 0.49 |
| 1:2A:582:G:H2' | 1:2A:583:G:C8 | 2.48 | 0.49 |
| 1:2A:1227:G:OP2 | 16:2U:16:LYS:NZ | 2.37 | 0.49 |
| 1:2A:2291:U:H2' | 1:2A:2292:C:C6 | 2.47 | 0.49 |
| 1:2A:2682:U:HO2' | 15:2T:58:ASN:ND2 | 2.11 | 0.49 |
| 21:2Z:154:ASP:OD1 | 21:2Z:154:ASP:N | 2.46 | 0.49 |
| 32:2a:946:A:H2' | 32:2a:947:G:C8 | 2.48 | 0.49 |
| 32:2a:1004:A:N3 | 32:2a:1038:C:C2 | 2.80 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 32:2a:1107:C:C4 | 32:2a:1108:G:C8 | 3.00 | 0.49 |
| 35:2d:194:LEU:HB3 | 35:2d:196:LEU:HD13 | 1.94 | 0.49 |
| 1:1A:768:G:O2' | 1:1A:1379:A:N1 | 2.46 | 0.49 |
| 1:1A:784:A:C5 | 3:1D:229:VAL:HG21 | 2.48 | 0.49 |
| 1:1A:1638:C:O3' | 1:1A:2709:G:N2 | 2.46 | 0.49 |
| 1:1A:2543:G:H2' | 1:1A:2544:G:C8 | 2.47 | 0.49 |
| 1:1A:2732:G:H3' | 1:1A:2733:A:O4' | 2.13 | 0.49 |
| 9:1N:73:THR:HB | 9:1N:82:LEU:HD11 | 1.95 | 0.49 |
| 21:1Z:53:ILE:HG22 | 21:1Z:71:VAL:HG12 | 1.95 | 0.49 |
| 21:1Z:126:VAL:HG12 | 21:1Z:128:VAL:HB | 1.95 | 0.49 |
| 32:1a:69:G:H2' | 32:1a:70:G:C8 | 2.48 | 0.49 |
| 32:1a:664:G:P | 49:1r:64:ARG:HH21 | 2.36 | 0.49 |
| 32:1a:1260:C:O5' | 32:1a:1284:C:H4' | 2.13 | 0.49 |
| 40:1i:23:ASN:HB2 | 40:1i:25:LYS:HE2 | 1.95 | 0.49 |
| 41:1j:50:ILE:HD11 | 41:1j:57:LYS:HD3 | 1.94 | 0.49 |
| 1:2A:1820:U:H4' | 1:2A:1821:A:OP2 | 2.13 | 0.49 |
| 1:2A:2126:A:N3 | 1:2A:2127:G:H1' | 2.28 | 0.49 |
| 1:2A:2630:G:H2' | 1:2A:2631:G:H8 | 1.78 | 0.49 |
| 8:2I:78:THR:H | 8:2I:104:GLN:HE22 | 1.60 | 0.49 |
| 32:2a:16:A:H4' | 36:2e:17:ALA:H | 1.78 | 0.49 |
| 32:2a:147:G:H2' | 32:2a:148:G:C8 | 2.48 | 0.49 |
| 32:2a:528:C:H5' | 32:2a:529:G:OP2 | 2.13 | 0.49 |
| 32:2a:971:G:N2 | 32:2a:1363(A):A:OP2 | 2.36 | 0.49 |
| 34:2c:77:ILE:HG22 | 34:2c:103:VAL:HG21 | 1.95 | 0.49 |
| 1:1A:153:C:OP2 | 23:11:92:LYS:NZ | 2.28 | 0.49 |
| 1:1A:570:G:H2' | 1:1A:2030:A:C5 | 2.48 | 0.49 |
| 1:1A:1009:A:OP2 | 9:1N:37:LYS:NZ | 2.45 | 0.49 |
| 1:1A:1188:U:H2' | 1:1A:1189:A:H5' | 1.95 | 0.49 |
| 1:1A:2347:C:OP1 | 28:16:38:LYS:NZ | 2.46 | 0.49 |
| 4:1E:1:MET:HE1 | 4:1E:200:GLU:O | 2.12 | 0.49 |
| 19:1X:54:VAL:HG13 | 19:1X:81:VAL:HG12 | 1.95 | 0.49 |
| 34:1c:190:ARG:HA | 34:1c:195:VAL:HG23 | 1.94 | 0.49 |
| 39:1h:14:ARG:NH2 | 39:1h:83:ILE:O | 2.39 | 0.49 |
| 40:1i:37:PHE:HD1 | 40:1i:40:LEU:HD12 | 1.76 | 0.49 |
| 50:1s:11:VAL:HG11 | 50:1s:16:LEU:HB2 | 1.94 | 0.49 |
| 1:2A:1268:A:H2' | 1:2A:1269:A:O4' | 2.13 | 0.49 |
| 1:2A:1364:G:N7 | 23:21:3:LYS:HD2 | 2.28 | 0.49 |
| 1:2A:1782:C:H1' | 1:2A:2609:U:H5" | 1.95 | 0.49 |
| 1:2A:2549:G:H2' | 1:2A:2550:G:H8 | 1.77 | 0.49 |
| 4:2E:179:GLU:HG3 | 15:2T:9:LEU:HD21 | 1.93 | 0.49 |
| 8:2I:71:ILE:O | 8:2I:75:LEU:N | 2.46 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 9:2N:38:HIS:CE1 | 9:2N:39:ARG:HG3 | 2.48 | 0.49 |
| 31:29:29:ASN:HD22 | 31:29:32:HIS:CE1 | 2.31 | 0.49 |
| 32:2a:450:G:H4' | 47:2p:41:PRO:HB2 | 1.95 | 0.49 |
| 32:2a:1305:G:H5' | 52:2u:4:GLY:HA3 | 1.95 | 0.49 |
| 33:2b:189:ASP:OD2 | 33:2b:189:ASP:N | 2.35 | 0.49 |
| 41:2j:7:LYS:HG3 | 41:2j:71:LEU:HD13 | 1.95 | 0.49 |
| 50:2s:23:ASN:HD21 | 50:2s:47:HIS:HE1 | 1.61 | 0.49 |
| 1:1A:826:U:C4' | 11:1P:55:ARG:HB3 | 2.43 | 0.48 |
| 1:1A:1298:C:H5" | 1:1A:1299:G:OP2 | 2.13 | 0.48 |
| 1:1A:1570:A:H2' | 1:1A:1571:A:C8 | 2.47 | 0.48 |
| 1:1A:2703:C:H2' | 1:1A:2704:C:H6 | 1.78 | 0.48 |
| 33:1b:54:THR:HG23 | 33:1b:199:TYR:HB3 | 1.94 | 0.48 |
| 39:1h:7:ALA:HB2 | 39:1h:85:ARG:HG3 | 1.95 | 0.48 |
| 41:1j:5:ARG:NE | 41:1j:73:ASP:OD1 | 2.41 | 0.48 |
| 44:1m:102:ARG:HH21 | 44:1m:105:THR:HG23 | 1.79 | 0.48 |
| 50:1s:50:ALA:HA | 50:1s:58:VAL:O | 2.13 | 0.48 |
| 54:1x:32:5MC:HM52 | 54:1x:33:U:O4 | 2.13 | 0.48 |
| 1:2A:443:A:H1' | 1:2A:1201:C:O4' | 2.13 | 0.48 |
| 1:2A:2116:G:N7 | 1:2A:2166:G:N2 | 2.61 | 0.48 |
| 1:2A:2576:G:O2' | 1:2A:2579:C:OP2 | 2.22 | 0.48 |
| 1:2A:2732:G:H3' | 1:2A:2733:A:O4' | 2.12 | 0.48 |
| 3:2D:77:ALA:HA | 3:2D:97:TYR:HA | 1.95 | 0.48 |
| 6:2G:144:ILE:HA | 6:2G:148:MET:SD | 2.53 | 0.48 |
| 32:2a:187:C:H5" | 51:2t:86:ARG:HG3 | 1.94 | 0.48 |
| 32:2a:767:A:H2' | 32:2a:768:A:O4' | 2.12 | 0.48 |
| 33:2b:101:MET:HA | 33:2b:108:ILE:HD12 | 1.95 | 0.48 |
| 34:2c:155:GLY:HA3 | 34:2c:196:LEU:HD13 | 1.95 | 0.48 |
| 40:2i:53:VAL:O | 40:2i:55:ALA:N | 2.46 | 0.48 |
| 44:2m:33:ALA:HA | 44:2m:59:TYR:CE2 | 2.48 | 0.48 |
| 1:1A:64:A:O3' | 19:1X:71:GLY:HA3 | 2.13 | 0.48 |
| 1:1A:1557:C:H5" | 1:1A:1558:A:OP2 | 2.12 | 0.48 |
| 3:1D:206:LEU:HD22 | 3:1D:211:ARG:HG2 | 1.95 | 0.48 |
| 4:1E:60:ASN:OD1 | 4:1E:63:LEU:HG | 2.13 | 0.48 |
| 17:1V:62:LEU:HD12 | 17:1V:93:GLU:HG2 | 1.94 | 0.48 |
| 32:1a:656:C:C2' | 46:1o:28:GLN:HE22 | 2.26 | 0.48 |
| 32:1a:728:A:H2' | 32:1a:729:A:C8 | 2.47 | 0.48 |
| 40:1i:40:LEU:HD11 | 40:1i:70:LYS:HD3 | 1.95 | 0.48 |
| 41:1j:13:HIS:HA | 41:1j:16:LEU:HB3 | 1.94 | 0.48 |
| 47:1p:19:ILE:HG22 | 47:1p:36:ILE:HG13 | 1.94 | 0.48 |
| 1:2A:1133:U:O4 | 1:2A:2026:C:H1' | 2.13 | 0.48 |
| 1:2A:1385:G:O2' | 1:2A:1396:U:O2 | 2.24 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:2A:1821:A:H2' | 1:2A:1822:G:C8 | 2.46 | 0.48 |
| 8:2I:93:THR:O | 8:2I:97:ILE:HG12 | 2.14 | 0.48 |
| 8:2I:126:TYR:HD2 | 8:2I:142:VAL:HB | 1.78 | 0.48 |
| 15:2T:61:PHE:CE2 | 15:2T:76:PHE:HB2 | 2.48 | 0.48 |
| 32:2a:662:G:H2' | 32:2a:663:A:H8 | 1.78 | 0.48 |
| 32:2a:664:G:N2 | 32:2a:741:G:H1 | 2.10 | 0.48 |
| 32:2a:1106:G:H2' | 32:2a:1107:C:H6 | 1.78 | 0.48 |
| 1:1A:27:G:N2 | 1:1A:512:G:H1' | 2.28 | 0.48 |
| 1:1A:1047:G:O2' | 1:1A:1048:A:H8 | 1.96 | 0.48 |
| 1:1A:2086:U:H2' | 1:1A:2087:G:C8 | 2.48 | 0.48 |
| 1:1A:2443:C:OP1 | 5:1F:68:LYS:HD3 | 2.13 | 0.48 |
| 1:1A:2841:C:H2' | 1:1A:2842:G:C8 | 2.48 | 0.48 |
| 1:1A:2848:G:H8 | 15:1T:97:ALA:HB2 | 1.77 | 0.48 |
| 3:1D:254:THR:O | 3:1D:254:THR:OG1 | 2.30 | 0.48 |
| 4:1E:2:LYS:HB2 | 4:1E:95:ILE:HD12 | 1.94 | 0.48 |
| 4:1E:67:PHE:CE1 | 4:1E:75:VAL:HG22 | 2.49 | 0.48 |
| 15:1T:91:ARG:HH11 | 15:1T:120:ARG:HH12 | 1.61 | 0.48 |
| 32:1a:68:G:H1 | 32:1a:101:A:H61 | 1.60 | 0.48 |
| 32:1a:1062:U:H2' | 32:1a:1063:C:C6 | 2.48 | 0.48 |
| 32:1a:1118:C:P | 40:1i:104:ARG:HH11 | 2.34 | 0.48 |
| 33:1b:36:ARG:C | 33:1b:38:GLY:H | 2.21 | 0.48 |
| 39:1h:35:ILE:HD11 | 39:1h:134:ILE:HG21 | 1.94 | 0.48 |
| 39:1h:124:ALA:O | 39:1h:128:GLY:N | 2.44 | 0.48 |
| 1:2A:286:C:H42 | 1:2A:355:G:H1 | 1.61 | 0.48 |
| 1:2A:819:A:OP2 | 1:2A:1187:G:N2 | 2.32 | 0.48 |
| 1:2A:1507:A:O2' | 1:2A:1508:A:O5' | 2.32 | 0.48 |
| 1:2A:2030:A:H4' | 1:2A:2031:A:C8 | 2.49 | 0.48 |
| 1:2A:2690:C:N4 | 1:2A:2713:A:H1' | 2.27 | 0.48 |
| 5:2F:129:PHE:CD2 | 5:2F:163:VAL:HG21 | 2.48 | 0.48 |
| 8:2I:51:ILE:HB | 8:2I:52:ARG:NH1 | 2.28 | 0.48 |
| 8:2I:84:GLY:HA3 | 8:2I:87:LYS:HE2 | 1.95 | 0.48 |
| 17:2V:58:VAL:O | 17:2V:97:LYS:N | 2.44 | 0.48 |
| 30:28:14:VAL:HG13 | 30:28:22:VAL:HG13 | 1.94 | 0.48 |
| 30:28:34:TRP:CG | 30:28:35:GLN:N | 2.81 | 0.48 |
| 32:2a:447:G:O5' | 32:2a:447:G:H8 | 1.96 | 0.48 |
| 32:2a:1352:C:H2' | 32:2a:1353:G:C8 | 2.47 | 0.48 |
| 44:2m:5:ALA:HB2 | 44:2m:22:ILE:HD13 | 1.95 | 0.48 |
| 50:2s:36:ARG:NH1 | 50:2s:53:ASN:HA | 2.28 | 0.48 |
| 1:1A:1495:A:C6 | 1:1A:1496:A:C6 | 3.02 | 0.48 |
| 5:1F:170:LEU:HD13 | 5:1F:172:TRP:CZ2 | 2.49 | 0.48 |
| 15:1T:100:TYR:HB3 | 15:1T:103:ARG:NH1 | 2.28 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 32:1a:755:G:OP2 | 46:1o:65:ARG:HD2 | 2.13 | 0.48 |
| 35:1d:98:GLU:O | 35:1d:103:ASN:ND2 | 2.47 | 0.48 |
| 36:1e:88:LYS:HB3 | 36:1e:123:LEU:HB2 | 1.94 | 0.48 |
| 37:1f:82:ARG:HB2 | 37:1f:85:VAL:HG23 | 1.94 | 0.48 |
| 1:2A:271(Z):C:H1' | 1:2A:272(C):G:H1' | 1.95 | 0.48 |
| 1:2A:2615:U:C2 | 27:25:7:PRO:HA | 2.48 | 0.48 |
| 5:2F:126:VAL:HG22 | 5:2F:195:ASP:HA | 1.95 | 0.48 |
| 6:2G:161:THR:C | 6:2G:163:ALA:H | 2.22 | 0.48 |
| 32:2a:110:C:H2' | 32:2a:111:G:O4' | 2.13 | 0.48 |
| 32:2a:1359:C:O2' | 32:2a:1362:C:N4 | 2.46 | 0.48 |
| 39:2h:12:ARG:NH1 | 39:2h:27:PRO:HD3 | 2.28 | 0.48 |
| 39:2h:87:SER:HB2 | 39:2h:93:VAL:HB | 1.94 | 0.48 |
| 50:2s:32:LYS:HA | 50:2s:50:ALA:HB3 | 1.95 | 0.48 |
| 1:1A:271(P):C:O3' | 8:1I:42:SER:OG | 2.32 | 0.48 |
| 1:1A:1082:U:C4 | 1:1A:1086:A:N1 | 2.78 | 0.48 |
| 1:1A:1791:A:H3' | 1:1A:1792:G:H8 | 1.79 | 0.48 |
| 1:1A:1796:U:H2' | 1:1A:1797:C:C6 | 2.48 | 0.48 |
| 1:1A:2705:A:O2' | 1:1A:2852:G:OP1 | 2.28 | 0.48 |
| 6:1G:67:LYS:HE2 | 26:14:5:ILE:HD12 | 1.96 | 0.48 |
| 15:1T:24:PRO:HD3 | 15:1T:52:ILE:HD12 | 1.94 | 0.48 |
| 28:16:18:ARG:HD2 | 28:16:42:TRP:CD1 | 2.48 | 0.48 |
| 32:1a:297:G:N2 | 32:1a:300:A:OP2 | 2.43 | 0.48 |
| 32:1a:476:G:H2' | 32:1a:477:A:H8 | 1.76 | 0.48 |
| 32:1a:1425:U:H2' | 32:1a:1426:C:H6 | 1.77 | 0.48 |
| 32:1a:1429:C:H2' | 32:1a:1430:C:C6 | 2.47 | 0.48 |
| 33:1b:88:ALA:HB2 | 33:1b:219:VAL:HG13 | 1.95 | 0.48 |
| 35:1d:128:VAL:HG12 | 35:1d:129:ASN:ND2 | 2.28 | 0.48 |
| 37:1f:97:PHE:HB2 | 49:1r:32:ARG:HD2 | 1.96 | 0.48 |
| 44:1m:59:TYR:O | 44:1m:63:THR:OG1 | 2.22 | 0.48 |
| 47:1p:20:VAL:HG21 | 47:1p:32:TYR:CD2 | 2.49 | 0.48 |
| 1:2A:189:G:H2' | 1:2A:205:G:N2 | 2.29 | 0.48 |
| 1:2A:484:C:H2' | 1:2A:485:C:C6 | 2.48 | 0.48 |
| 1:2A:577:G:O2' | 1:2A:1254:A:OP1 | 2.28 | 0.48 |
| 1:2A:675:A:OP1 | 5:2F:63:LYS:NZ | 2.44 | 0.48 |
| 21:2Z:52:SER:C | 21:2Z:54:HIS:H | 2.22 | 0.48 |
| 32:2a:153:C:N3 | 32:2a:169:C:N4 | 2.61 | 0.48 |
| 32:2a:542:G:P | 35:2d:10:ARG:HH22 | 2.36 | 0.48 |
| 32:2a:1121:U:O2' | 32:2a:1122:U:H5' | 2.13 | 0.48 |
| 33:2b:80:ILE:HD12 | 33:2b:208:ILE:HD13 | 1.96 | 0.48 |
| 39:2h:9:MET:HE3 | 39:2h:32:LYS:HE2 | 1.95 | 0.48 |
| 54:2x:25:C:H2' | 54:2x:26:G:O4' | 2.13 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1A:296:C:H2' | 1:1A:297:C:C6 | 2.49 | 0.48 |
| 1:1A:1655:A:H3' | 1:1A:1656:C:C6 | 2.48 | 0.48 |
| 1:1A:2628:C:O2' | 1:1A:2781:A:H2' | 2.13 | 0.48 |
| 32:1a:266:G:H4' | 32:1a:267:C:C5 | 2.48 | 0.48 |
| 32:1a:544:G:OP2 | 35:1d:66:ARG:NH2 | 2.47 | 0.48 |
| 32:1a:741:G:H2' | 32:1a:742:G:O4' | 2.13 | 0.48 |
| 32:1a:1033:G:H2' | 32:1a:1034:G:C8 | 2.47 | 0.48 |
| 33:1b:183:PRO:HA | 33:1b:198:ASP:OD2 | 2.14 | 0.48 |
| 44:1m:84:ILE:HB | 50:1s:66:MET:HE2 | 1.96 | 0.48 |
| 1:2A:613:G:O2' | 1:2A:614(C):A:N1 | 2.42 | 0.48 |
| 1:2A:729:G:C6 | 3:2D:208:LYS:HB2 | 2.48 | 0.48 |
| 1:2A:852:G:H2' | 1:2A:853:G:C8 | 2.48 | 0.48 |
| 1:2A:2774:C:H2' | 1:2A:2775:A:O4' | 2.13 | 0.48 |
| 2:2B:5:C:H42 | 2:2B:116:G:H1 | 1.60 | 0.48 |
| 2:2B:7:G:H5' | 14:2S:29:PHE:CE2 | 2.48 | 0.48 |
| 3:2D:175:LEU:HD12 | 3:2D:185:VAL:HG21 | 1.96 | 0.48 |
| 5:2F:20:LEU:HD23 | 5:2F:22:ALA:HB2 | 1.94 | 0.48 |
| 8:2I:9:LEU:HD21 | 8:2I:35:LEU:HD13 | 1.95 | 0.48 |
| 9:2N:30:ILE:HG23 | 9:2N:52:VAL:HG11 | 1.95 | 0.48 |
| 10:2O:64:ARG:NH2 | 10:2O:99:PHE:O | 2.47 | 0.48 |
| 15:2T:74:ARG:HG2 | 15:2T:76:PHE:CZ | 2.48 | 0.48 |
| 32:2a:187:C:H2' | 32:2a:188:C:C6 | 2.48 | 0.48 |
| 32:2a:1023:G:H3' | 32:2a:1024:G:H8 | 1.78 | 0.48 |
| 35:2d:94:LEU:HA | 35:2d:97:LEU:HD12 | 1.94 | 0.48 |
| 1:1A:323:G:C8 | 5:1F:171:PRO:HG3 | 2.48 | 0.48 |
| 1:1A:2467:C:H4' | 12:1Q:123:HIS:CG | 2.48 | 0.48 |
| 1:1A:2637:U:C2' | 1:1A:2638:G:H5' | 2.44 | 0.48 |
| 1:1A:2819:G:OP1 | 59:1A:4289:HOH:O | 2.19 | 0.48 |
| 7:1H:3:ARG:NH1 | 7:1H:4:ILE:H | 2.11 | 0.48 |
| 7:1H:86:GLU:HB2 | 7:1H:165:ALA:HB2 | 1.96 | 0.48 |
| 9:1N:14:VAL:HB | 9:1N:138:LEU:HD12 | 1.95 | 0.48 |
| 14:1S:10:ARG:HG2 | 14:1S:91:PRO:HA | 1.95 | 0.48 |
| 20:1Y:28:LYS:HB3 | 20:1Y:38:ILE:HG22 | 1.94 | 0.48 |
| 32:1a:1316:G:H5" | 45:1n:17:LYS:HE3 | 1.95 | 0.48 |
| 1:2A:489:G:H2' | 1:2A:491:G:O4' | 2.13 | 0.48 |
| 1:2A:1125:G:H5' | 31:29:37:GLY:HA2 | 1.96 | 0.48 |
| 1:2A:1628:G:H2' | 1:2A:1629:U:C6 | 2.48 | 0.48 |
| 1:2A:2111:C:O4' | 1:2A:2118:U:H1' | 2.14 | 0.48 |
| 1:2A:2136:C:N4 | 1:2A:2155:G:H1 | 2.11 | 0.48 |
| 1:2A:2788:C:OP1 | 4:2E:61:ARG:NH2 | 2.47 | 0.48 |
| 2:2B:31:C:H4' | 6:2G:29:TRP:CZ2 | 2.48 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 15:2T:39:ARG:NH2 | 32:2a:345:C:OP2 | 2.41 | 0.48 |
| 26:24:46:GLN:HG2 | 26:24:48:ARG:H | 1.79 | 0.48 |
| 32:2a:601:C:H2' | 32:2a:602:A:C8 | 2.48 | 0.48 |
| 32:2a:998:G:H1 | 32:2a:1043:C:N4 | 2.11 | 0.48 |
| 32:2a:1271:G:N2 | 32:2a:1272:G:N7 | 2.61 | 0.48 |
| 32:2a:1326:C:H2' | 32:2a:1327:C:C6 | 2.49 | 0.48 |
| 46:2o:82:ILE:HD11 | 46:2o:88:ARG:HH11 | 1.78 | 0.48 |
| 1:1A:862:G:H2' | 1:1A:863:A:O4' | 2.14 | 0.48 |
| 1:1A:1081:U:H2' | 1:1A:1082:U:C6 | 2.49 | 0.48 |
| 1:1A:2683:C:H2' | 1:1A:2684:U:C6 | 2.48 | 0.48 |
| 2:1B:42:C:O2 | 6:1G:93:THR:N | 2.40 | 0.48 |
| 8:1I:6:LEU:O | 8:1I:7:GLU:HG3 | 2.13 | 0.48 |
| 11:1P:106:LEU:HD22 | 11:1P:112:LEU:HB2 | 1.94 | 0.48 |
| 11:1P:138:LEU:HD23 | 11:1P:145:PRO:HB3 | 1.95 | 0.48 |
| 32:1a:176:C:H2' | 32:1a:177:C:C6 | 2.49 | 0.48 |
| 32:1a:881:G:P | 43:1l:12:ARG:HH22 | 2.36 | 0.48 |
| 32:1a:1218:C:H2' | 32:1a:1219:U:C6 | 2.48 | 0.48 |
| 38:1g:22:LEU:HD11 | 38:1g:101:LEU:HD21 | 1.96 | 0.48 |
| 1:2A:412:A:OP2 | 1:2A:412:A:H8 | 1.96 | 0.48 |
| 1:2A:445:C:O2' | 1:2A:449:A:N3 | 2.41 | 0.48 |
| 1:2A:1291:C:H2' | 1:2A:1292:U:C6 | 2.49 | 0.48 |
| 16:2U:110:VAL:O | 16:2U:114:LYS:HG2 | 2.14 | 0.48 |
| 21:2Z:138:GLU:HG2 | 21:2Z:156:LYS:NZ | 2.29 | 0.48 |
| 32:2a:303:A:HO2' | 32:2a:555:C:HO2' | 1.61 | 0.48 |
| 32:2a:973:G:OP1 | 41:2j:57:LYS:NZ | 2.40 | 0.48 |
| 32:2a:1015:A:H2' | 32:2a:1016:A:C8 | 2.47 | 0.48 |
| 32:2a:1121:U:H2' | 32:2a:1122:U:C6 | 2.49 | 0.48 |
| 32:2a:1149:C:O2' | 32:2a:1280:A:N1 | 2.46 | 0.48 |
| 32:2a:1414:U:H3 | 32:2a:1486:G:H1 | 1.61 | 0.48 |
| 1:1A:239:U:H2' | 1:1A:240:G:O4' | 2.13 | 0.48 |
| 1:1A:945:A:C4 | 1:1A:2448:A:C2 | 3.02 | 0.48 |
| 1:1A:1429:G:H2' | 1:1A:1430:C:H6 | 1.79 | 0.48 |
| 1:1A:1698:A:OP2 | 59:1A:4291:HOH:O | 2.20 | 0.48 |
| 23:11:8:SER:HB3 | 23:11:66:HIS:CD2 | 2.49 | 0.48 |
| 23:11:64:ALA:HA | 23:11:67:ILE:HG13 | 1.95 | 0.48 |
| 32:1a:341:C:H2' | 32:1a:342:C:C6 | 2.49 | 0.48 |
| 32:1a:373:A:O2' | 32:1a:451:A:N7 | 2.47 | 0.48 |
| 32:1a:435:C:H2' | 32:1a:436:C:H6 | 1.79 | 0.48 |
| 32:1a:865:A:C2 | 32:1a:918:A:H4' | 2.48 | 0.48 |
| 32:1a:973:G:H3' | 32:1a:974:A:H5" | 1.94 | 0.48 |
| 34:1c:150:LYS:HE2 | 34:1c:152:ILE:HD11 | 1.95 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:1j:78:ASN:O | 41:1j:80:LYS:N | 2.47 | 0.48 |
| 1:2A:139:G:H2' | 1:2A:140:G:N7 | 2.29 | 0.48 |
| 1:2A:286:C:H2' | 1:2A:287:C:C6 | 2.49 | 0.48 |
| 1:2A:322:A:OP1 | 5:2F:168:ARG:HD2 | 2.14 | 0.48 |
| 1:2A:884:C:H3' | 1:2A:885:C:H6 | 1.78 | 0.48 |
| 1:2A:1257:C:H4' | 5:2F:83:PHE:CD1 | 2.49 | 0.48 |
| 1:2A:1913:A:H4' | 1:2A:1914:C:C5' | 2.44 | 0.48 |
| 3:2D:70:TRP:CE2 | 3:2D:150:LYS:HD2 | 2.48 | 0.48 |
| 6:2G:103:LEU:HD23 | 6:2G:106:LEU:HD12 | 1.96 | 0.48 |
| 12:2Q:27:VAL:HG21 | 12:2Q:134:ARG:HG3 | 1.96 | 0.48 |
| 22:20:27:GLU:HB2 | 22:20:69:PHE:HD1 | 1.79 | 0.48 |
| 35:2d:129:ASN:OD1 | 35:2d:145:GLU:N | 2.47 | 0.48 |
| 46:2o:5:LYS:O | 46:2o:9:GLN:HG2 | 2.13 | 0.48 |
| 1:1A:1063:G:H2' | 1:1A:1064:C:H6 | 1.78 | 0.48 |
| 1:1A:1766:U:H2' | 1:1A:1767:C:H6 | 1.79 | 0.48 |
| 1:1A:2482:G:O6 | 12:1Q:124:LYS:NZ | 2.47 | 0.48 |
| 1:1A:2627:G:N2 | 1:1A:2777:G:OP2 | 2.46 | 0.48 |
| 7:1H:9:ILE:HB | 7:1H:50:VAL:HG12 | 1.96 | 0.48 |
| 7:1H:40:GLU:CD | 7:1H:60:ARG:HH21 | 2.22 | 0.48 |
| 26:14:58:ARG:O | 26:14:61:ARG:HG2 | 2.14 | 0.48 |
| 29:17:18:PHE:N | 29:17:43:THR:HG21 | 2.29 | 0.48 |
| 32:1a:175:C:H2' | 32:1a:176:C:C6 | 2.49 | 0.48 |
| 32:1a:670:G:H2' | 32:1a:671:G:O4' | 2.14 | 0.48 |
| 32:1a:688:G:H2' | 32:1a:689:C:C6 | 2.49 | 0.48 |
| 38:1g:107:ALA:HB2 | 38:1g:134:ALA:HB2 | 1.96 | 0.48 |
| 1:2A:496:G:H2' | 1:2A:497:A:H5' | 1.95 | 0.48 |
| 1:2A:851:U:O2' | 25:23:42:ALA:O | 2.31 | 0.48 |
| 1:2A:1431:U:H2' | 1:2A:1432:C:C6 | 2.49 | 0.48 |
| 1:2A:2786:U:H2' | 1:2A:2787:C:C6 | 2.49 | 0.48 |
| 6:2G:15:VAL:HG11 | 6:2G:176:LEU:HD23 | 1.96 | 0.48 |
| 11:2P:84:ASN:OD1 | 11:2P:117:GLU:HB2 | 2.14 | 0.48 |
| 32:2a:545:C:H5' | 35:2d:72:GLU:HB2 | 1.96 | 0.48 |
| 33:2b:165:VAL:HG13 | 33:2b:166:ASP:H | 1.78 | 0.48 |
| 42:2k:41:THR:HG21 | 42:2k:71:LYS:HB2 | 1.96 | 0.48 |
| 42:2k:105:VAL:HG23 | 42:2k:105:VAL:O | 2.12 | 0.48 |
| 1:1A:214:G:N3 | 1:1A:216:A:O2' | 2.43 | 0.47 |
| 1:1A:220:G:O2' | 1:1A:233:A:N3 | 2.44 | 0.47 |
| 1:1A:247:G:H4' | 1:1A:386:G:C5 | 2.49 | 0.47 |
| 1:1A:358:U:H2' | 1:1A:359:A:C8 | 2.49 | 0.47 |
| 1:1A:1665:A:H2' | 1:1A:1666:G:O4' | 2.13 | 0.47 |
| 1:1A:2243:U:H2' | 1:1A:2244:U:C6 | 2.49 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1A:2849:U:H4' | 1:1A:2868:A:C2 | 2.49 | 0.47 |
| 1:1A:2853:C:H2' | 1:1A:2854:G:C8 | 2.49 | 0.47 |
| 1:1A:2853:C:H2' | 1:1A:2854:G:H8 | 1.79 | 0.47 |
| 3:1D:68:LYS:HE3 | 3:1D:70:TRP:CH2 | 2.49 | 0.47 |
| 4:1E:101:ARG:HG2 | 4:1E:169:ASN:OD1 | 2.14 | 0.47 |
| 5:1F:106:ARG:H | 5:1F:106:ARG:HG2 | 1.46 | 0.47 |
| 7:1H:119:GLU:O | 7:1H:140:LYS:NZ | 2.46 | 0.47 |
| 10:1O:73:ASP:OD1 | 10:1O:75:SER:HB3 | 2.13 | 0.47 |
| 21:1Z:150:LEU:HD11 | 21:1Z:154:ASP:OD2 | 2.13 | 0.47 |
| 32:1a:106:C:O2' | 32:1a:379:C:H5" | 2.14 | 0.47 |
| 32:1a:757:U:H2' | 32:1a:758:G:O4' | 2.14 | 0.47 |
| 32:1a:1106:G:H2' | 32:1a:1107:C:C6 | 2.49 | 0.47 |
| 41:1j:40:LEU:HB2 | 41:1j:69:ASN:CB | 2.44 | 0.47 |
| 1:2A:483:A:O2' | 20:2Y:49:VAL:O | 2.21 | 0.47 |
| 1:2A:1301:A:H2 | 1:2A:1626:G:N3 | 2.12 | 0.47 |
| 1:2A:2555:U:H5" | 1:2A:2556:C:OP2 | 2.13 | 0.47 |
| 1:2A:2679:A:OP2 | 4:2E:160:TYR:OH | 2.27 | 0.47 |
| 1:2A:2785:C:O3' | 4:2E:69:LYS:NZ | 2.46 | 0.47 |
| 1:2A:2884:U:P | 27:25:43:HIS:HE2 | 2.37 | 0.47 |
| 32:2a:852:G:H2' | 32:2a:853:G:O4' | 2.14 | 0.47 |
| 32:2a:919:A:H8 | 32:2a:919:A:O5' | 1.95 | 0.47 |
| 32:2a:1014:A:N3 | 32:2a:1219:U:H1' | 2.28 | 0.47 |
| 32:2a:1026:G:N2 | 32:2a:1027:C:O4' | 2.47 | 0.47 |
| 32:2a:1368:G:H5' | 40:2i:112:LYS:HB3 | 1.95 | 0.47 |
| 41:2j:12:ASP:O | 41:2j:15:THR:OG1 | 2.28 | 0.47 |
| 43:2l:7:ILE:O | 43:2l:11:VAL:HG23 | 2.13 | 0.47 |
| 1:1A:443:A:C5 | 5:1F:45:ARG:HD2 | 2.49 | 0.47 |
| 1:1A:989:G:OP2 | 25:13:11:SER:OG | 2.23 | 0.47 |
| 1:1A:1783:A:OP1 | 59:1A:4241:HOH:O | 2.20 | 0.47 |
| 1:1A:2408:U:H2' | 1:1A:2409:G:H8 | 1.79 | 0.47 |
| 1:1A:2564:A:OP1 | 1:1A:2648:C:H4' | 2.14 | 0.47 |
| 1:1A:2699:C:H2' | 1:1A:2700:C:O4' | 2.13 | 0.47 |
| 2:1B:2:C:H2' | 2:1B:3:C:C6 | 2.49 | 0.47 |
| 9:1N:6:PRO:HD2 | 9:1N:43:THR:OG1 | 2.14 | 0.47 |
| 18:1W:78:GLU:OE2 | 18:1W:99:ARG:NH1 | 2.35 | 0.47 |
| 32:1a:313:A:H2' | 32:1a:314:C:C6 | 2.49 | 0.47 |
| 32:1a:921:U:O2 | 36:1e:19:MET:HB2 | 2.14 | 0.47 |
| 32:1a:977:A:H1' | 32:1a:982:U:O4 | 2.14 | 0.47 |
| 33:1b:185:ILE:HG22 | 33:1b:199:TYR:HB2 | 1.96 | 0.47 |
| 47:1p:6:LEU:HB3 | 47:1p:17:TYR:CD1 | 2.49 | 0.47 |
| 1:2A:910:A:N1 | 1:2A:2277:G:H1' | 2.29 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:2A:1651:G:N7 | 13:2R:11:ASN:ND2 | 2.61 | 0.47 |
| 1:2A:2136:C:N4 | 1:2A:2155:G:N1 | 2.62 | 0.47 |
| 2:2B:117:G:H8 | 2:2B:117:G:O5' | 1.97 | 0.47 |
| 6:2G:106:LEU:HD22 | 6:2G:111:LEU:HG | 1.96 | 0.47 |
| 9:2N:19:GLU:HG3 | 9:2N:59:LYS:HB3 | 1.96 | 0.47 |
| 14:2S:3:ARG:NH1 | 14:2S:4:LEU:H | 2.12 | 0.47 |
| 32:2a:109:A:C6 | 32:2a:326:G:C6 | 3.02 | 0.47 |
| 32:2a:1305:G:H22 | 32:2a:1331:G:H1' | 1.78 | 0.47 |
| 32:2a:1328:C:OP1 | 52:2u:21:TYR:OH | 2.19 | 0.47 |
| 42:2k:73:MET:HG2 | 42:2k:103:LEU:HD21 | 1.96 | 0.47 |
| 48:2q:58:GLU:O | 48:2q:74:LEU:N | 2.41 | 0.47 |
| 1:1A:285:C:H2' | 1:1A:286:C:C6 | 2.49 | 0.47 |
| 1:1A:1983:C:H4' | 1:1A:2606:C:H4' | 1.96 | 0.47 |
| 11:1P:1:MET:HE2 | 11:1P:1:MET:HB2 | 1.82 | 0.47 |
| 18:1W:71:VAL:HA | 18:1W:107:LEU:HD12 | 1.95 | 0.47 |
| 28:16:12:GLU:HA | 28:16:19:ARG:HA | 1.97 | 0.47 |
| 32:1a:7:G:H2' | 36:1e:119:LEU:HD22 | 1.96 | 0.47 |
| 32:1a:1255:G:N7 | 41:1j:43:ARG:NH2 | 2.60 | 0.47 |
| 34:1c:35:GLU:O | 34:1c:39:ILE:N | 2.42 | 0.47 |
| 39:1h:46:LYS:HE2 | 39:1h:63:LEU:O | 2.14 | 0.47 |
| 43:1l:23:LYS:C | 43:1l:25:PRO:HD3 | 2.39 | 0.47 |
| 48:1q:45:HIS:O | 48:1q:73:VAL:HG23 | 2.15 | 0.47 |
| 1:2A:1296:G:OP1 | 1:2A:2709:G:O2' | 2.22 | 0.47 |
| 1:2A:1639:U:O2' | 1:2A:2699:C:H4' | 2.14 | 0.47 |
| 1:2A:1709:U:H2' | 1:2A:1710:C:H6 | 1.78 | 0.47 |
| 1:2A:1981:A:N7 | 59:2A:4036:HOH:O | 2.35 | 0.47 |
| 1:2A:2294:C:OP2 | 14:2S:89:ARG:NH2 | 2.29 | 0.47 |
| 14:2S:34:HIS:O | 14:2S:97:ARG:NH2 | 2.47 | 0.47 |
| 19:2X:49:VAL:HG11 | 19:2X:89:ILE:HG12 | 1.95 | 0.47 |
| 28:26:9:LEU:HA | 28:26:54:ILE:HB | 1.95 | 0.47 |
| 32:2a:629:G:H2' | 32:2a:630:G:O4' | 2.14 | 0.47 |
| 32:2a:1186:G:O3' | 40:2i:113:LYS:NZ | 2.36 | 0.47 |
| 32:2a:1272:G:N2 | 32:2a:1273:G:C8 | 2.81 | 0.47 |
| 54:2x:8:4SU:O5' | 54:2x:8:4SU:H6 | 2.14 | 0.47 |
| 1:1A:174:C:H2' | 1:1A:175:G:O4' | 2.14 | 0.47 |
| 1:1A:300:A:OP1 | 20:1Y:86:ARG:NH2 | 2.44 | 0.47 |
| 1:1A:1371:G:H2' | 1:1A:1372:U:H5 | 1.79 | 0.47 |
| 1:1A:2279:G:O6 | 22:10:14:ARG:HG3 | 2.15 | 0.47 |
| 5:1F:13:SER:OG | 5:1F:127:GLU:OE1 | 2.32 | 0.47 |
| 6:1G:3:LEU:O | 6:1G:8:LYS:NZ | 2.41 | 0.47 |
| 6:1G:103:LEU:HD23 | 6:1G:106:LEU:HD23 | 1.97 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:1G:111:LEU:HD22 | 6:1G:120:LEU:HD21 | 1.96 | 0.47 |
| 12:1Q:16:ARG:HG2 | 12:1Q:18:LYS:HE2 | 1.97 | 0.47 |
| 13:1R:9:LYS:O | 13:1R:17:ARG:NH1 | 2.46 | 0.47 |
| 13:1R:14:SER:OG | 13:1R:15:SER:N | 2.47 | 0.47 |
| 13:1R:28:LEU:HD23 | 13:1R:48:VAL:HG21 | 1.95 | 0.47 |
| 26:14:44:THR:O | 26:14:46:GLN:N | 2.48 | 0.47 |
| 32:1a:316:G:OP2 | 32:1a:351:G:O2' | 2.30 | 0.47 |
| 32:1a:1442:G:O2' | 32:1a:1442(A):G:H5' | 2.14 | 0.47 |
| 33:1b:21:ARG:C | 33:1b:23:ARG:H | 2.23 | 0.47 |
| 44:1m:15:VAL:HG11 | 44:1m:48:LEU:HD21 | 1.95 | 0.47 |
| 45:1n:48:ALA:HB2 | 45:1n:53:LEU:HD12 | 1.96 | 0.47 |
| 47:1p:49:LEU:HD11 | 47:1p:73:LEU:HB3 | 1.95 | 0.47 |
| 1:2A:69:C:N4 | 59:2A:4001:HOH:O | 2.47 | 0.47 |
| 1:2A:195:A:H2' | 1:2A:198:C:N4 | 2.28 | 0.47 |
| 1:2A:608:A:H2' | 1:2A:609:A:O4' | 2.14 | 0.47 |
| 1:2A:1580:A:H3' | 1:2A:1581:G:C8 | 2.49 | 0.47 |
| 1:2A:2261:C:C6 | 22:20:16:SER:HB3 | 2.49 | 0.47 |
| 1:2A:2687:U:H2' | 1:2A:2688:U:O4' | 2.15 | 0.47 |
| 1:2A:2850:A:H2 | 13:2R:61:HIS:CG | 2.32 | 0.47 |
| 6:2G:50:ALA:O | 6:2G:52:ILE:N | 2.48 | 0.47 |
| 14:2S:38:GLN:NE2 | 14:2S:47:THR:OG1 | 2.25 | 0.47 |
| 32:2a:34:C:H2' | 32:2a:35:G:H8 | 1.76 | 0.47 |
| 32:2a:933:G:N2 | 32:2a:935:A:O4' | 2.47 | 0.47 |
| 32:2a:957:U:H2' | 32:2a:959:A:OP2 | 2.14 | 0.47 |
| 32:2a:967:5MC:H2' | 32:2a:968:A:C8 | 2.49 | 0.47 |
| 35:2d:57:ARG:N | 35:2d:57:ARG:HD2 | 2.30 | 0.47 |
| 40:2i:108:VAL:HG22 | 40:2i:109:VAL:H | 1.80 | 0.47 |
| 1:1A:700:G:H2' | 1:1A:701:G:O4' | 2.15 | 0.47 |
| 1:1A:795:C:H2' | 1:1A:796:C:C6 | 2.49 | 0.47 |
| 1:1A:820:A:H1' | 1:1A:943:U:H1' | 1.96 | 0.47 |
| 1:1A:1268:A:C2 | 1:1A:2013:A:C4 | 3.03 | 0.47 |
| 1:1A:2097:C:H2' | 1:1A:2098:U:C6 | 2.50 | 0.47 |
| 7:1H:83:TYR:CE2 | 7:1H:138:LYS:HB2 | 2.50 | 0.47 |
| 15:1T:27:THR:HB | 15:1T:90:GLN:HB3 | 1.96 | 0.47 |
| 28:16:38:LYS:HB2 | 28:16:49:HIS:CD2 | 2.49 | 0.47 |
| 32:1a:437:U:H5' | 35:1d:155:LEU:HD11 | 1.97 | 0.47 |
| 1:2A:10:G:H1' | 1:2A:2801(A):A:N7 | 2.29 | 0.47 |
| 1:2A:55:G:H2' | 1:2A:56:A:C8 | 2.49 | 0.47 |
| 1:2A:271(H):G:H2' | 1:2A:271(I):G:C8 | 2.49 | 0.47 |
| 1:2A:302:C:H42 | 1:2A:315:G:H1 | 1.63 | 0.47 |
| 1:2A:1027:A:C6 | 1:2A:1126:A:C4 | 3.03 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:2A:1341:U:OP1 | 1:2A:1397:U:N3 | 2.43 | 0.47 |
| 1:2A:1607:C:H5" | 1:2A:1608:A:H5' | 1.97 | 0.47 |
| 1:2A:1794:U:H2' | 1:2A:1795:C:C6 | 2.50 | 0.47 |
| 1:2A:2050:C:N4 | 1:2A:2051:A:C6 | 2.83 | 0.47 |
| 1:2A:2427:C:H5" | 1:2A:2428:G:OP1 | 2.14 | 0.47 |
| 1:2A:2785:C:O2' | 4:2E:66:HIS:ND1 | 2.46 | 0.47 |
| 6:2G:63:ILE:HD13 | 6:2G:143:GLU:HB2 | 1.96 | 0.47 |
| 10:2O:122:LEU:HD13 | 15:2T:72:VAL:HG11 | 1.95 | 0.47 |
| 15:2T:26:ASP:O | 15:2T:49:VAL:HG22 | 2.14 | 0.47 |
| 15:2T:65:LYS:HE3 | 15:2T:67:SER:HB2 | 1.95 | 0.47 |
| 32:2a:728:A:N7 | 46:2o:54:ARG:HD3 | 2.30 | 0.47 |
| 35:2d:176:LEU:HG | 35:2d:178:VAL:HG22 | 1.96 | 0.47 |
| 39:2h:6:ILE:O | 39:2h:10:LEU:HG | 2.14 | 0.47 |
| 54:2x:58:A:H4' | 54:2x:59:A:OP1 | 2.13 | 0.47 |
| 1:1A:566:U:H5" | 11:1P:29:LYS:HE3 | 1.96 | 0.47 |
| 1:1A:662:G:H5" | 11:1P:16:ARG:HG2 | 1.97 | 0.47 |
| 13:1R:26:LYS:HE2 | 13:1R:70:LEU:O | 2.15 | 0.47 |
| 18:1W:35:ILE:O | 18:1W:39:THR:OG1 | 2.28 | 0.47 |
| 30:18:8:LYS:O | 30:18:12:LYS:HG3 | 2.15 | 0.47 |
| 33:1b:71:VAL:HA | 33:1b:93:VAL:HG22 | 1.96 | 0.47 |
| 54:1x:19:G:H4' | 54:1x:20:U:OP2 | 2.15 | 0.47 |
| 1:2A:996:A:H4' | 16:2U:91:ASP:OD2 | 2.13 | 0.47 |
| 1:2A:1196:C:H2' | 1:2A:1197:G:C8 | 2.49 | 0.47 |
| 1:2A:2330:G:H2' | 1:2A:2331:G:O4' | 2.14 | 0.47 |
| 11:2P:59:LEU:HD23 | 11:2P:60:MET:HE2 | 1.96 | 0.47 |
| 21:2Z:24:LEU:HD12 | 21:2Z:25:PRO:HD2 | 1.96 | 0.47 |
| 32:2a:1118:C:H1' | 32:2a:1179:A:C5 | 2.48 | 0.47 |
| 32:2a:1129:C:H2' | 32:2a:1139:G:N7 | 2.29 | 0.47 |
| 33:2b:24:TRP:CZ3 | 33:2b:26:PRO:HA | 2.49 | 0.47 |
| 33:2b:84:GLU:O | 33:2b:219:VAL:HG21 | 2.14 | 0.47 |
| 1:1A:414:C:H4' | 1:1A:1879:C:O2 | 2.15 | 0.47 |
| 1:1A:1074:G:N1 | 1:1A:1075:C:H1' | 2.29 | 0.47 |
| 1:1A:1427:A:H4' | 1:1A:1428:C:O4' | 2.14 | 0.47 |
| 1:1A:1495:A:H2' | 1:1A:1496:A:C8 | 2.48 | 0.47 |
| 1:1A:1926:U:O2' | 1:1A:1928:A:N7 | 2.46 | 0.47 |
| 1:1A:2291:U:H2' | 1:1A:2292:C:C6 | 2.50 | 0.47 |
| 5:1F:95:ARG:HD3 | 5:1F:97:TYR:CZ | 2.49 | 0.47 |
| 8:1I:27:ARG:HD3 | 23:11:71:TYR:CE2 | 2.50 | 0.47 |
| 32:1a:189(B):C:H2' | 32:1a:189(C):C:C6 | 2.50 | 0.47 |
| 32:1a:288:A:H2' | 32:1a:289:G:H4' | 1.97 | 0.47 |
| 32:1a:412:A:C6 | 35:1d:35:ARG:HG2 | 2.49 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 32:1a:414:A:H2' | 32:1a:415:A:H8 | 1.78 | 0.47 |
| 32:1a:444:C:H2' | 32:1a:445:G:H8 | 1.79 | 0.47 |
| 32:1a:711:G:OP1 | 37:1f:54:LYS:NZ | 2.40 | 0.47 |
| 32:1a:1008:C:N3 | 32:1a:1021:G:C6 | 2.81 | 0.47 |
| 32:1a:1112:C:H1' | 34:1c:179:ARG:HG2 | 1.96 | 0.47 |
| 32:1a:1149:C:H2' | 32:1a:1150:U:H6 | 1.79 | 0.47 |
| 32:1a:1315:U:H2' | 32:1a:1316:G:O4' | 2.14 | 0.47 |
| 32:1a:1343:G:H4' | 40:1i:122:ALA:HB3 | 1.96 | 0.47 |
| 33:1b:208:ILE:HA | 33:1b:211:ILE:HG13 | 1.97 | 0.47 |
| 34:1c:134:ILE:O | 34:1c:138:VAL:HG23 | 2.15 | 0.47 |
| 37:1f:27:GLN:HA | 37:1f:30:LEU:HD12 | 1.95 | 0.47 |
| 41:1j:15:THR:O | 41:1j:19:SER:OG | 2.25 | 0.47 |
| 41:1j:42:THR:HG21 | 41:1j:66:ARG:HH11 | 1.79 | 0.47 |
| 43:1l:7:ILE:HA | 43:1l:10:LEU:HD12 | 1.97 | 0.47 |
| 51:1t:10:LEU:HD12 | 51:1t:12:ALA:H | 1.80 | 0.47 |
| 1:2A:656:G:H2' | 1:2A:657:U:O4' | 2.15 | 0.47 |
| 1:2A:763:G:H1' | 1:2A:765:G:O4' | 2.15 | 0.47 |
| 1:2A:992:C:OP1 | 16:2U:47:TYR:OH | 2.24 | 0.47 |
| 1:2A:1011:G:OP2 | 16:2U:66:ASN:ND2 | 2.48 | 0.47 |
| 1:2A:1376:C:OP1 | 59:2A:3963:HOH:O | 2.20 | 0.47 |
| 1:2A:1428:C:N4 | 1:2A:1570:A:OP2 | 2.44 | 0.47 |
| 1:2A:1486:A:H2' | 1:2A:1487:G:C8 | 2.49 | 0.47 |
| 1:2A:1550:C:H2' | 1:2A:1551:C:H6 | 1.79 | 0.47 |
| 1:2A:1671:U:O2' | 1:2A:1673:U:H5 | 1.98 | 0.47 |
| 1:2A:1817:G:OP1 | 3:2D:88:ARG:NH2 | 2.45 | 0.47 |
| 1:2A:2466:C:H5" | 31:29:6:SER:HB2 | 1.95 | 0.47 |
| 1:2A:2601:C:H2' | 1:2A:2603:G:C8 | 2.50 | 0.47 |
| 2:2B:25:A:H2' | 2:2B:26:A:C8 | 2.50 | 0.47 |
| 2:2B:90:A:C5 | 2:2B:91:C:H1' | 2.50 | 0.47 |
| 4:2E:174:ASP:OD1 | 4:2E:175:VAL:N | 2.44 | 0.47 |
| 8:2I:73:GLU:HG2 | 8:2I:73:GLU:O | 2.15 | 0.47 |
| 10:2O:15:GLY:O | 10:2O:47:ILE:HG12 | 2.15 | 0.47 |
| 12:2Q:54:MET:HB3 | 12:2Q:117:ALA:HB1 | 1.95 | 0.47 |
| 16:2U:86:ALA:O | 17:2V:49:THR:HG23 | 2.14 | 0.47 |
| 18:2W:17:VAL:HG11 | 18:2W:103:ILE:HD11 | 1.96 | 0.47 |
| 19:2X:2:LYS:NZ | 19:2X:38:GLU:OE2 | 2.38 | 0.47 |
| 26:24:50:VAL:HG11 | 44:2m:65:LYS:HG3 | 1.97 | 0.47 |
| 32:2a:223:U:H2' | 32:2a:224:C:H6 | 1.79 | 0.47 |
| 32:2a:352:C:H4' | 32:2a:354:G:OP1 | 2.15 | 0.47 |
| 32:2a:406:G:H21 | 35:2d:119:GLN:NE2 | 2.12 | 0.47 |
| 32:2a:449:C:H3' | 32:2a:450:G:C8 | 2.50 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 32:2a:458:C:H2' | 32:2a:460:G:O4' | 2.15 | 0.47 |
| 32:2a:707:C:H2' | 32:2a:708:C:H6 | 1.77 | 0.47 |
| 32:2a:936:C:H2' | 32:2a:937:A:O4' | 2.14 | 0.47 |
| 32:2a:980:C:H3' | 32:2a:981:U:C6 | 2.50 | 0.47 |
| 32:2a:1100:C:H2' | 32:2a:1102:A:O5' | 2.15 | 0.47 |
| 32:2a:1151:A:O2' | 32:2a:1152:A:H8 | 1.97 | 0.47 |
| 32:2a:1174:G:N7 | 59:2a:3317:HOH:O | 2.35 | 0.47 |
| 32:2a:1518:MA6:H93 | 32:2a:1519:MA6:H92 | 1.96 | 0.47 |
| 35:2d:64:LEU:HB2 | 35:2d:198:VAL:HG21 | 1.96 | 0.47 |
| 38:2g:70:LYS:HD2 | 38:2g:96:GLN:HB3 | 1.97 | 0.47 |
| 38:2g:108:ALA:HA | 38:2g:111:ARG:HD2 | 1.97 | 0.47 |
| 38:2g:153:HIS:CE1 | 42:2k:57:THR:HB | 2.49 | 0.47 |
| 39:2h:29:SER:HB3 | 39:2h:32:LYS:HG3 | 1.96 | 0.47 |
| 44:2m:60:VAL:HG22 | 44:2m:64:TRP:HZ3 | 1.79 | 0.47 |
| 47:2p:42:ARG:HB3 | 47:2p:44:THR:HG23 | 1.96 | 0.47 |
| 1:1A:443:A:H1' | 1:1A:1201:C:O4' | 2.14 | 0.47 |
| 1:1A:631:A:H2' | 1:1A:632:A:O4' | 2.15 | 0.47 |
| 1:1A:657:U:H2' | 1:1A:658:C:C6 | 2.50 | 0.47 |
| 1:1A:721:C:H2' | 1:1A:722:A:C8 | 2.50 | 0.47 |
| 1:1A:1441:G:H2' | 1:1A:1442:G:H8 | 1.80 | 0.47 |
| 1:1A:1829:A:N3 | 3:1D:15:PHE:HZ | 2.13 | 0.47 |
| 1:1A:1935:G:H1' | 1:1A:1964:G:N2 | 2.29 | 0.47 |
| 2:1B:17:C:H2' | 2:1B:18:G:O4' | 2.15 | 0.47 |
| 2:1B:48:A:H4' | 14:1S:95:HIS:HD2 | 1.80 | 0.47 |
| 20:1Y:6:HIS:H | 20:1Y:6:HIS:CD2 | 2.32 | 0.47 |
| 24:12:14:ARG:O | 24:12:67:LYS:NZ | 2.43 | 0.47 |
| 26:14:8:LYS:HE2 | 26:14:8:LYS:HB3 | 1.64 | 0.47 |
| 32:1a:277:C:H5" | 48:1q:68:ARG:NH2 | 2.29 | 0.47 |
| 33:1b:109:SER:O | 33:1b:112:VAL:HG22 | 2.15 | 0.47 |
| 43:1l:77:LEU:HD21 | 43:1l:107:ALA:HB2 | 1.96 | 0.47 |
| 1:2A:705:A:H1' | 3:2D:9:TYR:CE2 | 2.50 | 0.47 |
| 3:2D:108:PRO:HB3 | 3:2D:143:HIS:HE1 | 1.79 | 0.47 |
| 11:2P:138:LEU:HD23 | 11:2P:145:PRO:HB3 | 1.97 | 0.47 |
| 13:2R:50:HIS:O | 13:2R:54:LEU:HG | 2.15 | 0.47 |
| 15:2T:31:SER:OG | 15:2T:44:ASP:OD1 | 2.21 | 0.47 |
| 32:2a:45:U:OP1 | 32:2a:307:C:O2' | 2.28 | 0.47 |
| 32:2a:114:U:H2' | 32:2a:115:G:C8 | 2.50 | 0.47 |
| 32:2a:519:C:H2' | 32:2a:520:A:O4' | 2.15 | 0.47 |
| 32:2a:1370:G:C8 | 40:2i:109:VAL:HG11 | 2.50 | 0.47 |
| 32:2a:1401:G:C2 | 32:2a:1402:4OC:H1' | 2.50 | 0.47 |
| 40:2i:3:GLN:HE21 | 40:2i:20:ARG:HH21 | 1.63 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:2i:21:PRO:HA | 40:2i:59:PHE:HA | 1.97 | 0.47 |
| 1:1A:628:G:H2' | 1:1A:629:G:H8 | 1.78 | 0.47 |
| 1:1A:644:A:H4' | 1:1A:645:C:H5 | 1.80 | 0.47 |
| 1:1A:686:G:N2 | 1:1A:788:A:H61 | 2.13 | 0.47 |
| 1:1A:2017:U:O2 | 27:15:10:LYS:HB2 | 2.15 | 0.47 |
| 1:1A:2633:G:H2' | 1:1A:2634:G:O4' | 2.15 | 0.47 |
| 1:1A:2771:C:H2' | 1:1A:2772:C:C6 | 2.49 | 0.47 |
| 4:1E:7:VAL:HG23 | 4:1E:51:PHE:CE2 | 2.50 | 0.47 |
| 6:1G:25:TYR:CZ | 6:1G:32:PRO:HD3 | 2.50 | 0.47 |
| 7:1H:7:LEU:HD12 | 7:1H:8:PRO:HD2 | 1.97 | 0.47 |
| 14:1S:15:ARG:HE | 14:1S:88:ASP:CG | 2.20 | 0.47 |
| 32:1a:135:C:O2 | 47:1p:1:MET:N | 2.48 | 0.47 |
| 32:1a:219:C:H2' | 32:1a:220:G:O4' | 2.15 | 0.47 |
| 32:1a:263:A:OP1 | 51:1t:79:ARG:NH1 | 2.48 | 0.47 |
| 32:1a:436:C:H2' | 32:1a:437:U:O4' | 2.15 | 0.47 |
| 32:1a:487:A:C2 | 32:1a:488:C:H1' | 2.50 | 0.47 |
| 32:1a:676:A:H1' | 42:1k:115:PRO:HB3 | 1.96 | 0.47 |
| 32:1a:826:C:H4' | 39:1h:12:ARG:HD3 | 1.96 | 0.47 |
| 32:1a:938:A:C6 | 32:1a:939:G:C5 | 3.03 | 0.47 |
| 32:1a:1187:G:H2' | 32:1a:1188:A:C8 | 2.50 | 0.47 |
| 32:1a:1291:G:OP1 | 38:1g:37:ASN:ND2 | 2.48 | 0.47 |
| 32:1a:1349:A:OP1 | 40:1i:118:LYS:HB2 | 2.14 | 0.47 |
| 41:1j:64:GLU:HB3 | 45:1n:59:ALA:HB2 | 1.97 | 0.47 |
| 48:1q:67:LYS:HA | 48:1q:70:ARG:NH1 | 2.30 | 0.47 |
| 50:1s:31:ILE:HB | 50:1s:49:ILE:HG23 | 1.97 | 0.47 |
| 1:2A:196:A:N3 | 1:2A:196:A:H2' | 2.30 | 0.47 |
| 1:2A:395:U:O2' | 59:2A:3961:HOH:O | 2.20 | 0.47 |
| 1:2A:632:A:H2' | 1:2A:633:A:C8 | 2.50 | 0.47 |
| 1:2A:1580:A:H3' | 1:2A:1581:G:H8 | 1.80 | 0.47 |
| 1:2A:2247:A:H2' | 1:2A:2248:C:H6 | 1.80 | 0.47 |
| 6:2G:102:PHE:O | 6:2G:106:LEU:HB2 | 2.15 | 0.47 |
| 11:2P:6:LEU:HA | 11:2P:6:LEU:HD23 | 1.66 | 0.47 |
| 12:2Q:24:GLY:HA2 | 12:2Q:67:ARG:NH2 | 2.29 | 0.47 |
| 14:2S:36:TYR:OH | 14:2S:54:LEU:HD22 | 2.15 | 0.47 |
| 20:2Y:19:LYS:HE2 | 20:2Y:20:TYR:HE2 | 1.80 | 0.47 |
| 21:2Z:147:GLY:N | 21:2Z:174:VAL:O | 2.45 | 0.47 |
| 24:22:35:LEU:HD13 | 24:22:53:LEU:HD12 | 1.96 | 0.47 |
| 32:2a:19:C:H5" | 36:2e:86:ALA:HB1 | 1.97 | 0.47 |
| 32:2a:174:C:H2' | 32:2a:175:C:C6 | 2.50 | 0.47 |
| 32:2a:932:C:H2' | 32:2a:933:G:C8 | 2.49 | 0.47 |
| 42:2k:61:ALA:HB1 | 42:2k:94:ALA:HB2 | 1.97 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 44:2m:90:LEU:HA | 44:2m:93:ARG:HE | 1.80 | 0.47 |
| 48:2q:41:LYS:NZ | 48:2q:92:ARG:HH21 | 2.13 | 0.47 |
| 1:1A:234:C:H2' | 1:1A:235:U:H6 | 1.79 | 0.47 |
| 6:1G:56:ALA:HA | 6:1G:59:GLU:HG2 | 1.95 | 0.47 |
| 8:1I:94:ALA:H | 8:1I:116:LEU:HD22 | 1.79 | 0.47 |
| 32:1a:475:G:O2' | 32:1a:476:G:H5' | 2.15 | 0.47 |
| 32:1a:874:G:H21 | 39:1h:15:ASN:ND2 | 2.13 | 0.47 |
| 32:1a:1014:A:H4' | 50:1s:14:HIS:CE1 | 2.49 | 0.47 |
| 45:1n:15:LYS:HD2 | 45:1n:16:PHE:CE2 | 2.50 | 0.47 |
| 1:2A:607:U:OP1 | 5:2F:102:PRO:HA | 2.14 | 0.47 |
| 1:2A:637:A:C8 | 11:2P:117:GLU:HG3 | 2.42 | 0.47 |
| 1:2A:783:A:O2' | 1:2A:785:G:OP1 | 2.25 | 0.47 |
| 1:2A:955:C:OP1 | 12:2Q:87:LYS:HE3 | 2.15 | 0.47 |
| 1:2A:1221(A):C:C2 | 1:2A:1229:G:C2 | 3.03 | 0.47 |
| 1:2A:1252:G:OP2 | 16:2U:14:HIS:NE2 | 2.33 | 0.47 |
| 1:2A:1359:A:H2' | 1:2A:1360:A:H5' | 1.97 | 0.47 |
| 1:2A:1926:U:O2' | 1:2A:1928:A:N7 | 2.39 | 0.47 |
| 1:2A:2250:G:OP1 | 12:2Q:85:LYS:NZ | 2.48 | 0.47 |
| 1:2A:2530:A:O2' | 1:2A:2532:G:OP2 | 2.24 | 0.47 |
| 1:2A:2556:C:H2' | 1:2A:2557:G:O4' | 2.15 | 0.47 |
| 1:2A:2823:A:OP1 | 4:2E:113:PHE:HB2 | 2.14 | 0.47 |
| 3:2D:184:LYS:HE3 | 3:2D:271:ILE:HD11 | 1.97 | 0.47 |
| 6:2G:12:TYR:HA | 6:2G:16:ARG:HB2 | 1.97 | 0.47 |
| 11:2P:38:GLN:C | 11:2P:40:SER:H | 2.23 | 0.47 |
| 21:2Z:77:ASP:CG | 21:2Z:80:ARG:HH11 | 2.23 | 0.47 |
| 31:29:3:VAL:HA | 31:29:35:ARG:O | 2.15 | 0.47 |
| 32:2a:121:C:H4' | 32:2a:122:G:OP1 | 2.15 | 0.47 |
| 38:2g:62:PHE:O | 38:2g:66:VAL:HG12 | 2.14 | 0.47 |
| 41:2j:38:ILE:HD11 | 41:2j:71:LEU:HD23 | 1.97 | 0.47 |
| 1:1A:1027:A:C2 | 1:1A:2488:A:H5' | 2.50 | 0.46 |
| 1:1A:1056:G:H5" | 1:1A:1057:A:O4' | 2.15 | 0.46 |
| 1:1A:1862:G:H2' | 1:1A:1863:G:H8 | 1.80 | 0.46 |
| 1:1A:2487:G:OP2 | 59:1A:4293:HOH:O | 2.21 | 0.46 |
| 1:1A:2706:G:N7 | 59:1A:4412:HOH:O | 2.36 | 0.46 |
| 8:1I:5:LEU:HD13 | 8:1I:17:GLN:HB3 | 1.97 | 0.46 |
| 32:1a:1009:G:O6 | 32:1a:1020:U:C2 | 2.68 | 0.46 |
| 32:1a:1217:C:H5" | 45:1n:9:LYS:HE2 | 1.96 | 0.46 |
| 32:1a:1235:U:H2' | 32:1a:1236:A:O4' | 2.14 | 0.46 |
| 32:1a:1425:U:H2' | 32:1a:1426:C:C6 | 2.50 | 0.46 |
| 42:1k:23:ALA:O | 42:1k:86:GLY:HA3 | 2.15 | 0.46 |
| 1:2A:271(M):G:H4' | 1:2A:271(N):U:OP1 | 2.16 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:2A:271(P):C:H2' | 1:2A:271(Q):G:O4' | 2.15 | 0.46 |
| 1:2A:1636:C:H2' | 1:2A:1637:A:C8 | 2.49 | 0.46 |
| 1:2A:2552:2MU:H2' | 1:2A:2554:U:H5" | 1.97 | 0.46 |
| 2:2B:89:G:C6 | 2:2B:90:A:C6 | 3.03 | 0.46 |
| 6:2G:79:ASN:OD1 | 6:2G:79:ASN:N | 2.29 | 0.46 |
| 25:23:46:ASN:O | 25:23:50:VAL:HG22 | 2.14 | 0.46 |
| 32:2a:1274:G:H2' | 32:2a:1275:A:H5" | 1.96 | 0.46 |
| 38:2g:9:VAL:HG13 | 38:2g:94:ARG:HE | 1.80 | 0.46 |
| 1:1A:588:U:O4 | 1:1A:670:A:H1' | 2.15 | 0.46 |
| 1:1A:1866:C:H2' | 1:1A:1876:A:O4' | 2.15 | 0.46 |
| 1:1A:1882:C:H2' | 1:1A:1883:G:O4' | 2.15 | 0.46 |
| 1:1A:2074:U:H2' | 1:1A:2075:U:C6 | 2.50 | 0.46 |
| 10:1O:4:PRO:O | 10:1O:5:GLN:HB2 | 2.15 | 0.46 |
| 33:1b:126:GLU:O | 33:1b:127:ILE:HG23 | 2.15 | 0.46 |
| 34:1c:138:VAL:HG13 | 34:1c:149:ALA:HB3 | 1.96 | 0.46 |
| 38:1g:26:PHE:O | 38:1g:30:ILE:HG13 | 2.15 | 0.46 |
| 1:2A:224:G:O6 | 1:2A:420:C:H5' | 2.16 | 0.46 |
| 1:2A:307:G:N1 | 1:2A:310:A:OP2 | 2.47 | 0.46 |
| 1:2A:861:A:H2' | 1:2A:862:G:O4' | 2.14 | 0.46 |
| 1:2A:1412:A:H2' | 1:2A:1413:G:C8 | 2.50 | 0.46 |
| 1:2A:1428:C:O2' | 1:2A:1429:G:H5' | 2.15 | 0.46 |
| 1:2A:1557:C:OP2 | 1:2A:1558:A:O2' | 2.21 | 0.46 |
| 1:2A:1834:U:H4' | 1:2A:1969:A:C6 | 2.50 | 0.46 |
| 1:2A:2061:G:H5" | 1:2A:2503:2MA:C2 | 2.45 | 0.46 |
| 1:2A:2151:G:C2 | 1:2A:2152:G:C4 | 3.04 | 0.46 |
| 1:2A:2379:G:O2' | 14:2S:17:ARG:NH1 | 2.47 | 0.46 |
| 6:2G:16:ARG:HD2 | 6:2G:16:ARG:HA | 1.70 | 0.46 |
| 8:2I:75:LEU:HD12 | 8:2I:140:LEU:HD11 | 1.97 | 0.46 |
| 10:2O:87:ILE:HD12 | 10:2O:91:LEU:HA | 1.97 | 0.46 |
| 26:24:46:GLN:C | 26:24:48:ARG:H | 2.23 | 0.46 |
| 32:2a:1091:U:H2' | 32:2a:1093:A:OP2 | 2.15 | 0.46 |
| 1:1A:2743:C:H2' | 1:1A:2744:G:O4' | 2.15 | 0.46 |
| 6:1G:114:ILE:HG12 | 6:1G:140:ILE:HG12 | 1.96 | 0.46 |
| 8:1I:45:LYS:HB3 | 8:1I:45:LYS:HE2 | 1.75 | 0.46 |
| 9:1N:131:GLN:H | 9:1N:131:GLN:HG2 | 1.44 | 0.46 |
| 35:1d:60:GLU:HG3 | 35:1d:202:LEU:HD12 | 1.98 | 0.46 |
| 1:2A:251:A:C4 | 1:2A:252:G:H1' | 2.51 | 0.46 |
| 1:2A:307:G:H21 | 1:2A:330:A:H62 | 1.62 | 0.46 |
| 1:2A:489:G:N7 | 18:2W:49:LYS:NZ | 2.63 | 0.46 |
| 1:2A:500:G:C2 | 1:2A:503:A:C8 | 3.04 | 0.46 |
| 1:2A:1027:A:C2 | 1:2A:2488:A:H5' | 2.50 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:2A:1420:U:O2' | 1:2A:1421:G:OP1 | 2.29 | 0.46 |
| 1:2A:1702:G:H2' | 1:2A:1703:G:O4' | 2.16 | 0.46 |
| 1:2A:1777:U:H2' | 1:2A:1778:U:C6 | 2.50 | 0.46 |
| 1:2A:1936:A:OP2 | 1:2A:1962:5MC:N4 | 2.44 | 0.46 |
| 1:2A:2419:U:H2' | 1:2A:2420:C:C6 | 2.51 | 0.46 |
| 4:2E:170:LEU:HB3 | 4:2E:184:VAL:CG2 | 2.45 | 0.46 |
| 5:2F:65:TRP:CZ2 | 5:2F:75:HIS:HD2 | 2.34 | 0.46 |
| 8:2I:65:ALA:HA | 8:2I:68:LEU:HD12 | 1.97 | 0.46 |
| 32:2a:160:A:H1' | 32:2a:344:A:C8 | 2.50 | 0.46 |
| 32:2a:637:G:H2' | 32:2a:638:G:C8 | 2.50 | 0.46 |
| 33:2b:8:LYS:HD3 | 33:2b:51:LEU:HD13 | 1.98 | 0.46 |
| 34:2c:157:ILE:HD13 | 34:2c:164:ARG:HB3 | 1.96 | 0.46 |
| 35:2d:108:LEU:HD11 | 35:2d:174:LEU:HB3 | 1.96 | 0.46 |
| 43:2l:92:0TD:H4 | 43:2l:92:0TD:H8 | 1.78 | 0.46 |
| 1:1A:34:C:H5" | 1:1A:35:G:OP2 | 2.15 | 0.46 |
| 1:1A:142:A:O2' | 1:1A:1407:C:O2' | 2.32 | 0.46 |
| 1:1A:2123:G:N2 | 1:1A:2175:C:N3 | 2.55 | 0.46 |
| 4:1E:178:GLU:N | 4:1E:178:GLU:OE2 | 2.47 | 0.46 |
| 10:1O:35:VAL:HA | 10:1O:62:VAL:HG12 | 1.97 | 0.46 |
| 12:1Q:2:LEU:HD23 | 12:1Q:2:LEU:HA | 1.74 | 0.46 |
| 32:1a:812:C:OP1 | 32:1a:903:G:H1' | 2.15 | 0.46 |
| 32:1a:1257:U:O4 | 45:1n:17:LYS:NZ | 2.46 | 0.46 |
| 32:1a:1273:G:H3' | 32:1a:1274:G:C8 | 2.50 | 0.46 |
| 33:1b:18:GLY:HA3 | 33:1b:42:ILE:HG13 | 1.98 | 0.46 |
| 37:1f:72:VAL:CG1 | 37:1f:90:VAL:HG11 | 2.45 | 0.46 |
| 40:1i:17:VAL:HG23 | 40:1i:63:ILE:HG12 | 1.97 | 0.46 |
| 51:1t:16:HIS:O | 51:1t:19:SER:OG | 2.27 | 0.46 |
| 51:1t:45:GLN:HG2 | 51:1t:91:LEU:HG | 1.97 | 0.46 |
| 1:2A:1410:G:H2' | 1:2A:1411:C:C6 | 2.50 | 0.46 |
| 1:2A:2579:C:H2' | 1:2A:2580:U:O4' | 2.16 | 0.46 |
| 1:2A:2820:A:O2' | 1:2A:2821:A:OP1 | 2.31 | 0.46 |
| 5:2F:167:ALA:HB1 | 5:2F:173:VAL:HG11 | 1.97 | 0.46 |
| 15:2T:107:ASP:O | 15:2T:111:ARG:HG3 | 2.14 | 0.46 |
| 32:2a:130:A:N3 | 32:2a:263:A:O2' | 2.42 | 0.46 |
| 32:2a:1226:C:O2' | 44:2m:111:LYS:NZ | 2.29 | 0.46 |
| 32:2a:1400:5MC:N4 | 54:2x:34:C:H1' | 2.31 | 0.46 |
| 34:2c:135:LYS:HZ3 | 36:2e:52:PRO:HG2 | 1.79 | 0.46 |
| 38:2g:116:ALA:O | 38:2g:120:ILE:HG13 | 2.16 | 0.46 |
| 46:2o:39:LEU:HD23 | 46:2o:39:LEU:HA | 1.70 | 0.46 |
| 48:2q:25:ARG:HG2 | 48:2q:38:ARG:O | 2.15 | 0.46 |
| 1:1A:153:C:H2' | 1:1A:154:G:C8 | 2.50 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1A:515:A:H1' | 1:1A:581:C:H1' | 1.98 | 0.46 |
| 1:1A:818:G:H4' | 1:1A:838:C:O3' | 2.16 | 0.46 |
| 1:1A:1242:A:N1 | 11:1P:4:SER:OG | 2.49 | 0.46 |
| 1:1A:1826:G:H2' | 1:1A:1827:C:O4' | 2.16 | 0.46 |
| 1:1A:2101:G:H2' | 1:1A:2102:U:C6 | 2.50 | 0.46 |
| 1:1A:2147:G:H3' | 1:1A:2147:G:N3 | 2.31 | 0.46 |
| 2:1B:90:A:C5 | 2:1B:91:C:H1' | 2.50 | 0.46 |
| 6:1G:124:SER:HB3 | 6:1G:132:ASN:O | 2.15 | 0.46 |
| 32:1a:42:G:O2' | 32:1a:622:A:N1 | 2.48 | 0.46 |
| 32:1a:399:G:H2' | 32:1a:400:C:C6 | 2.50 | 0.46 |
| 32:1a:713:G:H2' | 32:1a:714:G:C8 | 2.51 | 0.46 |
| 39:1h:38:ILE:HG23 | 39:1h:120:THR:HG22 | 1.98 | 0.46 |
| 1:2A:937:U:H2' | 1:2A:938:G:O4' | 2.16 | 0.46 |
| 1:2A:1011:G:OP1 | 16:2U:77:SER:OG | 2.22 | 0.46 |
| 1:2A:1291:C:H2' | 1:2A:1292:U:H6 | 1.80 | 0.46 |
| 1:2A:2262:U:H4' | 1:2A:2328:A:C2 | 2.50 | 0.46 |
| 5:2F:192:LEU:HD21 | 5:2F:194:MET:HE2 | 1.97 | 0.46 |
| 6:2G:73:ALA:HB3 | 6:2G:85:GLY:N | 2.24 | 0.46 |
| 8:2I:45:LYS:HE2 | 8:2I:45:LYS:HB3 | 1.57 | 0.46 |
| 10:2O:48:PRO:CB | 32:2a:1422:G:H5" | 2.39 | 0.46 |
| 13:2R:13:HIS:CE1 | 13:2R:16:HIS:HB2 | 2.50 | 0.46 |
| 21:2Z:3:TYR:CD2 | 21:2Z:51:ALA:HB2 | 2.50 | 0.46 |
| 21:2Z:5:LEU:HD12 | 21:2Z:47:VAL:HB | 1.97 | 0.46 |
| 32:2a:237:C:H5" | 48:2q:25:ARG:CZ | 2.46 | 0.46 |
| 32:2a:1118:C:N3 | 32:2a:1156:G:N2 | 2.63 | 0.46 |
| 32:2a:1238:A:N7 | 32:2a:1303:C:H1' | 2.30 | 0.46 |
| 33:2b:208:ILE:C | 33:2b:210:SER:H | 2.23 | 0.46 |
| 36:2e:102:ALA:HB2 | 36:2e:120:THR:HG21 | 1.96 | 0.46 |
| 38:2g:74:GLU:HG2 | 38:2g:91:VAL:HG22 | 1.98 | 0.46 |
| 38:2g:152:ALA:O | 38:2g:155:ARG:HD3 | 2.15 | 0.46 |
| 44:2m:13:LYS:O | 44:2m:45:VAL:HG23 | 2.14 | 0.46 |
| 47:2p:28:ARG:HG2 | 47:2p:29:ASP:OD1 | 2.16 | 0.46 |
| 1:1A:469:G:O6 | 29:17:37:LYS:HE2 | 2.16 | 0.46 |
| 1:1A:1094:U:H2' | 1:1A:1095:A:C8 | 2.50 | 0.46 |
| 1:1A:1999:C:H4' | 1:1A:2723:C:O2 | 2.15 | 0.46 |
| 3:1D:184:LYS:HE3 | 3:1D:271:ILE:HD11 | 1.98 | 0.46 |
| 5:1F:17:ARG:NH2 | 5:1F:19:GLU:OE2 | 2.48 | 0.46 |
| 21:1Z:11:GLU:O | 21:1Z:36:LYS:NZ | 2.28 | 0.46 |
| 32:1a:114:U:H1' | 32:1a:353:A:H1' | 1.98 | 0.46 |
| 32:1a:1429:C:H2' | 32:1a:1430:C:H6 | 1.80 | 0.46 |
| 33:1b:77:ALA:HB2 | 33:1b:211:ILE:HG21 | 1.96 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 33:1b:124:SER:HA | 33:1b:125:PRO:HA | 1.64 | 0.46 |
| 43:1l:53:ARG:HB3 | 43:1l:69:TYR:HE1 | 1.80 | 0.46 |
| 1:2A:588:U:H1' | 5:2F:90:PHE:CG | 2.51 | 0.46 |
| 1:2A:1952:A:OP1 | 10:2O:42:SER:OG | 2.31 | 0.46 |
| 1:2A:2647:U:H2' | 1:2A:2648:C:C6 | 2.50 | 0.46 |
| 4:2E:3:GLY:HA3 | 4:2E:81:ILE:HG21 | 1.98 | 0.46 |
| 8:2I:126:TYR:CD2 | 8:2I:142:VAL:HB | 2.51 | 0.46 |
| 9:2N:15:LEU:HB2 | 9:2N:135:PRO:HB2 | 1.97 | 0.46 |
| 18:2W:71:VAL:HA | 18:2W:107:LEU:HD12 | 1.97 | 0.46 |
| 32:2a:189(C):C:H2' | 32:2a:189(D):C:O4' | 2.15 | 0.46 |
| 32:2a:728:A:H2' | 32:2a:729:A:H8 | 1.79 | 0.46 |
| 32:2a:814:A:H2' | 32:2a:816:A:H5" | 1.98 | 0.46 |
| 32:2a:1046:A:H3' | 32:2a:1047:G:H8 | 1.80 | 0.46 |
| 32:2a:1179:A:H4' | 40:2i:103:THR:HA | 1.98 | 0.46 |
| 33:2b:134:GLU:O | 33:2b:138:LEU:HG | 2.15 | 0.46 |
| 36:2e:42:GLY:HA2 | 36:2e:65:ASN:O | 2.15 | 0.46 |
| 36:2e:146:ALA:O | 36:2e:150:ARG:HG2 | 2.16 | 0.46 |
| 47:2p:2:VAL:O | 47:2p:64:ALA:HA | 2.16 | 0.46 |
| 1:1A:253:C:OP2 | 30:18:5:LYS:NZ | 2.41 | 0.46 |
| 1:1A:667:U:O2 | 30:18:2:PRO:HD2 | 2.15 | 0.46 |
| 1:1A:1670:C:O2 | 4:1E:129:HIS:NE2 | 2.39 | 0.46 |
| 1:1A:1939:5MU:OP1 | 1:1A:2604:U:O2' | 2.32 | 0.46 |
| 6:1G:37:VAL:HG22 | 6:1G:159:VAL:HG13 | 1.98 | 0.46 |
| 8:1I:109:ILE:HD12 | 8:1I:109:ILE:HA | 1.72 | 0.46 |
| 11:1P:47:ASP:OD2 | 11:1P:49:ARG:NH2 | 2.48 | 0.46 |
| 11:1P:112:LEU:HD21 | 11:1P:114:ILE:HD11 | 1.97 | 0.46 |
| 12:1Q:17:LEU:HD21 | 12:1Q:41:TRP:HE1 | 1.80 | 0.46 |
| 12:1Q:137:TYR:O | 12:1Q:141:GLN:HG2 | 2.16 | 0.46 |
| 14:1S:61:ASN:HD21 | 14:1S:63:THR:HB | 1.79 | 0.46 |
| 32:1a:262:A:C6 | 32:1a:263:A:C6 | 3.03 | 0.46 |
| 38:1g:13:GLN:O | 38:1g:24:THR:HG21 | 2.15 | 0.46 |
| 41:1j:38:ILE:H | 41:1j:38:ILE:HG12 | 1.48 | 0.46 |
| 42:1k:30:VAL:HG21 | 42:1k:65:ALA:HA | 1.98 | 0.46 |
| 43:1l:101:VAL:O | 43:1l:104:VAL:HG22 | 2.16 | 0.46 |
| 46:1o:4:THR:HG23 | 46:1o:7:GLU:HG2 | 1.97 | 0.46 |
| 54:1x:25:C:H2' | 54:1x:26:G:O4' | 2.16 | 0.46 |
| 1:2A:184:C:O2' | 1:2A:217:G:N3 | 2.46 | 0.46 |
| 1:2A:1292:U:H2' | 1:2A:1293:C:C6 | 2.51 | 0.46 |
| 1:2A:1952:A:N6 | 1:2A:1953:A:N1 | 2.63 | 0.46 |
| 1:2A:2401:U:OP1 | 28:26:18:ARG:NH2 | 2.42 | 0.46 |
| 1:2A:2853:C:H2' | 1:2A:2854:G:C8 | 2.51 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:2B:7:G:H21 | 14:2S:38:GLN:NE2 | 2.13 | 0.46 |
| 22:20:69:PHE:CE2 | 22:20:79:VAL:HG22 | 2.50 | 0.46 |
| 26:24:15:ILE:HD13 | 26:24:21:VAL:HG23 | 1.98 | 0.46 |
| 32:2a:445:G:H2' | 32:2a:446:G:C8 | 2.50 | 0.46 |
| 32:2a:620:C:C2 | 35:2d:135:LEU:HG | 2.51 | 0.46 |
| 32:2a:1010:G:N2 | 32:2a:1020:U:O2' | 2.49 | 0.46 |
| 32:2a:1269:A:C8 | 32:2a:1270:C:H1' | 2.50 | 0.46 |
| 34:2c:125:GLU:O | 34:2c:190:ARG:NH1 | 2.46 | 0.46 |
| 36:2e:95:ALA:O | 36:2e:98:THR:HG23 | 2.15 | 0.46 |
| 36:2e:152:ARG:HG2 | 39:2h:42:GLU:O | 2.15 | 0.46 |
| 37:2f:33:TYR:CE2 | 37:2f:78:GLU:HG3 | 2.51 | 0.46 |
| 37:2f:89:MET:HG3 | 37:2f:90:VAL:N | 2.30 | 0.46 |
| 39:2h:123:GLU:H | 39:2h:123:GLU:HG2 | 1.56 | 0.46 |
| 42:2k:21:ILE:HB | 42:2k:84:VAL:HG12 | 1.97 | 0.46 |
| 1:1A:26:G:C6 | 1:1A:27:G:N1 | 2.84 | 0.46 |
| 1:1A:581:C:H2' | 1:1A:582:G:C8 | 2.50 | 0.46 |
| 1:1A:911:A:H2' | 12:1Q:9:TYR:OH | 2.16 | 0.46 |
| 1:1A:1062:G:H5" | 1:1A:1070:A:C1' | 2.46 | 0.46 |
| 1:1A:2114:A:C2 | 1:1A:2168:G:H1' | 2.51 | 0.46 |
| 1:1A:2693:A:H2' | 1:1A:2694:G:H8 | 1.81 | 0.46 |
| 2:1B:11:C:H3' | 2:1B:12:C:H6 | 1.81 | 0.46 |
| 30:18:4:MET:HE3 | 30:18:63:PRO:HG3 | 1.98 | 0.46 |
| 32:1a:392:G:H2' | 32:1a:393:A:C8 | 2.50 | 0.46 |
| 32:1a:737:A:H2' | 32:1a:738:C:C6 | 2.50 | 0.46 |
| 32:1a:858:G:O6 | 32:1a:869:G:H3' | 2.16 | 0.46 |
| 44:1m:11:ARG:HA | 44:1m:45:VAL:HB | 1.98 | 0.46 |
| 1:2A:57:C:H2' | 1:2A:58:G:O4' | 2.16 | 0.46 |
| 1:2A:1005:C:H2' | 1:2A:1006:C:C6 | 2.50 | 0.46 |
| 1:2A:1264:G:H2' | 1:2A:2014:A:N6 | 2.30 | 0.46 |
| 1:2A:1355:G:C6 | 1:2A:1356:G:C5 | 3.04 | 0.46 |
| 1:2A:1399:C:H2' | 1:2A:1400:G:H8 | 1.81 | 0.46 |
| 1:2A:1987:G:H2' | 1:2A:1988:C:C6 | 2.50 | 0.46 |
| 1:2A:2839:G:C5' | 13:2R:46:GLY:HA2 | 2.45 | 0.46 |
| 2:2B:11:C:OP2 | 2:2B:12:C:N4 | 2.36 | 0.46 |
| 4:2E:25:VAL:HG21 | 15:2T:10:VAL:HG21 | 1.97 | 0.46 |
| 6:2G:31:VAL:O | 6:2G:33:ARG:NH1 | 2.48 | 0.46 |
| 9:2N:34:LEU:HD12 | 9:2N:107:LEU:HD21 | 1.97 | 0.46 |
| 9:2N:91:LEU:HG | 9:2N:98:VAL:HG21 | 1.97 | 0.46 |
| 23:21:80:LEU:HD23 | 23:21:82:LEU:HD21 | 1.97 | 0.46 |
| 26:24:48:ARG:NH1 | 26:24:51:ASP:O | 2.49 | 0.46 |
| 32:2a:427:U:H3' | 32:2a:428:G:H2' | 1.98 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 32:2a:859:A:H2' | 32:2a:860:A:O4' | 2.16 | 0.46 |
| 32:2a:997:U:H3 | 32:2a:1044:A:H61 | 1.62 | 0.46 |
| 32:2a:1005:A:H5" | 32:2a:1006:C:C5 | 2.51 | 0.46 |
| 32:2a:1176:A:H2' | 32:2a:1177:G:H8 | 1.78 | 0.46 |
| 34:2c:6:HIS:HB3 | 45:2n:49:HIS:ND1 | 2.31 | 0.46 |
| 35:2d:92:VAL:O | 35:2d:96:LEU:HG | 2.15 | 0.46 |
| 36:2e:9:LYS:O | 36:2e:33:VAL:HG12 | 2.16 | 0.46 |
| 1:1A:469:G:OP1 | 5:1F:60:SER:N | 2.44 | 0.46 |
| 1:1A:684:G:OP1 | 29:17:16:HIS:ND1 | 2.45 | 0.46 |
| 1:1A:824:A:H1' | 1:1A:2358:G:N7 | 2.31 | 0.46 |
| 1:1A:952:G:P | 12:1Q:16:ARG:HH21 | 2.39 | 0.46 |
| 1:1A:1271:G:OP2 | 59:1A:4227:HOH:O | 2.20 | 0.46 |
| 1:1A:1279:G:H4' | 13:1R:31:HIS:CD2 | 2.50 | 0.46 |
| 1:1A:1547:C:H2' | 1:1A:1548:C:C6 | 2.51 | 0.46 |
| 1:1A:1641:A:H2' | 1:1A:1642:G:O4' | 2.16 | 0.46 |
| 1:1A:2341:G:H2' | 1:1A:2342:C:C6 | 2.51 | 0.46 |
| 1:1A:2364:C:H4' | 22:10:56:ASP:OD1 | 2.16 | 0.46 |
| 1:1A:2417:C:OP1 | 11:1P:65:ARG:NH2 | 2.48 | 0.46 |
| 7:1H:41:MET:HE2 | 7:1H:65:HIS:HA | 1.98 | 0.46 |
| 23:11:72:GLU:O | 23:11:76:ARG:HG2 | 2.16 | 0.46 |
| 32:1a:7:G:O2' | 36:1e:120:THR:O | 2.34 | 0.46 |
| 32:1a:134:A:H61 | 47:1p:25:ARG:NH1 | 2.14 | 0.46 |
| 32:1a:410:G:H2' | 32:1a:429:U:C5 | 2.51 | 0.46 |
| 32:1a:1166:G:N2 | 32:1a:1170:A:OP2 | 2.49 | 0.46 |
| 41:1j:7:LYS:HD3 | 41:1j:71:LEU:HD13 | 1.96 | 0.46 |
| 1:2A:236:C:H2' | 1:2A:237:C:C6 | 2.50 | 0.46 |
| 1:2A:251:A:P | 30:28:7:HIS:HE2 | 2.38 | 0.46 |
| 1:2A:661:C:N4 | 59:2A:4100:HOH:O | 2.48 | 0.46 |
| 1:2A:2302:G:N2 | 6:2G:126:ASP:OD1 | 2.40 | 0.46 |
| 1:2A:2674:G:H2' | 1:2A:2675:A:C8 | 2.51 | 0.46 |
| 4:2E:181:LEU:HD12 | 4:2E:181:LEU:HA | 1.69 | 0.46 |
| 5:2F:64:ILE:HG21 | 5:2F:78:ILE:HG23 | 1.96 | 0.46 |
| 5:2F:107:LYS:HG3 | 5:2F:206:ILE:HA | 1.98 | 0.46 |
| 10:2O:49:ARG:NH1 | 32:2a:1422:G:O3' | 2.45 | 0.46 |
| 11:2P:1:MET:HE2 | 11:2P:1:MET:HB2 | 1.73 | 0.46 |
| 12:2Q:18:LYS:O | 12:2Q:98:LYS:NZ | 2.27 | 0.46 |
| 14:2S:15:ARG:O | 14:2S:18:ILE:N | 2.48 | 0.46 |
| 30:28:39:LYS:HA | 30:28:42:ARG:NH1 | 2.30 | 0.46 |
| 32:2a:520:A:N1 | 32:2a:536:C:H1' | 2.30 | 0.46 |
| 32:2a:678:U:H2' | 32:2a:679:C:C6 | 2.50 | 0.46 |
| 32:2a:1089:G:H1 | 32:2a:1096:C:N4 | 2.14 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 32:2a:1287:A:H2 | 32:2a:1353:G:H1' | 1.80 | 0.46 |
| 35:2d:172:PRO:HD2 | 35:2d:173:TRP:CZ3 | 2.51 | 0.46 |
| 39:2h:7:ALA:O | 39:2h:11:THR:HG23 | 2.15 | 0.46 |
| 39:2h:78:GLN:O | 39:2h:81:HIS:NE2 | 2.49 | 0.46 |
| 40:2i:23:ASN:ND2 | 40:2i:25:LYS:HG2 | 2.27 | 0.46 |
| 1:1A:1257:C:H4' | 5:1F:83:PHE:CD1 | 2.51 | 0.46 |
| 2:1B:11:C:H3' | 2:1B:12:C:C6 | 2.52 | 0.46 |
| 17:1V:34:GLU:HB3 | 17:1V:56:SER:HB2 | 1.98 | 0.46 |
| 19:1X:32:PRO:HA | 19:1X:77:LYS:HB2 | 1.98 | 0.46 |
| 27:15:40:LYS:HD3 | 27:15:46:CYS:HA | 1.98 | 0.46 |
| 32:1a:128:G:O3' | 48:1q:3:LYS:NZ | 2.49 | 0.46 |
| 32:1a:1130:A:O3' | 40:1i:3:GLN:NE2 | 2.47 | 0.46 |
| 32:1a:1252:A:H2' | 32:1a:1253:G:O4' | 2.16 | 0.46 |
| 33:1b:115:LEU:HD12 | 33:1b:145:LEU:HB3 | 1.97 | 0.46 |
| 40:1i:32:ASP:OD1 | 40:1i:33:PHE:N | 2.48 | 0.46 |
| 1:2A:116:C:H2' | 1:2A:117:G:O4' | 2.16 | 0.46 |
| 1:2A:918:A:H5" | 2:2B:98:G:O2' | 2.16 | 0.46 |
| 1:2A:1897:G:H2' | 1:2A:1898:U:H6 | 1.81 | 0.46 |
| 1:2A:2632:A:O2' | 1:2A:2811:G:O2' | 2.20 | 0.46 |
| 1:2A:2635:C:O2' | 4:2E:80:GLU:OE2 | 2.33 | 0.46 |
| 1:2A:2643:G:H2' | 1:2A:2644:G:O4' | 2.16 | 0.46 |
| 1:2A:2895:U:H2' | 1:2A:2896:C:O4' | 2.15 | 0.46 |
| 2:2B:79:C:H2' | 2:2B:80:U:O4' | 2.16 | 0.46 |
| 6:2G:17:PRO:HA | 6:2G:20:ILE:HG22 | 1.98 | 0.46 |
| 13:2R:59:ASP:OD2 | 13:2R:61:HIS:HB3 | 2.15 | 0.46 |
| 15:2T:117:ASP:O | 15:2T:121:ILE:HG13 | 2.15 | 0.46 |
| 32:2a:158:G:H2' | 32:2a:159:G:O4' | 2.16 | 0.46 |
| 32:2a:186:C:H2' | 32:2a:187:C:C6 | 2.51 | 0.46 |
| 32:2a:216:G:H2' | 32:2a:217:C:C6 | 2.51 | 0.46 |
| 32:2a:814:A:N7 | 32:2a:816:A:C4 | 2.84 | 0.46 |
| 32:2a:1097:C:H1' | 32:2a:1170:A:H1' | 1.97 | 0.46 |
| 32:2a:1113:C:O2' | 34:2c:14:ILE:HD11 | 2.16 | 0.46 |
| 35:2d:150:GLU:HA | 35:2d:153:ARG:HG3 | 1.98 | 0.46 |
| 1:1A:534:U:H2' | 1:1A:535:C:C6 | 2.51 | 0.45 |
| 1:1A:827:U:H5' | 1:1A:828:U:O5' | 2.16 | 0.45 |
| 1:1A:1637:A:H4' | 1:1A:2711:A:O2' | 2.16 | 0.45 |
| 1:1A:2661:G:H2' | 1:1A:2662:A:C8 | 2.51 | 0.45 |
| 4:1E:21:VAL:O | 4:1E:23:VAL:HG13 | 2.16 | 0.45 |
| 8:1I:104:GLN:HB3 | 8:1I:105:HIS:ND1 | 2.31 | 0.45 |
| 32:1a:940:C:H2' | 32:1a:941:G:C8 | 2.52 | 0.45 |
| 35:1d:65:ARG:HG2 | 35:1d:75:PHE:CD1 | 2.51 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 37:1f:69:GLU:O | 37:1f:72:VAL:HG23 | 2.16 | 0.45 |
| 1:2A:1802:A:N1 | 1:2A:1822:G:H1' | 2.31 | 0.45 |
| 1:2A:2067:G:O2' | 1:2A:2069:G:H5' | 2.15 | 0.45 |
| 7:2H:54:ARG:HG2 | 7:2H:65:HIS:CE1 | 2.51 | 0.45 |
| 32:2a:189(L):G:H2' | 32:2a:190:U:H6 | 1.81 | 0.45 |
| 32:2a:1005:A:H3' | 32:2a:1006:C:C6 | 2.51 | 0.45 |
| 33:2b:24:TRP:CD1 | 33:2b:24:TRP:H | 2.34 | 0.45 |
| 38:2g:59:LEU:O | 38:2g:63:LYS:HG3 | 2.16 | 0.45 |
| 1:1A:782:A:N7 | 3:1D:221:VAL:HG21 | 2.31 | 0.45 |
| 1:1A:1472:A:H2' | 1:1A:1473:G:O4' | 2.16 | 0.45 |
| 1:1A:1810:A:H2' | 1:1A:1811:G:O4' | 2.16 | 0.45 |
| 1:1A:2262:U:OP2 | 22:10:19:LYS:NZ | 2.49 | 0.45 |
| 1:1A:2698:U:H2' | 1:1A:2699:C:C6 | 2.51 | 0.45 |
| 1:1A:2747:G:O6 | 1:1A:2755:C:H5" | 2.16 | 0.45 |
| 8:1I:65:ALA:HB1 | 8:1I:136:VAL:HG11 | 1.98 | 0.45 |
| 8:1I:77:LEU:HD23 | 8:1I:97:ILE:HG23 | 1.97 | 0.45 |
| 26:14:56:VAL:O | 26:14:60:GLN:HB2 | 2.17 | 0.45 |
| 32:1a:1028:C:H2' | 32:1a:1029:C:O4' | 2.17 | 0.45 |
| 32:1a:1068:G:N2 | 32:1a:1191:A:N3 | 2.60 | 0.45 |
| 35:1d:110:PHE:CE1 | 35:1d:148:VAL:HG23 | 2.50 | 0.45 |
| 41:1j:24:VAL:O | 41:1j:28:ARG:N | 2.49 | 0.45 |
| 45:1n:29:ARG:HH21 | 45:1n:42:ILE:HD11 | 1.80 | 0.45 |
| 1:2A:37:C:H2' | 1:2A:38:A:C8 | 2.51 | 0.45 |
| 1:2A:264:C:O2' | 1:2A:265:A:H2' | 2.17 | 0.45 |
| 1:2A:745:G:O2' | 1:2A:750:A:N6 | 2.48 | 0.45 |
| 1:2A:1161:C:H2' | 1:2A:1162:G:C8 | 2.50 | 0.45 |
| 1:2A:1479:G:H5" | 1:2A:1560:G:H4' | 1.98 | 0.45 |
| 1:2A:1792:G:H5' | 3:2D:205:VAL:HG13 | 1.97 | 0.45 |
| 1:2A:2287:A:C8 | 1:2A:2289:G:C8 | 3.04 | 0.45 |
| 1:2A:2340:G:H2' | 1:2A:2341:G:H8 | 1.82 | 0.45 |
| 2:2B:24:G:N7 | 2:2B:56:G:H2' | 2.32 | 0.45 |
| 6:2G:11:TYR:O | 6:2G:15:VAL:HG22 | 2.16 | 0.45 |
| 8:2I:93:THR:OG1 | 8:2I:116:LEU:HD22 | 2.15 | 0.45 |
| 8:2I:102:SER:OG | 8:2I:108:THR:HG23 | 2.17 | 0.45 |
| 17:2V:69:LYS:HA | 17:2V:88:ARG:HG2 | 1.98 | 0.45 |
| 23:21:3:LYS:HB3 | 23:21:4:VAL:H | 1.50 | 0.45 |
| 32:2a:6:G:H22 | 36:2e:98:THR:HG22 | 1.80 | 0.45 |
| 32:2a:186:C:H2' | 32:2a:187:C:H6 | 1.82 | 0.45 |
| 32:2a:397:A:H3' | 32:2a:397:A:N3 | 2.31 | 0.45 |
| 32:2a:837:G:H2' | 32:2a:838:G:C8 | 2.52 | 0.45 |
| 33:2b:31:TYR:HE2 | 33:2b:194:PRO:HB3 | 1.81 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 33:2b:126:GLU:CD | 33:2b:126:GLU:H | 2.24 | 0.45 |
| 34:2c:157:ILE:C | 34:2c:159:GLY:H | 2.24 | 0.45 |
| 37:2f:76:ALA:O | 37:2f:80:ARG:HG3 | 2.16 | 0.45 |
| 51:2t:10:LEU:HD12 | 51:2t:10:LEU:HA | 1.84 | 0.45 |
| 51:2t:98:PRO:O | 51:2t:99:LEU:HB2 | 2.15 | 0.45 |
| 1:1A:220:G:H5" | 1:1A:221:A:OP1 | 2.15 | 0.45 |
| 1:1A:548:A:H1' | 1:1A:549:G:OP1 | 2.16 | 0.45 |
| 1:1A:670:A:H4' | 1:1A:671:C:O5' | 2.16 | 0.45 |
| 1:1A:748:G:C8 | 18:1W:89:ALA:HB1 | 2.51 | 0.45 |
| 1:1A:780:G:H1' | 1:1A:785:G:C2 | 2.52 | 0.45 |
| 1:1A:1076:C:H4' | 1:1A:1077:A:OP1 | 2.16 | 0.45 |
| 1:1A:1190:G:H5" | 11:1P:32:THR:O | 2.16 | 0.45 |
| 1:1A:1418:G:O5' | 1:1A:1418:G:H8 | 1.99 | 0.45 |
| 1:1A:1824:G:O3' | 3:1D:249:PRO:HD3 | 2.16 | 0.45 |
| 2:1B:29:A:H2' | 2:1B:30:C:O4' | 2.17 | 0.45 |
| 11:1P:98:GLU:O | 11:1P:101:VAL:HG12 | 2.17 | 0.45 |
| 24:12:22:GLU:OE2 | 24:12:68:ARG:NH2 | 2.48 | 0.45 |
| 26:14:43:TYR:O | 26:14:45:GLY:N | 2.48 | 0.45 |
| 32:1a:625:G:H2' | 32:1a:626:U:C6 | 2.51 | 0.45 |
| 32:1a:673:G:O3' | 37:1f:87:ARG:NH2 | 2.50 | 0.45 |
| 32:1a:1221:G:H1' | 50:1s:54:GLY:HA3 | 1.97 | 0.45 |
| 33:1b:78:GLN:HA | 33:1b:78:GLN:HE21 | 1.80 | 0.45 |
| 1:2A:948:G:H21 | 1:2A:985:C:P | 2.39 | 0.45 |
| 1:2A:1239:G:H2' | 1:2A:1240:U:O4' | 2.16 | 0.45 |
| 1:2A:2284:C:OP2 | 28:26:2:ALA:N | 2.50 | 0.45 |
| 7:2H:143:GLN:HG3 | 7:2H:147:ASN:ND2 | 2.32 | 0.45 |
| 8:2I:62:LYS:NZ | 8:2I:136:VAL:HG22 | 2.31 | 0.45 |
| 9:2N:67:LEU:O | 9:2N:88:GLU:HG3 | 2.16 | 0.45 |
| 13:2R:72:ASP:HB3 | 13:2R:75:LEU:HB3 | 1.96 | 0.45 |
| 20:2Y:5:MET:HE2 | 20:2Y:5:MET:HB3 | 1.83 | 0.45 |
| 32:2a:147:G:H1 | 32:2a:175:C:H42 | 1.65 | 0.45 |
| 32:2a:1101:A:N3 | 32:2a:1102:A:H1' | 2.31 | 0.45 |
| 32:2a:1273:G:H5' | 32:2a:1274:G:OP2 | 2.16 | 0.45 |
| 32:2a:1308:U:P | 44:2m:99:ARG:HG3 | 2.57 | 0.45 |
| 32:2a:1469:G:H2' | 32:2a:1470:G:C8 | 2.51 | 0.45 |
| 36:2e:79:GLU:HA | 36:2e:91:LEU:O | 2.17 | 0.45 |
| 38:2g:75:VAL:HB | 38:2g:86:GLN:HB3 | 1.98 | 0.45 |
| 41:2j:8:LEU:HB3 | 41:2j:96:ILE:HG23 | 1.98 | 0.45 |
| 44:2m:19:LEU:HD21 | 44:2m:56:LEU:HD21 | 1.98 | 0.45 |
| 44:2m:23:TYR:CE2 | 44:2m:71:ARG:HG3 | 2.52 | 0.45 |
| 1:1A:36:G:H4' | 1:1A:451:C:C2 | 2.52 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1A:55:G:O2' | 1:1A:127:A:N1 | 2.42 | 0.45 |
| 1:1A:245:G:O5' | 11:1P:73:GLY:HA2 | 2.16 | 0.45 |
| 1:1A:493:G:H2' | 1:1A:494:G:O4' | 2.16 | 0.45 |
| 1:1A:524:U:H4' | 1:1A:555:U:H4' | 1.97 | 0.45 |
| 1:1A:987:G:O2' | 1:1A:1000:A:N3 | 2.45 | 0.45 |
| 1:1A:1059:G:H2' | 1:1A:1060:U:C5 | 2.50 | 0.45 |
| 1:1A:1203:G:H5' | 11:1P:3:LEU:HD13 | 1.97 | 0.45 |
| 1:1A:1474:C:H2' | 1:1A:1475:G:C8 | 2.51 | 0.45 |
| 1:1A:1711:C:H2' | 1:1A:1712:C:C6 | 2.51 | 0.45 |
| 1:1A:1889:A:H1' | 1:1A:2087:G:O4' | 2.16 | 0.45 |
| 1:1A:1952:A:C6 | 1:1A:1953:A:N1 | 2.85 | 0.45 |
| 1:1A:2640:G:P | 9:1N:97:ARG:HH22 | 2.39 | 0.45 |
| 2:1B:14:U:O2 | 2:1B:108:U:H4' | 2.16 | 0.45 |
| 5:1F:28:ILE:O | 5:1F:30:PRO:HD3 | 2.16 | 0.45 |
| 5:1F:34:TRP:CE2 | 11:1P:8:PRO:HB3 | 2.51 | 0.45 |
| 12:1Q:68:ILE:HG23 | 12:1Q:103:MET:HA | 1.97 | 0.45 |
| 14:1S:66:ALA:O | 14:1S:69:VAL:HG13 | 2.15 | 0.45 |
| 19:1X:61:GLY:HA3 | 19:1X:73:ARG:O | 2.16 | 0.45 |
| 24:12:32:LEU:HD22 | 24:12:36:ARG:NH1 | 2.28 | 0.45 |
| 30:18:62:LEU:HB3 | 30:18:65:GLU:CG | 2.46 | 0.45 |
| 32:1a:224:C:H2' | 32:1a:225:C:C6 | 2.51 | 0.45 |
| 32:1a:1084:G:C5 | 32:1a:1085:U:C4 | 3.03 | 0.45 |
| 32:1a:1511:G:H2' | 32:1a:1512:U:O4' | 2.17 | 0.45 |
| 35:1d:18:LYS:HB3 | 35:1d:33:MET:CB | 2.47 | 0.45 |
| 39:1h:82:HIS:CD2 | 39:1h:82:HIS:C | 2.94 | 0.45 |
| 45:1n:50:LYS:HG2 | 45:1n:52:GLN:HG3 | 1.99 | 0.45 |
| 1:2A:668:G:H5' | 1:2A:669:G:OP2 | 2.16 | 0.45 |
| 1:2A:1639:U:C2' | 1:2A:1640:C:H5" | 2.47 | 0.45 |
| 1:2A:1814:G:H4' | 3:2D:51:VAL:HG21 | 1.98 | 0.45 |
| 1:2A:2282:G:H4' | 1:2A:2389:G:O2' | 2.16 | 0.45 |
| 3:2D:68:LYS:HE3 | 3:2D:70:TRP:CH2 | 2.51 | 0.45 |
| 4:2E:14:ILE:HB | 15:2T:14:TYR:CZ | 2.51 | 0.45 |
| 18:2W:46:PHE:O | 18:2W:50:VAL:HG23 | 2.16 | 0.45 |
| 20:2Y:86:ARG:HB2 | 20:2Y:98:VAL:HG22 | 1.97 | 0.45 |
| 32:2a:58:C:O2' | 32:2a:388:G:N7 | 2.37 | 0.45 |
| 32:2a:537:G:H2' | 32:2a:538:G:C8 | 2.51 | 0.45 |
| 32:2a:857:C:OP2 | 59:2a:3310:HOH:O | 2.21 | 0.45 |
| 32:2a:1251:A:H2' | 32:2a:1252:A:C8 | 2.51 | 0.45 |
| 32:2a:1297:C:H4' | 32:2a:1298:C:H5' | 1.98 | 0.45 |
| 33:2b:47:THR:HG23 | 33:2b:202:PRO:HG2 | 1.99 | 0.45 |
| 41:2j:5:ARG:O | 41:2j:98:ILE:HA | 2.16 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 44:2m:29:ARG:HD3 | 44:2m:64:TRP:CD1 | 2.51 | 0.45 |
| 1:1A:470:A:H5' | 59:1A:4360:HOH:O | 2.16 | 0.45 |
| 1:1A:478:A:C6 | 1:1A:480:A:C6 | 3.04 | 0.45 |
| 1:1A:588:U:H1' | 5:1F:90:PHE:CG | 2.52 | 0.45 |
| 1:1A:1028:A:H61 | 1:1A:1125:G:H2' | 1.81 | 0.45 |
| 1:1A:1252:G:C2 | 1:1A:1253:A:C2 | 3.05 | 0.45 |
| 1:1A:1803:A:H4' | 3:1D:259:THR:HG23 | 1.97 | 0.45 |
| 1:1A:2051:A:H5' | 1:1A:2578:G:O4' | 2.17 | 0.45 |
| 8:1I:75:LEU:HD22 | 8:1I:105:HIS:CD2 | 2.47 | 0.45 |
| 28:16:8:LYS:HG2 | 30:18:34:TRP:CD1 | 2.51 | 0.45 |
| 32:1a:1090:U:H2' | 32:1a:1091:U:H6 | 1.81 | 0.45 |
| 32:1a:1171:G:H2' | 32:1a:1172:C:C6 | 2.52 | 0.45 |
| 33:1b:54:THR:O | 33:1b:58:ILE:HD12 | 2.17 | 0.45 |
| 35:1d:39:PRO:O | 35:1d:44:GLY:HA3 | 2.15 | 0.45 |
| 36:1e:82:VAL:HG21 | 36:1e:138:ALA:HA | 1.99 | 0.45 |
| 40:1i:24:GLY:HA2 | 40:1i:59:PHE:O | 2.17 | 0.45 |
| 54:1x:37:A:H2' | 54:1x:38:A:O4' | 2.17 | 0.45 |
| 1:2A:93:G:H2' | 1:2A:94:C:C6 | 2.51 | 0.45 |
| 1:2A:249:C:H4' | 1:2A:250:G:O5' | 2.17 | 0.45 |
| 1:2A:807:U:OP2 | 11:2P:41:ARG:NH2 | 2.49 | 0.45 |
| 1:2A:1159:U:H2' | 1:2A:1160:G:C8 | 2.49 | 0.45 |
| 1:2A:1274:A:N3 | 1:2A:1297:C:H1' | 2.31 | 0.45 |
| 1:2A:1755:A:OP2 | 15:2T:113:LYS:NZ | 2.47 | 0.45 |
| 1:2A:1826:G:H4' | 3:2D:242:ARG:CZ | 2.45 | 0.45 |
| 1:2A:1999:C:H5" | 1:2A:2723:C:O2' | 2.16 | 0.45 |
| 1:2A:2515:C:H2' | 1:2A:2516:G:H8 | 1.82 | 0.45 |
| 1:2A:2704:C:H2' | 1:2A:2705:A:O4' | 2.16 | 0.45 |
| 1:2A:2836:U:H2' | 1:2A:2837:G:C8 | 2.52 | 0.45 |
| 2:2B:1:U:H2' | 2:2B:2:C:C6 | 2.51 | 0.45 |
| 4:2E:116:VAL:HG13 | 4:2E:122:PHE:HB2 | 1.98 | 0.45 |
| 8:2I:61:ARG:HH11 | 8:2I:61:ARG:N | 2.15 | 0.45 |
| 32:2a:968:A:H4' | 32:2a:969:A:OP2 | 2.17 | 0.45 |
| 32:2a:1024:G:H2' | 32:2a:1025:U:H5" | 1.99 | 0.45 |
| 32:2a:1121:U:H2' | 32:2a:1122:U:H6 | 1.81 | 0.45 |
| 33:2b:74:LYS:HG2 | 33:2b:169:LYS:HG2 | 1.98 | 0.45 |
| 37:2f:2:ARG:HB2 | 37:2f:4:TYR:CE2 | 2.52 | 0.45 |
| 37:2f:23:LYS:HG2 | 37:2f:61:LEU:HD21 | 1.97 | 0.45 |
| 44:2m:13:LYS:HA | 44:2m:44:ARG:HH11 | 1.80 | 0.45 |
| 44:2m:117:VAL:HG12 | 44:2m:118:ALA:H | 1.81 | 0.45 |
| 48:2q:23:VAL:HG21 | 48:2q:59:ILE:HD11 | 1.99 | 0.45 |
| 1:1A:84:A:H5" | 20:1Y:8:LYS:HG2 | 1.97 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1A:129:C:H2' | 1:1A:130:C:C6 | 2.52 | 0.45 |
| 1:1A:250:G:H2' | 1:1A:251:A:C8 | 2.51 | 0.45 |
| 1:1A:407:G:H2' | 1:1A:408:G:C8 | 2.51 | 0.45 |
| 1:1A:2299:G:H22 | 1:1A:2318:G:H1' | 1.81 | 0.45 |
| 2:1B:96:U:OP1 | 21:1Z:14:LYS:NZ | 2.49 | 0.45 |
| 8:1I:141:LYS:HE3 | 8:1I:141:LYS:HB2 | 1.81 | 0.45 |
| 20:1Y:20:TYR:HB3 | 20:1Y:23:ARG:HG3 | 1.98 | 0.45 |
| 25:13:7:LYS:NZ | 25:13:32:GLN:O | 2.50 | 0.45 |
| 30:18:26:LYS:HD2 | 30:18:48:PHE:CD2 | 2.51 | 0.45 |
| 32:1a:246:A:N1 | 32:1a:278:G:O2' | 2.50 | 0.45 |
| 32:1a:783:C:OP1 | 32:1a:1515:C:O2' | 2.28 | 0.45 |
| 32:1a:909:A:H2' | 32:1a:910:C:O4' | 2.15 | 0.45 |
| 36:1e:18:ARG:HH11 | 36:1e:27:ARG:HH12 | 1.63 | 0.45 |
| 1:2A:313:C:H2' | 1:2A:314:A:H8 | 1.82 | 0.45 |
| 1:2A:506:G:O3' | 1:2A:507:A:H8 | 1.99 | 0.45 |
| 1:2A:793:A:O2' | 59:2A:3966:HOH:O | 2.21 | 0.45 |
| 1:2A:911:A:H2' | 12:2Q:9:TYR:OH | 2.16 | 0.45 |
| 1:2A:1429:G:H2' | 1:2A:1430:C:C6 | 2.51 | 0.45 |
| 1:2A:1721:G:H5' | 1:2A:1722:A:OP2 | 2.16 | 0.45 |
| 32:2a:560:U:H6 | 32:2a:560:U:H2' | 1.58 | 0.45 |
| 32:2a:1371:G:OP1 | 40:2i:12:GLU:HB2 | 2.17 | 0.45 |
| 32:2a:1412:C:H2' | 32:2a:1413:A:C8 | 2.52 | 0.45 |
| 33:2b:94:ASN:HB3 | 33:2b:95:GLN:NE2 | 2.32 | 0.45 |
| 35:2d:31:CYS:SG | 35:2d:33:MET:N | 2.87 | 0.45 |
| 49:2r:74:ARG:H | 49:2r:74:ARG:HG3 | 1.62 | 0.45 |
| 1:1A:1636:C:H2' | 1:1A:1637:A:H8 | 1.78 | 0.45 |
| 1:1A:2101:G:H1 | 1:1A:2188:C:H42 | 1.65 | 0.45 |
| 1:1A:2161:C:HO2' | 1:1A:2162:G:H5" | 1.81 | 0.45 |
| 15:1T:111:ARG:NH2 | 32:1a:1464:G:OP2 | 2.50 | 0.45 |
| 18:1W:1:MET:HE3 | 18:1W:62:HIS:HB3 | 1.98 | 0.45 |
| 18:1W:20:VAL:HA | 18:1W:23:LEU:HD12 | 1.99 | 0.45 |
| 32:1a:491:G:H2' | 32:1a:492:G:O4' | 2.17 | 0.45 |
| 32:1a:536:C:H2' | 32:1a:537:G:C8 | 2.51 | 0.45 |
| 32:1a:630:G:H2' | 32:1a:631:G:C8 | 2.52 | 0.45 |
| 32:1a:986:A:H2' | 32:1a:987:G:O4' | 2.17 | 0.45 |
| 37:1f:19:LEU:HD11 | 37:1f:59:TYR:CE1 | 2.51 | 0.45 |
| 41:1j:51:ARG:HH11 | 45:1n:45:ARG:HH21 | 1.65 | 0.45 |
| 46:1o:8:LYS:O | 46:1o:12:ILE:HG13 | 2.16 | 0.45 |
| 1:2A:660:G:H5' | 5:2F:99:TYR:CE1 | 2.51 | 0.45 |
| 1:2A:2432:A:C6 | 1:2A:2433:A:C6 | 3.05 | 0.45 |
| 1:2A:2512:C:H2' | 1:2A:2513:G:O4' | 2.15 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 15:2T:118:ARG:HA | 15:2T:121:ILE:HD12 | 1.99 | 0.45 |
| 21:2Z:73:GLN:HB3 | 21:2Z:87:ASP:HB2 | 1.98 | 0.45 |
| 32:2a:67:C:H2' | 32:2a:68:G:C8 | 2.52 | 0.45 |
| 32:2a:103:C:O2' | 32:2a:172:A:N1 | 2.41 | 0.45 |
| 32:2a:1128:C:O2' | 32:2a:1129:C:OP1 | 2.35 | 0.45 |
| 32:2a:1323:G:H4' | 32:2a:1363:C:C2 | 2.51 | 0.45 |
| 39:2h:36:LEU:HA | 39:2h:39:LEU:HD12 | 1.99 | 0.45 |
| 1:1A:809:G:H2' | 1:1A:810:U:C6 | 2.51 | 0.45 |
| 1:1A:1018:C:O3' | 1:1A:1120:G:N2 | 2.49 | 0.45 |
| 1:1A:1366:A:H2' | 1:1A:1367:A:O4' | 2.16 | 0.45 |
| 1:1A:1826:G:OP1 | 3:1D:224:ALA:N | 2.43 | 0.45 |
| 1:1A:2078:C:C4 | 1:1A:2079:U:C4 | 3.05 | 0.45 |
| 1:1A:2099:U:O4 | 1:1A:2190:G:O6 | 2.34 | 0.45 |
| 1:1A:2345:G:N3 | 1:1A:2381:C:H2' | 2.31 | 0.45 |
| 1:1A:2691:C:O3' | 1:1A:2871:C:H4' | 2.17 | 0.45 |
| 32:1a:18:C:H5" | 36:1e:127:ASN:ND2 | 2.32 | 0.45 |
| 32:1a:219:C:O2' | 32:1a:381:C:H5' | 2.17 | 0.45 |
| 32:1a:1192:C:P | 34:1c:4:LYS:HZ1 | 2.40 | 0.45 |
| 32:1a:1223:C:P | 50:1s:78:ARG:HH21 | 2.40 | 0.45 |
| 35:1d:9:CYS:O | 35:1d:13:ARG:HG3 | 2.17 | 0.45 |
| 48:1q:67:LYS:HA | 48:1q:70:ARG:HH12 | 1.81 | 0.45 |
| 1:2A:884:C:N4 | 1:2A:893:C:O2 | 2.43 | 0.45 |
| 1:2A:1423:G:H2' | 1:2A:1424:G:H8 | 1.82 | 0.45 |
| 1:2A:2222:G:O2' | 3:2D:148:GLU:HG2 | 2.17 | 0.45 |
| 1:2A:2277:G:OP2 | 22:20:10:THR:HG21 | 2.17 | 0.45 |
| 1:2A:2465:C:O2 | 1:2A:2486:G:C2 | 2.70 | 0.45 |
| 1:2A:2683:C:OP1 | 15:2T:53:ARG:NH2 | 2.50 | 0.45 |
| 1:2A:2853:C:H2' | 1:2A:2854:G:H8 | 1.80 | 0.45 |
| 4:2E:105:THR:HG22 | 4:2E:106:GLY:H | 1.81 | 0.45 |
| 6:2G:114:ILE:HA | 6:2G:140:ILE:HD11 | 1.99 | 0.45 |
| 7:2H:89:ILE:H | 7:2H:89:ILE:HD12 | 1.81 | 0.45 |
| 7:2H:152:ARG:HD3 | 7:2H:152:ARG:HA | 1.68 | 0.45 |
| 9:2N:97:ARG:HA | 9:2N:100:GLU:HB2 | 1.98 | 0.45 |
| 32:2a:110:C:O2' | 47:2p:25:ARG:O | 2.27 | 0.45 |
| 32:2a:505:G:H2' | 32:2a:506:G:H8 | 1.82 | 0.45 |
| 32:2a:1148:U:H2' | 32:2a:1149:C:O4' | 2.17 | 0.45 |
| 33:2b:96:ARG:HB3 | 33:2b:148:TYR:CE1 | 2.52 | 0.45 |
| 33:2b:170:GLU:O | 33:2b:174:VAL:HG23 | 2.17 | 0.45 |
| 33:2b:218:ALA:O | 33:2b:222:ILE:HG23 | 2.16 | 0.45 |
| 37:2f:80:ARG:HG2 | 37:2f:88:VAL:HB | 1.99 | 0.45 |
| 39:2h:21:LYS:O | 39:2h:65:TYR:OH | 2.19 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 48:2q:12:SER:HB3 | 48:2q:20:THR:HB | 1.98 | 0.45 |
| 50:2s:41:VAL:HG22 | 50:2s:44:MET:SD | 2.57 | 0.45 |
| 1:1A:644:A:H4' | 1:1A:645:C:C5 | 2.51 | 0.45 |
| 1:1A:828:U:H4' | 1:1A:831:G:N1 | 2.31 | 0.45 |
| 1:1A:954:G:O2' | 1:1A:2274:A:N1 | 2.47 | 0.45 |
| 1:1A:1466:G:O2' | 1:1A:1546:C:O2' | 2.28 | 0.45 |
| 1:1A:2104:G:H2' | 1:1A:2105:C:C6 | 2.52 | 0.45 |
| 1:1A:2232:U:P | 23:11:40:ARG:HH12 | 2.39 | 0.45 |
| 1:1A:2328:A:H2' | 1:1A:2329:G:C8 | 2.52 | 0.45 |
| 1:1A:2646:C:H2' | 1:1A:2647:U:O4' | 2.17 | 0.45 |
| 1:1A:2846:G:H2' | 1:1A:2847:U:O4' | 2.17 | 0.45 |
| 4:1E:37:ARG:HB2 | 4:1E:46:ALA:H | 1.81 | 0.45 |
| 9:1N:30:ILE:HG23 | 9:1N:52:VAL:HG11 | 1.97 | 0.45 |
| 15:1T:23:ARG:N | 15:1T:26:ASP:OD2 | 2.44 | 0.45 |
| 32:1a:405:U:O4 | 35:1d:2:GLY:N | 2.50 | 0.45 |
| 32:1a:848:C:H2' | 32:1a:849:C:C6 | 2.51 | 0.45 |
| 32:1a:865:A:H2 | 32:1a:918:A:H4' | 1.82 | 0.45 |
| 34:1c:47:LEU:HD13 | 34:1c:70:VAL:HG11 | 1.99 | 0.45 |
| 39:1h:11:THR:HG22 | 39:1h:14:ARG:HH22 | 1.81 | 0.45 |
| 39:1h:81:HIS:N | 39:1h:138:TRP:O | 2.49 | 0.45 |
| 41:1j:38:ILE:CG1 | 41:1j:71:LEU:HB3 | 2.46 | 0.45 |
| 41:1j:81:THR:C | 41:1j:83:GLU:H | 2.23 | 0.45 |
| 47:1p:18:ARG:NH1 | 47:1p:32:TYR:OH | 2.50 | 0.45 |
| 1:2A:826:U:H5" | 1:2A:2428:G:O3' | 2.17 | 0.45 |
| 1:2A:884:C:H3' | 1:2A:885:C:C6 | 2.52 | 0.45 |
| 1:2A:1686:C:H2' | 1:2A:1687:G:O4' | 2.17 | 0.45 |
| 1:2A:1978:A:H2' | 1:2A:1979:C:O4' | 2.17 | 0.45 |
| 1:2A:2504:U:OP2 | 59:2A:3965:HOH:O | 2.21 | 0.45 |
| 6:2G:41:GLN:HG3 | 6:2G:154:GLY:O | 2.17 | 0.45 |
| 25:23:26:LEU:O | 25:23:35:ARG:NE | 2.50 | 0.45 |
| 26:24:47:GLN:O | 26:24:49:PHE:N | 2.40 | 0.45 |
| 32:2a:98:G:H5' | 32:2a:99:U:OP2 | 2.17 | 0.45 |
| 32:2a:189(K):U:H2' | 32:2a:189(L):G:C8 | 2.52 | 0.45 |
| 32:2a:659:U:OP1 | 46:2o:9:GLN:NE2 | 2.49 | 0.45 |
| 32:2a:684:A:O2' | 42:2k:39:PRO:O | 2.34 | 0.45 |
| 32:2a:922:G:N3 | 32:2a:1398:A:H2 | 2.15 | 0.45 |
| 32:2a:944:G:H1' | 32:2a:1339:A:H61 | 1.82 | 0.45 |
| 32:2a:946:A:O2' | 32:2a:1333:A:N3 | 2.38 | 0.45 |
| 32:2a:1080:A:OP1 | 36:2e:47:LYS:HD3 | 2.16 | 0.45 |
| 32:2a:1134:G:H2' | 32:2a:1135:U:O4' | 2.17 | 0.45 |
| 32:2a:1145:C:H4' | 32:2a:1146:A:H5' | 1.99 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 32:2a:1250:A:H4' | 40:2i:68:GLY:H | 1.81 | 0.45 |
| 38:2g:69:VAL:HG11 | 38:2g:134:ALA:HB1 | 1.99 | 0.45 |
| 1:1A:271(M):G:O2' | 1:1A:271(N):U:H5" | 2.17 | 0.45 |
| 1:1A:559:G:H22 | 16:1U:49:HIS:CE1 | 2.35 | 0.45 |
| 1:1A:810:U:C4 | 11:1P:29:LYS:O | 2.70 | 0.45 |
| 1:1A:1012:U:C5 | 9:1N:28:THR:HG21 | 2.52 | 0.45 |
| 1:1A:2840:C:H2' | 1:1A:2841:C:C6 | 2.52 | 0.45 |
| 3:1D:31:LYS:C | 3:1D:33:LEU:H | 2.25 | 0.45 |
| 3:1D:69:ARG:NH1 | 3:1D:128:GLY:O | 2.33 | 0.45 |
| 5:1F:53:THR:CG2 | 5:1F:55:GLY:H | 2.30 | 0.45 |
| 11:1P:67:MET:HE3 | 11:1P:67:MET:HB2 | 1.80 | 0.45 |
| 30:18:26:LYS:HG2 | 30:18:46:ARG:O | 2.16 | 0.45 |
| 32:1a:413:G:N2 | 32:1a:428:G:H1' | 2.32 | 0.45 |
| 32:1a:719:C:N4 | 49:1r:71:LYS:HE2 | 2.32 | 0.45 |
| 32:1a:839:U:H3' | 32:1a:840:C:H5' | 1.98 | 0.45 |
| 32:1a:1117:G:O3' | 40:1i:104:ARG:HD3 | 2.17 | 0.45 |
| 34:1c:131:ARG:NH1 | 34:1c:166:GLU:HG3 | 2.26 | 0.45 |
| 35:1d:110:PHE:CD1 | 35:1d:148:VAL:HG23 | 2.51 | 0.45 |
| 43:1l:54:LYS:HD2 | 43:1l:54:LYS:N | 2.32 | 0.45 |
| 51:1t:89:ARG:NH2 | 51:1t:103:GLY:HA3 | 2.27 | 0.45 |
| 1:2A:599:G:OP1 | 11:2P:9:ASN:ND2 | 2.50 | 0.45 |
| 1:2A:754:C:O2' | 1:2A:1272:A:N1 | 2.46 | 0.45 |
| 1:2A:1258:C:H5' | 59:2A:4334:HOH:O | 2.17 | 0.45 |
| 1:2A:2557:G:H2' | 1:2A:2558:C:H6 | 1.82 | 0.45 |
| 1:2A:2786:U:H2' | 1:2A:2787:C:H6 | 1.82 | 0.45 |
| 2:2B:55:U:H2' | 2:2B:56:G:O4' | 2.16 | 0.45 |
| 4:2E:35:GLN:H | 4:2E:48:GLN:HB3 | 1.82 | 0.45 |
| 5:2F:31:HIS:HB2 | 11:2P:9:ASN:OD1 | 2.17 | 0.45 |
| 6:2G:151:ALA:O | 6:2G:153:ARG:HG3 | 2.17 | 0.45 |
| 8:2I:4:ILE:HG12 | 8:2I:18:VAL:HG12 | 1.98 | 0.45 |
| 29:27:1:MET:HE3 | 29:27:3:ARG:NH2 | 2.32 | 0.45 |
| 32:2a:8:A:N6 | 35:2d:205:GLU:O | 2.44 | 0.45 |
| 32:2a:99:U:H2' | 32:2a:100:C:C6 | 2.52 | 0.45 |
| 32:2a:557:G:C6 | 32:2a:558:G:C6 | 3.05 | 0.45 |
| 32:2a:614:A:H2' | 32:2a:615:C:C6 | 2.52 | 0.45 |
| 32:2a:617:G:H4' | 47:2p:44:THR:O | 2.17 | 0.45 |
| 33:2b:22:LYS:HE3 | 33:2b:40:HIS:CE1 | 2.52 | 0.45 |
| 48:2q:50:LYS:HB2 | 48:2q:51:TYR:CE2 | 2.52 | 0.45 |
| 48:2q:67:LYS:CA | 48:2q:70:ARG:HH12 | 2.25 | 0.45 |
| 1:1A:518:G:H2' | 1:1A:519:U:C6 | 2.52 | 0.44 |
| 1:1A:531:C:H4' | 1:1A:532:A:H5" | 1.98 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1A:1688:U:H1' | 1:1A:1701:A:C6 | 2.53 | 0.44 |
| 1:1A:2023:G:H4' | 1:1A:2617:C:O3' | 2.17 | 0.44 |
| 1:1A:2037:G:H2' | 1:1A:2038:G:C8 | 2.52 | 0.44 |
| 1:1A:2136:C:C2 | 1:1A:2155:G:N2 | 2.85 | 0.44 |
| 1:1A:2471:C:H2' | 1:1A:2472:G:O4' | 2.17 | 0.44 |
| 1:1A:2695:C:H2' | 1:1A:2696:U:C6 | 2.52 | 0.44 |
| 1:1A:2742:C:OP1 | 31:19:1:MET:HE3 | 2.16 | 0.44 |
| 3:1D:168:ARG:HG2 | 3:1D:173:VAL:HG12 | 1.99 | 0.44 |
| 6:1G:105:LYS:O | 6:1G:109:VAL:HG22 | 2.17 | 0.44 |
| 11:1P:85:LEU:HD13 | 11:1P:120:ALA:HB2 | 1.98 | 0.44 |
| 16:1U:89:GLU:HG3 | 17:1V:50:PRO:HB3 | 1.97 | 0.44 |
| 24:12:21:LEU:HD13 | 24:12:64:LEU:HA | 1.99 | 0.44 |
| 32:1a:7:G:H5' | 32:1a:298:A:O4' | 2.17 | 0.44 |
| 32:1a:114:U:H2' | 32:1a:115:G:C8 | 2.52 | 0.44 |
| 32:1a:452:A:H4' | 47:1p:72:ARG:NH1 | 2.31 | 0.44 |
| 32:1a:1191:A:H5" | 34:1c:4:LYS:NZ | 2.32 | 0.44 |
| 32:1a:1273:G:C2 | 32:1a:1274:G:H1' | 2.52 | 0.44 |
| 34:1c:135:LYS:HE2 | 36:1e:53:LEU:HD11 | 1.99 | 0.44 |
| 36:1e:77:PRO:HD2 | 36:1e:142:LEU:HD13 | 1.99 | 0.44 |
| 37:1f:11:ASN:HB3 | 37:1f:14:LEU:HG | 1.99 | 0.44 |
| 39:1h:86:ILE:HG13 | 39:1h:133:LEU:HD22 | 1.99 | 0.44 |
| 50:1s:15:LEU:O | 50:1s:19:VAL:HG23 | 2.16 | 0.44 |
| 1:2A:388:G:O2' | 1:2A:389:G:N7 | 2.50 | 0.44 |
| 1:2A:879:G:H5' | 1:2A:880:G:OP2 | 2.17 | 0.44 |
| 1:2A:1359:A:N6 | 1:2A:1372:U:H3 | 2.14 | 0.44 |
| 1:2A:1794:U:H2' | 1:2A:1795:C:H6 | 1.82 | 0.44 |
| 1:2A:2001:A:H2' | 1:2A:2002:G:C8 | 2.52 | 0.44 |
| 1:2A:2319:G:H22 | 14:2S:3:ARG:HD2 | 1.81 | 0.44 |
| 1:2A:2416:C:H2' | 1:2A:2417:C:C6 | 2.51 | 0.44 |
| 1:2A:2843:G:H1 | 1:2A:2874:C:H42 | 1.65 | 0.44 |
| 6:2G:3:LEU:HD13 | 26:24:25:TYR:CE2 | 2.52 | 0.44 |
| 6:2G:56:ALA:HB2 | 6:2G:153:ARG:HD2 | 1.98 | 0.44 |
| 15:2T:118:ARG:HG2 | 32:2a:1442(A):G:C8 | 2.52 | 0.44 |
| 17:2V:57:VAL:HG22 | 17:2V:99:ILE:HG23 | 1.99 | 0.44 |
| 24:22:28:LYS:HD2 | 24:22:60:LEU:HD11 | 1.99 | 0.44 |
| 32:2a:160:A:H1' | 32:2a:344:A:N7 | 2.31 | 0.44 |
| 32:2a:1113:C:H2' | 32:2a:1114:C:C6 | 2.52 | 0.44 |
| 32:2a:1241:G:H2' | 32:2a:1242:C:C6 | 2.52 | 0.44 |
| 37:2f:62:TRP:CH2 | 37:2f:64:GLN:HB2 | 2.52 | 0.44 |
| 38:2g:42:ILE:H | 38:2g:42:ILE:HG13 | 1.43 | 0.44 |
| 40:2i:17:VAL:HA | 40:2i:63:ILE:HG23 | 1.99 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 45:2n:24:CYS:HB3 | 45:2n:29:ARG:HB2 | 1.99 | 0.44 |
| 47:2p:6:LEU:HD23 | 47:2p:17:TYR:CD2 | 2.52 | 0.44 |
| 47:2p:9:PHE:CE1 | 47:2p:18:ARG:HD2 | 2.52 | 0.44 |
| 47:2p:21:VAL:HG21 | 47:2p:59:TRP:CD2 | 2.52 | 0.44 |
| 1:1A:26:G:H1' | 1:1A:514:A:N6 | 2.32 | 0.44 |
| 1:1A:264:C:O2' | 1:1A:265:A:H2' | 2.17 | 0.44 |
| 1:1A:1093:G:C6 | 1:1A:1094:U:C5 | 3.05 | 0.44 |
| 1:1A:1348:G:H1' | 59:1A:4764:HOH:O | 2.18 | 0.44 |
| 1:1A:1972:A:H2' | 1:1A:1973:G:H8 | 1.83 | 0.44 |
| 1:1A:2497:A:H5" | 59:1A:4335:HOH:O | 2.16 | 0.44 |
| 12:1Q:27:VAL:HG23 | 12:1Q:138:ASP:OD2 | 2.17 | 0.44 |
| 32:1a:130:A:N3 | 32:1a:263:A:O2' | 2.46 | 0.44 |
| 32:1a:598:U:H4' | 39:1h:94:TYR:CG | 2.52 | 0.44 |
| 32:1a:857:C:H2' | 32:1a:858:G:O4' | 2.17 | 0.44 |
| 32:1a:974:A:H8 | 32:1a:974:A:OP1 | 2.01 | 0.44 |
| 34:1c:10:PHE:CE2 | 34:1c:178:LEU:HG | 2.53 | 0.44 |
| 35:1d:166:LYS:HA | 35:1d:178:VAL:HG21 | 1.98 | 0.44 |
| 48:1q:75:ARG:NH2 | 48:1q:77:VAL:HG22 | 2.32 | 0.44 |
| 1:2A:9:U:H2' | 1:2A:10:G:C8 | 2.52 | 0.44 |
| 1:2A:315:G:H2' | 1:2A:316:C:C6 | 2.52 | 0.44 |
| 1:2A:1003:G:N2 | 1:2A:1153:C:C2 | 2.86 | 0.44 |
| 1:2A:1598:C:H2' | 1:2A:1599:C:C6 | 2.53 | 0.44 |
| 1:2A:1833:U:O2' | 1:2A:1969:A:N1 | 2.41 | 0.44 |
| 2:2B:83:G:H1 | 2:2B:94:C:H42 | 1.65 | 0.44 |
| 5:2F:117:ARG:NH2 | 5:2F:186:ILE:O | 2.50 | 0.44 |
| 11:2P:93:GLY:H | 11:2P:123:LEU:HD22 | 1.82 | 0.44 |
| 18:2W:9:TYR:H | 18:2W:102:HIS:CE1 | 2.34 | 0.44 |
| 26:24:50:VAL:HG21 | 44:2m:64:TRP:C | 2.42 | 0.44 |
| 28:26:13:CYS:SG | 28:26:47:THR:HG21 | 2.57 | 0.44 |
| 32:2a:1029:C:N3 | 32:2a:1032:G:N2 | 2.65 | 0.44 |
| 32:2a:1130:A:H5" | 40:2i:62:TYR:HE2 | 1.81 | 0.44 |
| 32:2a:1310:G:H5' | 44:2m:77:ASN:ND2 | 2.33 | 0.44 |
| 32:2a:1320:C:H2' | 32:2a:1321:C:O4' | 2.17 | 0.44 |
| 32:2a:1435:G:H2' | 32:2a:1436:U:C6 | 2.52 | 0.44 |
| 33:2b:16:HIS:CB | 33:2b:210:SER:HB2 | 2.47 | 0.44 |
| 34:2c:152:ILE:HB | 34:2c:167:TRP:HB3 | 1.99 | 0.44 |
| 36:2e:32:VAL:HB | 36:2e:58:ALA:HB1 | 1.98 | 0.44 |
| 37:2f:44:GLY:HA2 | 37:2f:59:TYR:CE1 | 2.53 | 0.44 |
| 40:2i:111:ARG:HD2 | 45:2n:61:TRP:NE1 | 2.32 | 0.44 |
| 41:2j:89:ASP:O | 41:2j:91:PRO:HD3 | 2.18 | 0.44 |
| 1:1A:16:G:H5" | 27:15:17:ASP:HB2 | 2.00 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1A:734:A:C4 | 1:1A:735:A:C8 | 3.05 | 0.44 |
| 1:1A:2134:A:O2' | 1:1A:2135:A:OP1 | 2.31 | 0.44 |
| 1:1A:2406:U:H2' | 1:1A:2406:U:OP2 | 2.16 | 0.44 |
| 1:1A:2488:A:H2' | 1:1A:2489:G:O4' | 2.18 | 0.44 |
| 5:1F:65:TRP:CZ2 | 5:1F:75:HIS:HD2 | 2.36 | 0.44 |
| 8:1I:117:GLU:HG3 | 8:1I:118:LYS:H | 1.82 | 0.44 |
| 10:1O:122:LEU:HD13 | 15:1T:72:VAL:HG11 | 1.99 | 0.44 |
| 32:1a:323:U:H5' | 51:1t:23:ARG:HB2 | 1.99 | 0.44 |
| 32:1a:902:G:H2' | 32:1a:903:G:H8 | 1.81 | 0.44 |
| 32:1a:1027:C:N4 | 32:1a:1034:G:C6 | 2.85 | 0.44 |
| 32:1a:1111:A:N6 | 34:1c:176:HIS:O | 2.50 | 0.44 |
| 32:1a:1125:U:H4' | 41:1j:5:ARG:NH2 | 2.32 | 0.44 |
| 32:1a:1401:G:C2 | 32:1a:1402:4OC:H1' | 2.52 | 0.44 |
| 32:1a:1458:G:H5" | 51:1t:31:SER:HB2 | 1.98 | 0.44 |
| 34:1c:20:SER:HB3 | 45:1n:54:PRO:HG3 | 1.99 | 0.44 |
| 35:1d:121:VAL:O | 35:1d:134:ASP:HA | 2.18 | 0.44 |
| 35:1d:182:LYS:HG3 | 35:1d:182:LYS:O | 2.18 | 0.44 |
| 39:1h:51:VAL:HG12 | 39:1h:52:ASP:H | 1.82 | 0.44 |
| 40:1i:18:PHE:HB2 | 40:1i:62:TYR:O | 2.17 | 0.44 |
| 40:1i:79:LEU:HD22 | 40:1i:104:ARG:HB2 | 1.98 | 0.44 |
| 45:1n:11:LYS:HB2 | 45:1n:11:LYS:NZ | 2.31 | 0.44 |
| 1:2A:128:C:H2' | 1:2A:129:C:C6 | 2.52 | 0.44 |
| 1:2A:478:A:C6 | 1:2A:480:A:C6 | 3.05 | 0.44 |
| 1:2A:824:A:H2' | 1:2A:825:C:O4' | 2.18 | 0.44 |
| 1:2A:2698:U:H2' | 1:2A:2699:C:C6 | 2.53 | 0.44 |
| 7:2H:20:ALA:HB1 | 7:2H:21:PRO:HD2 | 1.98 | 0.44 |
| 8:2I:26:ALA:HA | 8:2I:30:LEU:HB2 | 1.99 | 0.44 |
| 8:2I:79:ILE:HG13 | 8:2I:81:VAL:HB | 1.98 | 0.44 |
| 8:2I:84:GLY:N | 8:2I:87:LYS:HE2 | 2.33 | 0.44 |
| 26:24:8:LYS:HD3 | 26:24:8:LYS:HA | 1.79 | 0.44 |
| 32:2a:181:G:H4' | 32:2a:182:U:H5' | 2.00 | 0.44 |
| 32:2a:955:U:O4 | 32:2a:1225:A:N1 | 2.50 | 0.44 |
| 32:2a:1286:A:H3' | 32:2a:1286:A:H8 | 1.83 | 0.44 |
| 32:2a:1511:G:H2' | 32:2a:1512:U:O4' | 2.18 | 0.44 |
| 33:2b:13:ALA:O | 33:2b:17:PHE:HD2 | 1.99 | 0.44 |
| 36:2e:82:VAL:HB | 36:2e:138:ALA:HB2 | 1.99 | 0.44 |
| 40:2i:63:ILE:HD13 | 40:2i:77:ILE:HG23 | 1.99 | 0.44 |
| 1:1A:620:G:N3 | 1:1A:620:G:H5' | 2.33 | 0.44 |
| 1:1A:833:U:OP1 | 11:1P:45:LEU:HD13 | 2.18 | 0.44 |
| 1:1A:969:U:H2' | 1:1A:970:C:C6 | 2.52 | 0.44 |
| 1:1A:1553:A:C6 | 1:1A:1555:G:H1' | 2.53 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1A:1800:C:OP1 | 3:1D:260:ARG:NH2 | 2.50 | 0.44 |
| 1:1A:2233:U:H2' | 1:1A:2234:G:C8 | 2.52 | 0.44 |
| 5:1F:184:TYR:CE1 | 11:1P:3:LEU:HD11 | 2.52 | 0.44 |
| 6:1G:23:PHE:HB2 | 6:1G:25:TYR:CE2 | 2.52 | 0.44 |
| 16:1U:69:CYS:HB3 | 16:1U:74:LEU:HD13 | 1.99 | 0.44 |
| 17:1V:61:VAL:HA | 17:1V:94:LEU:HD23 | 2.00 | 0.44 |
| 26:14:60:GLN:C | 26:14:62:ARG:H | 2.25 | 0.44 |
| 32:1a:524:G:H2' | 32:1a:525:C:C6 | 2.52 | 0.44 |
| 34:1c:22:TRP:CE2 | 45:1n:54:PRO:HG2 | 2.52 | 0.44 |
| 39:1h:9:MET:HB2 | 39:1h:32:LYS:HE3 | 1.98 | 0.44 |
| 42:1k:44:SER:OG | 42:1k:47:VAL:HG23 | 2.17 | 0.44 |
| 45:1n:21:TYR:HE1 | 45:1n:23:ARG:HD3 | 1.82 | 0.44 |
| 46:1o:40:SER:O | 46:1o:44:LYS:HG3 | 2.17 | 0.44 |
| 1:2A:195:A:OP1 | 11:2P:46:LYS:NZ | 2.43 | 0.44 |
| 1:2A:311:A:C6 | 1:2A:328:U:C4 | 3.05 | 0.44 |
| 1:2A:480:A:N1 | 1:2A:503:A:N6 | 2.66 | 0.44 |
| 1:2A:1170:G:O6 | 1:2A:1180:C:N4 | 2.51 | 0.44 |
| 1:2A:1916:A:O5' | 1:2A:1916:A:H8 | 2.00 | 0.44 |
| 7:2H:13:LYS:HA | 7:2H:14:GLY:HA2 | 1.48 | 0.44 |
| 13:2R:57:ARG:NE | 13:2R:59:ASP:OD1 | 2.45 | 0.44 |
| 16:2U:50:ARG:O | 16:2U:54:LYS:NZ | 2.46 | 0.44 |
| 21:2Z:30:ASN:HB3 | 21:2Z:90:VAL:HB | 2.00 | 0.44 |
| 26:24:32:TYR:CE2 | 44:2m:50:GLU:HG3 | 2.52 | 0.44 |
| 32:2a:59:A:H3' | 32:2a:331:G:H22 | 1.82 | 0.44 |
| 32:2a:433:C:H2' | 32:2a:434:U:C6 | 2.53 | 0.44 |
| 32:2a:840:C:H5" | 32:2a:841:U:H5 | 1.83 | 0.44 |
| 32:2a:947:G:O3' | 44:2m:109:THR:OG1 | 2.36 | 0.44 |
| 32:2a:1072:G:H2' | 32:2a:1073:U:C6 | 2.52 | 0.44 |
| 38:2g:101:LEU:O | 38:2g:105:VAL:HG23 | 2.17 | 0.44 |
| 39:2h:9:MET:HE1 | 39:2h:32:LYS:HB3 | 2.00 | 0.44 |
| 42:2k:98:LEU:O | 42:2k:101:SER:OG | 2.36 | 0.44 |
| 1:1A:18:C:O2' | 1:1A:554:U:OP1 | 2.29 | 0.44 |
| 1:1A:1366:A:OP1 | 23:11:3:LYS:NZ | 2.36 | 0.44 |
| 1:1A:1501:C:O4' | 3:1D:100:GLY:HA2 | 2.18 | 0.44 |
| 1:1A:2203:U:O2' | 1:1A:2205:C:H5' | 2.16 | 0.44 |
| 1:1A:2274:A:C5 | 1:1A:2276:G:C8 | 3.06 | 0.44 |
| 1:1A:2294:C:H2' | 1:1A:2295:C:H6 | 1.82 | 0.44 |
| 2:1B:15:A:OP2 | 2:1B:69:G:N2 | 2.45 | 0.44 |
| 9:1N:23:LEU:HA | 9:1N:60:ILE:HD11 | 2.00 | 0.44 |
| 13:1R:65:LEU:HA | 13:1R:65:LEU:HD12 | 1.76 | 0.44 |
| 23:11:3:LYS:HB3 | 23:11:4:VAL:H | 1.51 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 32:1a:92:C:H2' | 32:1a:93:G:H8 | 1.82 | 0.44 |
| 32:1a:450:G:OP1 | 47:1p:43:LYS:NZ | 2.38 | 0.44 |
| 32:1a:889:A:H61 | 32:1a:907:A:H5" | 1.82 | 0.44 |
| 32:1a:1221:G:H4' | 50:1s:77:THR:HG22 | 2.00 | 0.44 |
| 32:1a:1502:A:C8 | 32:1a:1505:G:N2 | 2.85 | 0.44 |
| 35:1d:104:VAL:HG11 | 35:1d:140:VAL:HG21 | 1.98 | 0.44 |
| 35:1d:109:GLY:HA3 | 35:1d:165:MET:CG | 2.47 | 0.44 |
| 36:1e:50:GLU:HB2 | 36:1e:53:LEU:HD13 | 1.99 | 0.44 |
| 46:1o:87:ILE:HG22 | 46:1o:88:ARG:H | 1.83 | 0.44 |
| 1:2A:407:G:H2' | 1:2A:408:G:H8 | 1.82 | 0.44 |
| 1:2A:515:A:H1' | 1:2A:581:C:H1' | 1.99 | 0.44 |
| 1:2A:697:C:H2' | 1:2A:698:C:C6 | 2.52 | 0.44 |
| 1:2A:833:U:H1' | 11:2P:55:ARG:HH21 | 1.82 | 0.44 |
| 1:2A:1288:U:C2 | 1:2A:1327:C:O2 | 2.70 | 0.44 |
| 1:2A:1805:U:O2 | 3:2D:50:THR:HB | 2.18 | 0.44 |
| 1:2A:1919:A:N1 | 32:2a:1495:U:O2' | 2.36 | 0.44 |
| 1:2A:2207:G:H2' | 1:2A:2208:A:C2 | 2.53 | 0.44 |
| 1:2A:2305:A:H2' | 1:2A:2306:C:O4' | 2.18 | 0.44 |
| 1:2A:2419:U:H2' | 1:2A:2420:C:H6 | 1.81 | 0.44 |
| 1:2A:2815:C:C5' | 27:25:29:THR:HG21 | 2.48 | 0.44 |
| 3:2D:43:ARG:HA | 3:2D:48:ARG:O | 2.18 | 0.44 |
| 16:2U:104:GLN:NE2 | 16:2U:105:VAL:HG23 | 2.33 | 0.44 |
| 20:2Y:102:CYS:SG | 20:2Y:103:GLY:N | 2.90 | 0.44 |
| 32:2a:196:A:OP1 | 51:2t:68:LYS:NZ | 2.43 | 0.44 |
| 32:2a:487:A:H3' | 32:2a:488:C:C6 | 2.53 | 0.44 |
| 32:2a:1260:C:P | 32:2a:1284:C:H4' | 2.58 | 0.44 |
| 35:2d:112:VAL:HG13 | 35:2d:116:GLN:HE22 | 1.82 | 0.44 |
| 38:2g:76:ARG:O | 38:2g:87:VAL:N | 2.43 | 0.44 |
| 39:2h:110:ALA:HB1 | 39:2h:133:LEU:HD11 | 2.00 | 0.44 |
| 40:2i:6:GLY:HA3 | 40:2i:80:GLY:O | 2.18 | 0.44 |
| 50:2s:18:LYS:HD3 | 50:2s:31:ILE:HG21 | 1.99 | 0.44 |
| 1:1A:218:A:C2 | 1:1A:235:U:H4' | 2.53 | 0.44 |
| 1:1A:322:A:OP2 | 5:1F:169:ASN:HB2 | 2.17 | 0.44 |
| 1:1A:518:G:H4' | 18:1W:18:ARG:NE | 2.32 | 0.44 |
| 1:1A:774:A:N3 | 1:1A:774:A:H2' | 2.32 | 0.44 |
| 1:1A:857:C:H4' | 22:10:23:VAL:HG21 | 1.99 | 0.44 |
| 1:1A:922:U:H2' | 1:1A:923:C:C6 | 2.52 | 0.44 |
| 1:1A:1069:A:H4' | 1:1A:1070:A:C8 | 2.53 | 0.44 |
| 1:1A:1371:G:H2' | 1:1A:1372:U:C5 | 2.53 | 0.44 |
| 1:1A:2848:G:H1' | 1:1A:2867:G:N2 | 2.32 | 0.44 |
| 4:1E:9:VAL:HG13 | 4:1E:25:VAL:O | 2.18 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:1F:152:GLU:HB3 | 5:1F:190:GLU:HB3 | 1.99 | 0.44 |
| 5:1F:182:ASN:HD21 | 5:1F:185:ASP:CG | 2.23 | 0.44 |
| 7:1H:13:LYS:HA | 7:1H:14:GLY:HA2 | 1.54 | 0.44 |
| 16:1U:110:VAL:O | 16:1U:114:LYS:HG2 | 2.17 | 0.44 |
| 18:1W:76:VAL:HG13 | 18:1W:101:SER:HB3 | 2.00 | 0.44 |
| 29:17:30:VAL:O | 29:17:34:ARG:HG3 | 2.18 | 0.44 |
| 32:1a:352:C:O2' | 32:1a:354:G:OP1 | 2.32 | 0.44 |
| 32:1a:1179:A:O3' | 40:1i:103:THR:HB | 2.18 | 0.44 |
| 35:1d:57:ARG:HD3 | 35:1d:205:GLU:HB3 | 1.99 | 0.44 |
| 41:1j:50:ILE:HB | 45:1n:41:ARG:HD2 | 1.99 | 0.44 |
| 43:1l:42:THR:HA | 43:1l:53:ARG:O | 2.17 | 0.44 |
| 51:1t:88:VAL:O | 51:1t:92:LEU:HG | 2.17 | 0.44 |
| 54:1x:31:G:C2 | 54:1x:40:C:C2 | 3.05 | 0.44 |
| 1:2A:24:G:H1' | 18:2W:77:ASP:HB3 | 2.00 | 0.44 |
| 1:2A:109:G:H2' | 1:2A:110:G:O4' | 2.17 | 0.44 |
| 1:2A:194:G:H2' | 1:2A:195:A:O4' | 2.18 | 0.44 |
| 1:2A:754:C:H2' | 1:2A:755:C:C6 | 2.52 | 0.44 |
| 1:2A:1131:G:O6 | 1:2A:2040:C:H1' | 2.17 | 0.44 |
| 1:2A:1499:C:H2' | 1:2A:1500:G:C8 | 2.50 | 0.44 |
| 1:2A:1504:C:H2' | 1:2A:1505:C:C6 | 2.53 | 0.44 |
| 1:2A:1530:C:O2' | 1:2A:1531:C:O5' | 2.31 | 0.44 |
| 1:2A:2255:G:O2' | 54:2x:3:C:H5' | 2.18 | 0.44 |
| 1:2A:2317:C:N4 | 1:2A:2318:G:O6 | 2.50 | 0.44 |
| 1:2A:2529:G:H5" | 1:2A:2530:A:H5" | 2.00 | 0.44 |
| 6:2G:56:ALA:HA | 6:2G:59:GLU:HG2 | 1.99 | 0.44 |
| 8:2I:133:HIS:O | 8:2I:136:VAL:HG23 | 2.17 | 0.44 |
| 17:2V:50:PRO:HG2 | 17:2V:51:VAL:HG23 | 1.98 | 0.44 |
| 18:2W:11:ARG:NH2 | 18:2W:98:LYS:HD3 | 2.32 | 0.44 |
| 20:2Y:20:TYR:CE2 | 20:2Y:43:ASN:HA | 2.53 | 0.44 |
| 21:2Z:28:MET:HB3 | 21:2Z:35:ARG:HB2 | 2.00 | 0.44 |
| 26:24:48:ARG:O | 26:24:50:VAL:N | 2.49 | 0.44 |
| 32:2a:136:C:H42 | 32:2a:227:G:H1 | 1.66 | 0.44 |
| 32:2a:645:C:H2' | 32:2a:646:U:C6 | 2.53 | 0.44 |
| 32:2a:1009:G:H22 | 32:2a:1021:G:H1' | 1.82 | 0.44 |
| 32:2a:1129:C:H5' | 32:2a:1130:A:OP1 | 2.17 | 0.44 |
| 32:2a:1270:C:H2' | 32:2a:1271:G:H8 | 1.83 | 0.44 |
| 39:2h:103:VAL:HG21 | 39:2h:110:ALA:HB2 | 1.98 | 0.44 |
| 51:2t:14:LYS:HA | 51:2t:17:ARG:CZ | 2.47 | 0.44 |
| 1:1A:185:U:H4' | 1:1A:218:A:H4' | 1.99 | 0.44 |
| 1:1A:320:A:H4' | 1:1A:322:A:C8 | 2.53 | 0.44 |
| 1:1A:1032:A:H2 | 1:1A:1122:G:H22 | 1.66 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1A:1342:A:O2' | 1:1A:1344:G:OP2 | 2.30 | 0.44 |
| 1:1A:2299:G:N2 | 1:1A:2318:G:H1' | 2.32 | 0.44 |
| 1:1A:2726:U:O2' | 1:1A:2727:G:H8 | 2.00 | 0.44 |
| 7:1H:33:LEU:HD21 | 7:1H:136:ILE:HG13 | 2.00 | 0.44 |
| 8:1I:72:LEU:HA | 8:1I:75:LEU:HD11 | 1.99 | 0.44 |
| 18:1W:20:VAL:HG11 | 18:1W:44:ALA:HA | 1.98 | 0.44 |
| 21:1Z:52:SER:C | 21:1Z:54:HIS:H | 2.24 | 0.44 |
| 24:12:64:LEU:HD11 | 24:12:68:ARG:HE | 1.83 | 0.44 |
| 24:12:64:LEU:HD11 | 24:12:68:ARG:HH21 | 1.82 | 0.44 |
| 32:1a:189(D):C:H2' | 32:1a:189(E):U:O4' | 2.18 | 0.44 |
| 32:1a:339:C:H2' | 32:1a:340:U:C6 | 2.53 | 0.44 |
| 32:1a:363:A:C6 | 43:1l:31:PRO:HD2 | 2.52 | 0.44 |
| 32:1a:447:G:O6 | 32:1a:485:G:O2' | 2.28 | 0.44 |
| 32:1a:872:A:C8 | 32:1a:874:G:C8 | 3.06 | 0.44 |
| 32:1a:875:C:O2' | 39:1h:14:ARG:NH1 | 2.44 | 0.44 |
| 34:1c:116:VAL:HG21 | 34:1c:202:ILE:HD11 | 1.99 | 0.44 |
| 54:1x:37:A:C4 | 54:1x:38:A:C8 | 3.06 | 0.44 |
| 1:2A:1599:C:H2' | 1:2A:1600:C:C6 | 2.52 | 0.44 |
| 1:2A:1996:C:H4' | 1:2A:1997:G:H5' | 2.00 | 0.44 |
| 3:2D:132:PRO:HD3 | 3:2D:190:TYR:CZ | 2.53 | 0.44 |
| 3:2D:218:ARG:CZ | 3:2D:218:ARG:HB3 | 2.47 | 0.44 |
| 6:2G:96:ARG:N | 6:2G:99:MET:HE2 | 2.31 | 0.44 |
| 9:2N:48:MET:HE2 | 9:2N:48:MET:HB2 | 1.83 | 0.44 |
| 12:2Q:110:THR:HB | 12:2Q:113:GLN:HB2 | 2.00 | 0.44 |
| 15:2T:2:ASN:OD1 | 15:2T:5:ALA:N | 2.43 | 0.44 |
| 32:2a:131:C:H2' | 32:2a:132:C:H6 | 1.83 | 0.44 |
| 32:2a:457:C:H2' | 32:2a:458:C:C6 | 2.53 | 0.44 |
| 32:2a:687:A:N3 | 32:2a:688:G:H1' | 2.33 | 0.44 |
| 32:2a:1132:C:H2' | 32:2a:1133:G:C8 | 2.53 | 0.44 |
| 32:2a:1330:U:H4' | 44:2m:23:TYR:CZ | 2.53 | 0.44 |
| 33:2b:19:HIS:CE1 | 33:2b:206:ASP:HB2 | 2.53 | 0.44 |
| 44:2m:27:LYS:HD2 | 44:2m:27:LYS:HA | 1.69 | 0.44 |
| 1:1A:272(J):C:H2' | 1:1A:274:G:C8 | 2.41 | 0.44 |
| 1:1A:897:C:H2' | 1:1A:898:C:H6 | 1.81 | 0.44 |
| 8:1I:50:ARG:HA | 8:1I:53:ALA:HB3 | 1.99 | 0.44 |
| 12:1Q:57:HIS:HD2 | 12:1Q:117:ALA:HB2 | 1.82 | 0.44 |
| 32:1a:299:G:H2' | 32:1a:300:A:C8 | 2.52 | 0.44 |
| 32:1a:501:C:H1' | 32:1a:549:C:H1' | 2.00 | 0.44 |
| 32:1a:720:C:OP2 | 32:1a:721:G:O2' | 2.32 | 0.44 |
| 41:1j:38:ILE:HG12 | 41:1j:71:LEU:O | 2.17 | 0.44 |
| 44:1m:74:VAL:O | 44:1m:78:ILE:HG13 | 2.17 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 50:1s:11:VAL:O | 50:1s:13:ASP:N | 2.51 | 0.44 |
| 1:2A:300:A:OP1 | 20:2Y:86:ARG:NH2 | 2.48 | 0.44 |
| 1:2A:400:G:O6 | 59:2A:3957:HOH:O | 2.19 | 0.44 |
| 1:2A:452:G:C4 | 1:2A:458:G:C6 | 3.05 | 0.44 |
| 1:2A:748:G:OP1 | 1:2A:2612:C:N4 | 2.51 | 0.44 |
| 1:2A:1486:A:H2' | 1:2A:1487:G:H8 | 1.83 | 0.44 |
| 1:2A:1721:G:H8 | 1:2A:1741:A:H62 | 1.65 | 0.44 |
| 1:2A:1914:C:C6 | 1:2A:1915:5MU:H72 | 2.52 | 0.44 |
| 1:2A:1992:G:O2' | 59:2A:3921:HOH:O | 2.09 | 0.44 |
| 1:2A:2626:C:H2' | 1:2A:2627:G:O4' | 2.18 | 0.44 |
| 1:2A:2745:C:C4 | 1:2A:2746:U:C4 | 3.06 | 0.44 |
| 1:2A:2850:A:N7 | 1:2A:2868:A:O2' | 2.49 | 0.44 |
| 6:2G:179:PRO:HB2 | 26:24:42:PHE:CE2 | 2.53 | 0.44 |
| 11:2P:99:LEU:HD23 | 11:2P:102:ARG:HH12 | 1.83 | 0.44 |
| 32:2a:333:G:H4' | 51:2t:16:HIS:CE1 | 2.53 | 0.44 |
| 32:2a:737:A:H2' | 32:2a:738:C:C6 | 2.53 | 0.44 |
| 32:2a:955:U:H2' | 32:2a:956:U:O4' | 2.18 | 0.44 |
| 32:2a:1299:A:H2' | 32:2a:1299:A:N3 | 2.33 | 0.44 |
| 35:2d:181:MET:HE3 | 35:2d:181:MET:HB2 | 1.85 | 0.44 |
| 35:2d:191:ARG:NH1 | 35:2d:194:LEU:O | 2.49 | 0.44 |
| 1:1A:242:G:C8 | 30:18:5:LYS:HG2 | 2.53 | 0.44 |
| 1:1A:287:C:H2' | 1:1A:288:C:C6 | 2.53 | 0.44 |
| 1:1A:740:U:OP2 | 59:1A:4241:HOH:O | 2.21 | 0.44 |
| 1:1A:963:U:H2' | 1:1A:964:C:C6 | 2.52 | 0.44 |
| 1:1A:1038:C:H42 | 1:1A:1117:G:H1 | 1.66 | 0.44 |
| 1:1A:1054:A:N1 | 1:1A:1105:U:O2 | 2.51 | 0.44 |
| 1:1A:1919:A:N1 | 32:1a:1495:U:O2' | 2.38 | 0.44 |
| 1:1A:2424:C:O2 | 1:1A:2429:G:O2' | 2.31 | 0.44 |
| 5:1F:34:TRP:CZ2 | 11:1P:8:PRO:HB3 | 2.52 | 0.44 |
| 11:1P:63:PRO:HD3 | 30:18:27:THR:HG22 | 2.00 | 0.44 |
| 32:1a:333:G:H2' | 32:1a:334:C:H6 | 1.83 | 0.44 |
| 32:1a:555:C:H2' | 32:1a:556:C:C6 | 2.53 | 0.44 |
| 32:1a:890:G:O2' | 32:1a:906:G:O6 | 2.28 | 0.44 |
| 32:1a:1149:C:H2' | 32:1a:1150:U:C6 | 2.52 | 0.44 |
| 32:1a:1261:A:H3' | 32:1a:1262:C:H6 | 1.82 | 0.44 |
| 40:1i:4:TYR:CZ | 40:1i:88:TYR:HD1 | 2.36 | 0.44 |
| 47:1p:69:THR:O | 47:1p:73:LEU:HG | 2.17 | 0.44 |
| 48:1q:56:VAL:HB | 48:1q:78:GLU:HB3 | 1.99 | 0.44 |
| 48:1q:86:GLU:O | 48:1q:90:ILE:HG13 | 2.17 | 0.44 |
| 52:1u:9:ARG:HH22 | 52:1u:10:ARG:NH2 | 2.16 | 0.44 |
| 1:2A:39:C:H2' | 1:2A:40:C:C6 | 2.53 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:2A:271(G):C:H2' | 1:2A:271(H):G:H8 | 1.83 | 0.44 |
| 1:2A:631:A:H2' | 1:2A:632:A:O4' | 2.18 | 0.44 |
| 1:2A:826:U:H2' | 1:2A:828:U:O4' | 2.18 | 0.44 |
| 1:2A:1430:C:H2' | 1:2A:1431:U:C6 | 2.53 | 0.44 |
| 1:2A:2224:G:OP1 | 3:2D:268:ARG:NE | 2.51 | 0.44 |
| 1:2A:2262:U:P | 22:20:19:LYS:HE2 | 2.57 | 0.44 |
| 1:2A:2345:G:H1' | 1:2A:2382:G:H5' | 2.00 | 0.44 |
| 8:2I:101:LEU:HB3 | 8:2I:107:VAL:O | 2.18 | 0.44 |
| 12:2Q:139:GLU:C | 12:2Q:141:GLN:H | 2.26 | 0.44 |
| 15:2T:23:ARG:HD3 | 15:2T:120:ARG:NH1 | 2.33 | 0.44 |
| 21:2Z:131:ARG:H | 21:2Z:131:ARG:HG3 | 1.49 | 0.44 |
| 23:21:73:LEU:HD23 | 23:21:73:LEU:HA | 1.81 | 0.44 |
| 32:2a:417:C:H2' | 32:2a:418:C:C6 | 2.52 | 0.44 |
| 32:2a:505:G:H2' | 32:2a:506:G:C8 | 2.53 | 0.44 |
| 32:2a:620:C:H2' | 32:2a:621:A:O4' | 2.18 | 0.44 |
| 32:2a:1122:U:C2 | 32:2a:1123:A:C8 | 3.05 | 0.44 |
| 32:2a:1395:C:N4 | 32:2a:1396:A:H62 | 2.16 | 0.44 |
| 34:2c:32:LEU:O | 34:2c:36:ASP:HB2 | 2.17 | 0.44 |
| 40:2i:102:LEU:H | 40:2i:102:LEU:HD23 | 1.83 | 0.44 |
| 1:1A:593:G:C4' | 30:18:4:MET:HE2 | 2.48 | 0.43 |
| 1:1A:836:G:C5 | 1:1A:837:C:C4 | 3.06 | 0.43 |
| 1:1A:1030:G:OP2 | 12:1Q:128:LYS:NZ | 2.51 | 0.43 |
| 1:1A:1174:A:H1' | 1:1A:1175:U:C5' | 2.48 | 0.43 |
| 1:1A:1210:A:H5" | 1:1A:1212:G:O4' | 2.18 | 0.43 |
| 1:1A:1912:A:HO2' | 32:1a:1494:G:HO2' | 1.54 | 0.43 |
| 1:1A:2346:A:C5 | 1:1A:2383:G:C2 | 3.05 | 0.43 |
| 1:1A:2552:2MU:O5' | 1:1A:2552:2MU:H6 | 2.18 | 0.43 |
| 7:1H:41:MET:HE1 | 7:1H:54:ARG:HB3 | 2.00 | 0.43 |
| 9:1N:75:TYR:CE2 | 9:1N:77:GLY:HA2 | 2.53 | 0.43 |
| 15:1T:91:ARG:HH11 | 15:1T:120:ARG:NH1 | 2.16 | 0.43 |
| 16:1U:76:TYR:CZ | 16:1U:80:ILE:HG13 | 2.53 | 0.43 |
| 32:1a:112:G:H21 | 32:1a:354:G:C4' | 2.31 | 0.43 |
| 32:1a:899:C:H2' | 32:1a:900:A:C8 | 2.53 | 0.43 |
| 32:1a:1034:G:C2 | 32:1a:1035:A:C4 | 3.05 | 0.43 |
| 33:1b:114:ARG:NH1 | 33:1b:117:GLU:OE1 | 2.51 | 0.43 |
| 35:1d:11:LEU:HG | 35:1d:66:ARG:HD3 | 2.00 | 0.43 |
| 37:1f:3:ARG:HA | 37:1f:65:VAL:O | 2.17 | 0.43 |
| 1:2A:312:G:H4' | 1:2A:331:A:N3 | 2.33 | 0.43 |
| 1:2A:493:G:H2' | 1:2A:494:G:O4' | 2.18 | 0.43 |
| 1:2A:1022:G:H22 | 1:2A:1142(A):A:H2 | 1.63 | 0.43 |
| 1:2A:1710:C:H5' | 1:2A:2859:G:H1' | 1.99 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:2A:1902:C:OP1 | 3:2D:242:ARG:HD2 | 2.18 | 0.43 |
| 1:2A:2019:A:N7 | 27:25:9:LYS:HE2 | 2.33 | 0.43 |
| 1:2A:2131:G:H1 | 1:2A:2158:A:H62 | 1.66 | 0.43 |
| 1:2A:2187:G:H2' | 1:2A:2188:C:O4' | 2.18 | 0.43 |
| 1:2A:2410:G:C2 | 1:2A:2411:A:H1' | 2.53 | 0.43 |
| 2:2B:11:C:H3' | 2:2B:12:C:H6 | 1.83 | 0.43 |
| 4:2E:11:MET:HE2 | 4:2E:11:MET:HB3 | 1.78 | 0.43 |
| 9:2N:13:TRP:CE2 | 9:2N:133:GLN:HG2 | 2.53 | 0.43 |
| 10:2O:71:ARG:NH2 | 10:2O:122:LEU:O | 2.40 | 0.43 |
| 32:2a:265:G:H5' | 48:2q:64:PRO:O | 2.17 | 0.43 |
| 32:2a:1051:C:H2' | 32:2a:1052:U:H6 | 1.82 | 0.43 |
| 57:2a:3210:V7A:OAZ | 57:2a:3210:V7A:OAY | 2.31 | 0.43 |
| 34:2c:50:ALA:HB1 | 34:2c:70:VAL:HG11 | 1.99 | 0.43 |
| 36:2e:67:VAL:HG22 | 36:2e:69:VAL:H | 1.83 | 0.43 |
| 41:2j:48:THR:HG23 | 41:2j:62:HIS:CE1 | 2.53 | 0.43 |
| 1:1A:709:U:H2' | 1:1A:710:G:C8 | 2.53 | 0.43 |
| 1:1A:1386:C:H2' | 1:1A:1387:C:C6 | 2.53 | 0.43 |
| 7:1H:127:GLU:OE2 | 7:1H:130:ARG:NE | 2.50 | 0.43 |
| 18:1W:62:HIS:O | 18:1W:64:MET:HG3 | 2.18 | 0.43 |
| 21:1Z:7:ALA:HB3 | 21:1Z:61:LEU:HD12 | 2.00 | 0.43 |
| 32:1a:193:C:H2' | 32:1a:194:C:C6 | 2.51 | 0.43 |
| 32:1a:841:U:O2 | 32:1a:841:U:H2' | 2.17 | 0.43 |
| 32:1a:1314:C:H2' | 32:1a:1315:U:C6 | 2.53 | 0.43 |
| 33:1b:15:VAL:HG13 | 33:1b:209:ARG:HG3 | 2.00 | 0.43 |
| 1:2A:68:G:H2' | 1:2A:69:C:O4' | 2.19 | 0.43 |
| 1:2A:357:A:H2' | 1:2A:358:U:C6 | 2.53 | 0.43 |
| 1:2A:740:U:H2' | 1:2A:741:G:H8 | 1.83 | 0.43 |
| 1:2A:2096:U:H2' | 1:2A:2097:C:C6 | 2.53 | 0.43 |
| 3:2D:71:ASP:CB | 3:2D:103:ARG:HH12 | 2.28 | 0.43 |
| 15:2T:106:SER:N | 15:2T:109:GLU:OE1 | 2.45 | 0.43 |
| 25:23:18:ASP:OD1 | 25:23:18:ASP:N | 2.51 | 0.43 |
| 32:2a:136:C:O2' | 47:2p:63:GLY:O | 2.31 | 0.43 |
| 32:2a:772:U:H2' | 32:2a:773:G:O4' | 2.18 | 0.43 |
| 32:2a:1225:A:OP1 | 44:2m:103:THR:OG1 | 2.31 | 0.43 |
| 33:2b:103:THR:HG23 | 33:2b:180:LEU:HD21 | 1.98 | 0.43 |
| 35:2d:150:GLU:H | 35:2d:150:GLU:HG3 | 1.59 | 0.43 |
| 39:2h:4:ASP:HB3 | 39:2h:7:ALA:HB3 | 2.00 | 0.43 |
| 43:2l:110:VAL:HG23 | 43:2l:120:TYR:HB3 | 2.00 | 0.43 |
| 1:1A:182:A:H8 | 1:1A:182:A:OP2 | 2.00 | 0.43 |
| 1:1A:572:A:H2' | 1:1A:573:G:O4' | 2.18 | 0.43 |
| 1:1A:893:C:H2' | 1:1A:894:C:C6 | 2.52 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1A:1693:U:OP1 | 59:1A:4295:HOH:O | 2.21 | 0.43 |
| 1:1A:2273:A:H2' | 1:1A:2274:A:C8 | 2.53 | 0.43 |
| 1:1A:2407:G:OP1 | 59:1A:4294:HOH:O | 2.21 | 0.43 |
| 1:1A:2556:C:H2' | 1:1A:2557:G:O4' | 2.18 | 0.43 |
| 2:1B:57:A:H1' | 6:1G:29:TRP:HB2 | 2.01 | 0.43 |
| 4:1E:37:ARG:O | 4:1E:45:THR:HA | 2.18 | 0.43 |
| 5:1F:116:ASP:OD1 | 5:1F:119:ARG:NH2 | 2.51 | 0.43 |
| 6:1G:131:TYR:CE2 | 6:1G:133:LEU:HD23 | 2.54 | 0.43 |
| 7:1H:137:ASP:HB3 | 7:1H:140:LYS:HB3 | 2.00 | 0.43 |
| 12:1Q:10:ARG:HH21 | 12:1Q:90:VAL:H | 1.64 | 0.43 |
| 13:1R:79:LEU:HA | 13:1R:83:ILE:HB | 1.99 | 0.43 |
| 13:1R:118:GLU:H | 13:1R:118:GLU:CD | 2.26 | 0.43 |
| 15:1T:106:SER:O | 15:1T:110:ILE:HG13 | 2.18 | 0.43 |
| 25:13:7:LYS:HA | 25:13:33:GLN:O | 2.18 | 0.43 |
| 29:17:12:ARG:NH2 | 29:17:44:PRO:HB3 | 2.33 | 0.43 |
| 32:1a:411:A:OP1 | 35:1d:30:LYS:HE3 | 2.17 | 0.43 |
| 32:1a:729:A:H2' | 32:1a:730:G:H8 | 1.83 | 0.43 |
| 32:1a:782:A:O3' | 32:1a:1515:C:H4' | 2.18 | 0.43 |
| 32:1a:831:U:H2' | 32:1a:832:C:H6 | 1.82 | 0.43 |
| 32:1a:1220:G:H2' | 32:1a:1221:G:H8 | 1.83 | 0.43 |
| 32:1a:1417:G:C6 | 32:1a:1482:G:C6 | 3.06 | 0.43 |
| 32:1a:1524:C:OP1 | 42:1k:120:ARG:NH1 | 2.52 | 0.43 |
| 44:1m:106:ASN:HB2 | 44:1m:107:ALA:H | 1.49 | 0.43 |
| 44:1m:121:LYS:HE3 | 44:1m:121:LYS:HB2 | 1.87 | 0.43 |
| 50:1s:11:VAL:C | 50:1s:13:ASP:H | 2.26 | 0.43 |
| 1:2A:17:G:H2' | 1:2A:18:C:C6 | 2.52 | 0.43 |
| 1:2A:71:A:H5" | 1:2A:73:A:C8 | 2.53 | 0.43 |
| 1:2A:873:G:N2 | 1:2A:905:U:O2 | 2.52 | 0.43 |
| 1:2A:1162:G:H2' | 1:2A:1163:G:H8 | 1.82 | 0.43 |
| 1:2A:1491:G:H2' | 1:2A:1492:G:H8 | 1.83 | 0.43 |
| 1:2A:1695:G:H8 | 3:2D:8:PRO:O | 2.00 | 0.43 |
| 1:2A:2397:G:N2 | 1:2A:2420:C:H1' | 2.33 | 0.43 |
| 2:2B:24:G:H4' | 2:2B:25:A:N7 | 2.33 | 0.43 |
| 3:2D:68:LYS:HE3 | 3:2D:70:TRP:CZ2 | 2.53 | 0.43 |
| 4:2E:37:ARG:HB2 | 4:2E:46:ALA:HB3 | 2.00 | 0.43 |
| 6:2G:96:ARG:O | 6:2G:99:MET:HB3 | 2.19 | 0.43 |
| 8:2I:84:GLY:CA | 8:2I:87:LYS:HE2 | 2.48 | 0.43 |
| 10:2O:64:ARG:HB2 | 10:2O:79:PHE:CG | 2.53 | 0.43 |
| 10:2O:68:GLU:HB3 | 10:2O:78:ARG:HB3 | 1.98 | 0.43 |
| 18:2W:70:TYR:OH | 18:2W:72:LYS:HG3 | 2.18 | 0.43 |
| 32:2a:302:G:N3 | 32:2a:556:C:H4' | 2.33 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 32:2a:309:G:O2' | 32:2a:607:A:N1 | 2.47 | 0.43 |
| 32:2a:596:C:N3 | 32:2a:644:G:N1 | 2.42 | 0.43 |
| 32:2a:1304:G:O2' | 32:2a:1333:A:N6 | 2.47 | 0.43 |
| 33:2b:120:ALA:O | 33:2b:125:PRO:HD2 | 2.18 | 0.43 |
| 51:2t:30:LYS:HE3 | 51:2t:30:LYS:HB2 | 1.73 | 0.43 |
| 1:1A:450:G:OP2 | 59:1A:4296:HOH:O | 2.21 | 0.43 |
| 1:1A:557:U:H2' | 1:1A:558:G:C8 | 2.53 | 0.43 |
| 1:1A:897:C:H2' | 1:1A:898:C:C6 | 2.54 | 0.43 |
| 1:1A:1107:G:O2' | 1:1A:1108:U:OP1 | 2.27 | 0.43 |
| 1:1A:2335:A:C8 | 1:1A:2337:G:C5 | 3.06 | 0.43 |
| 7:1H:109:PHE:HB3 | 7:1H:111:HIS:CD2 | 2.52 | 0.43 |
| 32:1a:107:G:H2' | 32:1a:108:G:O4' | 2.19 | 0.43 |
| 32:1a:872:A:H4' | 32:1a:873:A:OP1 | 2.18 | 0.43 |
| 32:1a:957:U:O2' | 32:1a:959:A:N7 | 2.34 | 0.43 |
| 32:1a:1508:G:H2' | 32:1a:1509:C:O4' | 2.18 | 0.43 |
| 33:1b:55:PHE:CE1 | 33:1b:218:ALA:HA | 2.53 | 0.43 |
| 34:1c:52:LEU:HD13 | 34:1c:70:VAL:HG12 | 2.00 | 0.43 |
| 36:1e:11:ILE:HB | 36:1e:31:LEU:HB3 | 2.01 | 0.43 |
| 39:1h:11:THR:HG22 | 39:1h:14:ARG:NH1 | 2.31 | 0.43 |
| 46:1o:74:ASP:OD2 | 46:1o:77:ARG:HD3 | 2.19 | 0.43 |
| 1:2A:464:U:H4' | 29:27:5:TRP:CZ3 | 2.53 | 0.43 |
| 1:2A:576:U:H2' | 1:2A:577:G:C8 | 2.52 | 0.43 |
| 1:2A:854:G:H2' | 1:2A:855:G:C8 | 2.48 | 0.43 |
| 1:2A:900:A:O2' | 1:2A:901:A:H5' | 2.18 | 0.43 |
| 1:2A:998:C:H2' | 1:2A:999:U:O4' | 2.18 | 0.43 |
| 1:2A:1479:G:H1' | 1:2A:1558:A:OP1 | 2.18 | 0.43 |
| 1:2A:2477:C:H2' | 31:29:2:LYS:HE2 | 2.00 | 0.43 |
| 5:2F:40:GLN:NE2 | 5:2F:182:ASN:HB2 | 2.33 | 0.43 |
| 34:2c:79:ARG:N | 34:2c:82:GLU:HB3 | 2.25 | 0.43 |
| 42:2k:20:TYR:CZ | 42:2k:83:ILE:HD13 | 2.53 | 0.43 |
| 1:1A:184:C:H2' | 1:1A:185:U:C6 | 2.54 | 0.43 |
| 1:1A:376:C:H2' | 1:1A:377:C:C6 | 2.53 | 0.43 |
| 1:1A:1114:G:H2' | 1:1A:1115:G:O4' | 2.19 | 0.43 |
| 1:1A:1827:C:OP2 | 3:1D:222:ARG:HD2 | 2.19 | 0.43 |
| 1:1A:2334:G:H4' | 1:1A:2335:A:OP2 | 2.19 | 0.43 |
| 8:1I:114:LEU:HD13 | 8:1I:130:TYR:HD1 | 1.84 | 0.43 |
| 10:1O:20:MET:HE2 | 10:1O:44:LYS:HE2 | 2.00 | 0.43 |
| 25:13:15:TYR:CE2 | 25:13:53:LEU:HD21 | 2.53 | 0.43 |
| 32:1a:1121:U:H2' | 32:1a:1122:U:C6 | 2.54 | 0.43 |
| 33:1b:70:PHE:O | 33:1b:92:TYR:HA | 2.18 | 0.43 |
| 35:1d:200:GLU:HG2 | 35:1d:201:GLN:N | 2.32 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 36:1e:41:VAL:O | 36:1e:66:MET:HA | 2.17 | 0.43 |
| 39:1h:28:ALA:HA | 39:1h:59:LEU:HG | 2.01 | 0.43 |
| 43:1l:28:LYS:HE3 | 43:1l:64:TYR:CE2 | 2.54 | 0.43 |
| 1:2A:250:G:C6 | 1:2A:251:A:C6 | 3.06 | 0.43 |
| 1:2A:764:A:O4' | 3:2D:213:ARG:HG3 | 2.19 | 0.43 |
| 1:2A:839:U:H2' | 1:2A:840:C:C6 | 2.53 | 0.43 |
| 1:2A:1814:G:O3' | 3:2D:54:ARG:NH2 | 2.52 | 0.43 |
| 1:2A:1815:A:OP2 | 3:2D:54:ARG:NH2 | 2.45 | 0.43 |
| 1:2A:1927:A:C6 | 1:2A:1928:A:C6 | 3.06 | 0.43 |
| 1:2A:2295:C:H1' | 1:2A:2338:G:N2 | 2.32 | 0.43 |
| 2:2B:3:C:H2' | 2:2B:4:C:C6 | 2.53 | 0.43 |
| 2:2B:54:G:H21 | 6:2G:29:TRP:HE1 | 1.66 | 0.43 |
| 3:2D:206:LEU:HD22 | 3:2D:211:ARG:HG2 | 1.99 | 0.43 |
| 7:2H:109:PHE:C | 7:2H:111:HIS:H | 2.27 | 0.43 |
| 8:2I:97:ILE:O | 8:2I:101:LEU:HB2 | 2.19 | 0.43 |
| 9:2N:1:MET:HE1 | 16:2U:94:ASN:ND2 | 2.33 | 0.43 |
| 10:2O:64:ARG:HB2 | 10:2O:79:PHE:CD2 | 2.54 | 0.43 |
| 13:2R:87:TYR:OH | 13:2R:117:VAL:O | 2.35 | 0.43 |
| 32:2a:187:C:O2 | 51:2t:103:GLY:HA2 | 2.19 | 0.43 |
| 32:2a:189(L):G:H2' | 32:2a:190:U:C6 | 2.53 | 0.43 |
| 32:2a:404:U:H2' | 32:2a:405:U:C6 | 2.52 | 0.43 |
| 32:2a:600:C:H5' | 39:2h:129:VAL:HA | 2.00 | 0.43 |
| 34:2c:104:GLN:HG3 | 34:2c:105:GLU:N | 2.33 | 0.43 |
| 1:1A:414:C:H2' | 1:1A:415:A:C8 | 2.54 | 0.43 |
| 1:1A:1916:A:H2' | 1:1A:1917:PSU:O4' | 2.19 | 0.43 |
| 1:1A:2319:G:C2 | 14:1S:3:ARG:HA | 2.53 | 0.43 |
| 1:1A:2375:G:O2' | 1:1A:2377:A:N7 | 2.46 | 0.43 |
| 1:1A:2393:A:H2' | 1:1A:2394:C:C6 | 2.50 | 0.43 |
| 1:1A:2729:G:H2' | 1:1A:2730:C:O4' | 2.19 | 0.43 |
| 5:1F:176:LEU:HA | 5:1F:176:LEU:HD23 | 1.81 | 0.43 |
| 7:1H:105:LEU:HB2 | 7:1H:113:VAL:HB | 2.01 | 0.43 |
| 9:1N:20:GLY:HA2 | 9:1N:61:ARG:HD2 | 2.01 | 0.43 |
| 21:1Z:24:LEU:HD21 | 21:1Z:86:VAL:HG13 | 2.00 | 0.43 |
| 32:1a:44:G:H2' | 32:1a:45:U:O4' | 2.19 | 0.43 |
| 32:1a:66:G:O4' | 32:1a:173:U:C4 | 2.72 | 0.43 |
| 32:1a:198:G:C5 | 32:1a:220:G:C2 | 3.07 | 0.43 |
| 32:1a:270:A:H2' | 32:1a:271:C:O4' | 2.18 | 0.43 |
| 32:1a:781:A:O2' | 32:1a:1522:U:O2 | 2.33 | 0.43 |
| 32:1a:866:C:C4 | 32:1a:867:G:H1' | 2.54 | 0.43 |
| 32:1a:1284:C:H3' | 32:1a:1285:A:H8 | 1.84 | 0.43 |
| 32:1a:1516:G:H2' | 32:1a:1518:MA6:OP2 | 2.19 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 48:1q:15:MET:HE1 | 48:1q:43:LEU:HD22 | 2.00 | 0.43 |
| 50:1s:40:ILE:HA | 50:1s:44:MET:SD | 2.59 | 0.43 |
| 1:2A:359:A:H2' | 1:2A:360:G:O4' | 2.17 | 0.43 |
| 1:2A:610:G:H2' | 1:2A:611:C:C6 | 2.53 | 0.43 |
| 1:2A:787:U:OP1 | 59:2A:3962:HOH:O | 2.20 | 0.43 |
| 1:2A:1121:C:H2' | 1:2A:1122:G:O4' | 2.18 | 0.43 |
| 1:2A:2540:C:O2' | 1:2A:2740:A:N3 | 2.48 | 0.43 |
| 1:2A:2654:A:N1 | 1:2A:2665:A:H5" | 2.34 | 0.43 |
| 2:2B:57:A:N3 | 6:2G:29:TRP:HB3 | 2.34 | 0.43 |
| 4:2E:12:THR:HG21 | 15:2T:11:GLU:HG2 | 2.00 | 0.43 |
| 9:2N:54:VAL:HB | 9:2N:122:VAL:HG22 | 2.00 | 0.43 |
| 32:2a:472:A:H5" | 47:2p:80:PHE:HB3 | 2.01 | 0.43 |
| 32:2a:515:G:H2' | 32:2a:516:PSU:H6 | 1.84 | 0.43 |
| 32:2a:1012:U:H2' | 32:2a:1013:G:C8 | 2.53 | 0.43 |
| 32:2a:1232:U:H5" | 40:2i:124:GLN:O | 2.18 | 0.43 |
| 33:2b:74:LYS:HD2 | 33:2b:166:ASP:HB2 | 1.99 | 0.43 |
| 34:2c:83:ARG:O | 34:2c:87:LEU:HB2 | 2.19 | 0.43 |
| 49:2r:58:LEU:HD23 | 49:2r:58:LEU:HA | 1.74 | 0.43 |
| 51:2t:36:LEU:CD2 | 51:2t:58:LYS:HG3 | 2.49 | 0.43 |
| 1:1A:250:G:P | 30:18:13:ARG:HH22 | 2.42 | 0.43 |
| 1:1A:253:C:H2' | 1:1A:254:G:O4' | 2.19 | 0.43 |
| 1:1A:459:U:H2' | 1:1A:460:A:H8 | 1.83 | 0.43 |
| 1:1A:725:G:C6 | 1:1A:726:G:N1 | 2.86 | 0.43 |
| 1:1A:858:U:O2 | 1:1A:2268:A:H2' | 2.19 | 0.43 |
| 1:1A:881:G:H3' | 1:1A:882:G:H8 | 1.83 | 0.43 |
| 1:1A:1142(A):A:C4 | 1:1A:1144:G:N7 | 2.87 | 0.43 |
| 1:1A:2259:G:H1' | 1:1A:2427:C:H2' | 2.01 | 0.43 |
| 1:1A:2292:C:H4' | 1:1A:2375:G:H4' | 2.01 | 0.43 |
| 5:1F:9:ILE:HG21 | 5:1F:125:LEU:HD13 | 1.99 | 0.43 |
| 10:1O:24:VAL:HG13 | 10:1O:33:ALA:HB2 | 2.01 | 0.43 |
| 12:1Q:130:LYS:HE2 | 12:1Q:130:LYS:HB3 | 1.71 | 0.43 |
| 15:1T:15:VAL:HG13 | 15:1T:79:HIS:CE1 | 2.54 | 0.43 |
| 15:1T:65:LYS:HG2 | 15:1T:66:VAL:N | 2.33 | 0.43 |
| 20:1Y:13:VAL:HG12 | 20:1Y:74:PRO:HA | 2.01 | 0.43 |
| 26:14:53:GLU:HG3 | 26:14:54:GLY:H | 1.84 | 0.43 |
| 28:16:9:LEU:HD13 | 28:16:51:GLU:HB2 | 2.01 | 0.43 |
| 32:1a:90:U:H4' | 32:1a:91:C:OP1 | 2.18 | 0.43 |
| 32:1a:567:G:O6 | 43:1l:5:PRO:HD3 | 2.18 | 0.43 |
| 34:1c:19:GLU:HB3 | 34:1c:40:ARG:HH21 | 1.83 | 0.43 |
| 36:1e:92:LYS:HB3 | 36:1e:119:LEU:HB2 | 1.99 | 0.43 |
| 44:1m:17:VAL:O | 44:1m:20:THR:OG1 | 2.27 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 44:1m:30:ALA:O | 44:1m:34:LEU:HG | 2.19 | 0.43 |
| 50:1s:12:ASP:C | 50:1s:14:HIS:H | 2.26 | 0.43 |
| 1:2A:652(B):A:N6 | 1:2A:655:A:H1' | 2.34 | 0.43 |
| 1:2A:679:C:H2' | 1:2A:680:G:C8 | 2.53 | 0.43 |
| 1:2A:1400:G:H2' | 1:2A:1401:G:C8 | 2.54 | 0.43 |
| 1:2A:1907:G:C6 | 1:2A:1908:C:C4 | 3.05 | 0.43 |
| 3:2D:184:LYS:CE | 3:2D:271:ILE:HD11 | 2.48 | 0.43 |
| 6:2G:173:LEU:HB3 | 6:2G:178:PHE:CG | 2.54 | 0.43 |
| 15:2T:6:LEU:O | 15:2T:10:VAL:HG23 | 2.19 | 0.43 |
| 15:2T:64:ARG:NH1 | 15:2T:103:ARG:HA | 2.34 | 0.43 |
| 32:2a:106:C:O2' | 32:2a:379:C:OP1 | 2.33 | 0.43 |
| 32:2a:232:G:O2' | 32:2a:263:A:N1 | 2.49 | 0.43 |
| 32:2a:247:G:O2' | 32:2a:282:A:N1 | 2.47 | 0.43 |
| 32:2a:353:A:OP1 | 59:2a:3311:HOH:O | 2.21 | 0.43 |
| 32:2a:781:A:OP1 | 32:2a:1523:G:H5' | 2.18 | 0.43 |
| 32:2a:1122:U:H2' | 32:2a:1123:A:O4' | 2.18 | 0.43 |
| 35:2d:12:CYS:O | 35:2d:16:GLY:N | 2.52 | 0.43 |
| 40:2i:3:GLN:NE2 | 40:2i:20:ARG:HH21 | 2.17 | 0.43 |
| 50:2s:16:LEU:HD23 | 50:2s:16:LEU:H | 1.83 | 0.43 |
| 54:2x:10:G:N2 | 54:2x:26:G:H1' | 2.34 | 0.43 |
| 1:1A:607:U:C5 | 1:1A:620:G:C5 | 3.07 | 0.43 |
| 1:1A:646:A:H2' | 1:1A:647:G:O4' | 2.19 | 0.43 |
| 1:1A:724:U:H2' | 1:1A:725:G:O4' | 2.19 | 0.43 |
| 1:1A:1794:U:H2' | 1:1A:1795:C:C6 | 2.54 | 0.43 |
| 1:1A:2469:A:C2 | 1:1A:2470:G:H1' | 2.54 | 0.43 |
| 2:1B:1:U:HO2' | 2:1B:2:C:P | 2.40 | 0.43 |
| 6:1G:131:TYR:HE2 | 6:1G:133:LEU:HD23 | 1.84 | 0.43 |
| 6:1G:179:PRO:HG3 | 26:14:43:TYR:CZ | 2.54 | 0.43 |
| 15:1T:26:ASP:OD1 | 15:1T:120:ARG:NH2 | 2.39 | 0.43 |
| 21:1Z:69:THR:HG22 | 21:1Z:90:VAL:HG22 | 2.01 | 0.43 |
| 28:16:40:CYS:SG | 28:16:42:TRP:HB2 | 2.59 | 0.43 |
| 32:1a:92:C:H2' | 32:1a:93:G:C8 | 2.53 | 0.43 |
| 32:1a:435:C:H2' | 32:1a:436:C:C6 | 2.53 | 0.43 |
| 32:1a:560:U:H6 | 32:1a:560:U:H2' | 1.61 | 0.43 |
| 32:1a:792:A:H4' | 32:1a:793:U:H5" | 2.00 | 0.43 |
| 32:1a:1223:C:OP2 | 50:1s:78:ARG:NH2 | 2.49 | 0.43 |
| 34:1c:53:ALA:HB3 | 34:1c:69:HIS:O | 2.19 | 0.43 |
| 38:1g:95:ARG:HE | 38:1g:99:LEU:HD11 | 1.83 | 0.43 |
| 44:1m:15:VAL:O | 44:1m:19:LEU:HD22 | 2.19 | 0.43 |
| 49:1r:22:VAL:HG12 | 49:1r:56:THR:HA | 2.01 | 0.43 |
| 1:2A:127:A:H5" | 1:2A:128:C:C6 | 2.54 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:2A:244:A:C2 | 1:2A:255:A:C4 | 3.07 | 0.43 |
| 1:2A:744:G:H2' | 1:2A:745:G:O4' | 2.18 | 0.43 |
| 1:2A:1043:C:P | 1:2A:1043:C:H3' | 2.59 | 0.43 |
| 1:2A:1910:G:H2' | 1:2A:1911:PSU:H6 | 1.82 | 0.43 |
| 1:2A:2057:A:H2' | 1:2A:2058:A:O4' | 2.19 | 0.43 |
| 1:2A:2364:C:H2' | 1:2A:2365:G:O4' | 2.19 | 0.43 |
| 1:2A:2750:A:H8 | 1:2A:2750:A:OP1 | 2.01 | 0.43 |
| 6:2G:114:ILE:HB | 6:2G:117:PHE:HB2 | 2.01 | 0.43 |
| 17:2V:40:LEU:HD23 | 17:2V:40:LEU:HA | 1.88 | 0.43 |
| 32:2a:270:A:H2' | 32:2a:271:C:C6 | 2.53 | 0.43 |
| 32:2a:745:C:OP1 | 32:2a:851:G:O2' | 2.27 | 0.43 |
| 32:2a:1124:G:H1 | 32:2a:1149:C:H42 | 1.66 | 0.43 |
| 32:2a:1126:U:N3 | 41:2j:40:LEU:HD11 | 2.34 | 0.43 |
| 32:2a:1225:A:H2' | 32:2a:1226:C:C5 | 2.54 | 0.43 |
| 32:2a:1436:U:H2' | 32:2a:1437:C:O4' | 2.19 | 0.43 |
| 35:2d:179:GLU:O | 35:2d:181:MET:HE2 | 2.19 | 0.43 |
| 39:2h:81:HIS:ND1 | 39:2h:138:TRP:OXT | 2.43 | 0.43 |
| 54:2x:8:4SU:H5" | 54:2x:49:G:H5' | 2.01 | 0.43 |
| 1:1A:690:G:O2' | 3:1D:43:ARG:NH2 | 2.50 | 0.43 |
| 1:1A:1059:G:O6 | 1:1A:1088:A:H1' | 2.18 | 0.43 |
| 1:1A:1152:C:H1' | 16:1U:77:SER:HB3 | 2.01 | 0.43 |
| 1:1A:1263:U:OP1 | 27:15:16:ARG:NH1 | 2.46 | 0.43 |
| 1:1A:1453:U:OP1 | 13:1R:77:ARG:NH1 | 2.41 | 0.43 |
| 1:1A:2330:G:H2' | 1:1A:2331:G:O4' | 2.18 | 0.43 |
| 1:1A:2636:U:H2' | 1:1A:2637:U:C6 | 2.54 | 0.43 |
| 1:1A:2801(A):A:H5" | 1:1A:2802:G:C8 | 2.53 | 0.43 |
| 8:1I:5:LEU:HD23 | 8:1I:9:LEU:HD12 | 2.00 | 0.43 |
| 9:1N:108:PRO:O | 9:1N:113:GLY:HA3 | 2.19 | 0.43 |
| 30:18:61:LEU:O | 30:18:63:PRO:HD3 | 2.18 | 0.43 |
| 32:1a:1304:G:C6 | 32:1a:1305:G:N1 | 2.87 | 0.43 |
| 44:1m:20:THR:C | 44:1m:22:ILE:H | 2.27 | 0.43 |
| 45:1n:13:THR:HA | 45:1n:14:PRO:HD3 | 1.87 | 0.43 |
| 46:1o:35:ARG:NH2 | 46:1o:59:MET:HE2 | 2.34 | 0.43 |
| 50:1s:19:VAL:HA | 50:1s:22:LEU:HD12 | 2.01 | 0.43 |
| 1:2A:237:C:O2 | 1:2A:609:A:O2' | 2.33 | 0.43 |
| 1:2A:271:A:N6 | 1:2A:271(X):G:H1' | 2.34 | 0.43 |
| 1:2A:484:C:H2' | 1:2A:485:C:H6 | 1.83 | 0.43 |
| 1:2A:846:C:H4' | 1:2A:847:U:O4' | 2.19 | 0.43 |
| 1:2A:1263:U:C4 | 1:2A:1264:G:C6 | 3.07 | 0.43 |
| 1:2A:1347:G:H2' | 1:2A:1348:G:H8 | 1.84 | 0.43 |
| 1:2A:1394:U:H2' | 1:2A:1395:A:O4' | 2.19 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:2A:1528(A):A:H2' | 1:2A:1529:G:O4' | 2.19 | 0.43 |
| 1:2A:2318:G:H21 | 14:2S:3:ARG:CD | 2.32 | 0.43 |
| 1:2A:2483:C:H2' | 1:2A:2484:G:O4' | 2.19 | 0.43 |
| 1:2A:2838:G:C6 | 1:2A:2839:G:C5 | 3.07 | 0.43 |
| 2:2B:55:U:H1' | 6:2G:29:TRP:CD1 | 2.53 | 0.43 |
| 4:2E:143:ASN:HD22 | 4:2E:147:PRO:CD | 2.28 | 0.43 |
| 10:2O:108:GLU:H | 10:2O:108:GLU:HG2 | 1.68 | 0.43 |
| 15:2T:19:LEU:HD13 | 15:2T:86:ILE:HD12 | 2.01 | 0.43 |
| 20:2Y:44:ILE:HA | 20:2Y:63:LYS:O | 2.19 | 0.43 |
| 26:24:48:ARG:HG3 | 26:24:52:THR:HA | 2.01 | 0.43 |
| 32:2a:163:C:H2' | 32:2a:164:U:O4' | 2.19 | 0.43 |
| 32:2a:354:G:N2 | 32:2a:388:G:O2' | 2.22 | 0.43 |
| 32:2a:1029:C:N4 | 32:2a:1032:G:N1 | 2.67 | 0.43 |
| 32:2a:1037:C:H2' | 32:2a:1038:C:C6 | 2.53 | 0.43 |
| 32:2a:1145:C:H4' | 32:2a:1146:A:H8 | 1.84 | 0.43 |
| 32:2a:1262:C:H2' | 32:2a:1263:C:H5' | 1.99 | 0.43 |
| 32:2a:1263:C:N3 | 32:2a:1272:G:O6 | 2.51 | 0.43 |
| 32:2a:1286:A:C8 | 32:2a:1286:A:H3' | 2.53 | 0.43 |
| 32:2a:1502:A:C8 | 32:2a:1505:G:N2 | 2.87 | 0.43 |
| 35:2d:119:GLN:HG3 | 35:2d:123:HIS:CD2 | 2.52 | 0.43 |
| 35:2d:199:ASN:HB3 | 35:2d:202:LEU:HD12 | 2.01 | 0.43 |
| 1:1A:191:A:H2' | 1:1A:192:C:C6 | 2.54 | 0.43 |
| 1:1A:444:C:H4' | 5:1F:49:ALA:HB2 | 2.00 | 0.43 |
| 1:1A:571:A:H5' | 1:1A:2030:A:N7 | 2.34 | 0.43 |
| 1:1A:671:C:H2' | 1:1A:672:C:C6 | 2.54 | 0.43 |
| 1:1A:848:G:O6 | 1:1A:928:G:H2' | 2.19 | 0.43 |
| 1:1A:849:A:H2 | 25:13:24:LYS:HB3 | 1.84 | 0.43 |
| 1:1A:864:G:O2' | 1:1A:865:C:H5' | 2.19 | 0.43 |
| 1:1A:1379:A:H4' | 1:1A:1380:G:OP2 | 2.18 | 0.43 |
| 1:1A:1400:G:H2' | 1:1A:1401:G:C8 | 2.53 | 0.43 |
| 1:1A:1580:A:OP2 | 1:1A:1580:A:H8 | 2.02 | 0.43 |
| 3:1D:89:SER:HB2 | 3:1D:201:HIS:CD2 | 2.53 | 0.43 |
| 5:1F:51:THR:HG23 | 5:1F:92:PRO:HD2 | 2.00 | 0.43 |
| 7:1H:3:ARG:CZ | 7:1H:5:GLY:H | 2.32 | 0.43 |
| 8:1I:92:VAL:HG11 | 8:1I:144:VAL:HG11 | 2.01 | 0.43 |
| 21:1Z:98:MET:O | 21:1Z:125:LEU:HA | 2.19 | 0.43 |
| 28:16:33:LYS:HA | 28:16:33:LYS:HD3 | 1.88 | 0.43 |
| 30:18:29:LYS:HD3 | 30:18:44:LYS:C | 2.43 | 0.43 |
| 32:1a:474:G:H5' | 32:1a:475:G:OP2 | 2.18 | 0.43 |
| 32:1a:724:G:C2 | 32:1a:725:G:C8 | 3.07 | 0.43 |
| 32:1a:731:G:H5' | 32:1a:766:A:H4' | 2.01 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 36:1e:103:GLY:O | 36:1e:106:PRO:HD2 | 2.19 | 0.43 |
| 37:1f:86:ARG:O | 37:1f:87:ARG:HG2 | 2.18 | 0.43 |
| 40:1i:46:ALA:HB2 | 40:1i:74:ILE:HG23 | 2.01 | 0.43 |
| 47:1p:26:ARG:HG3 | 47:1p:27:LYS:O | 2.19 | 0.43 |
| 1:2A:118:A:H1' | 1:2A:178:G:O4' | 2.18 | 0.43 |
| 1:2A:1024:G:C6 | 1:2A:1025:G:C6 | 3.07 | 0.43 |
| 1:2A:1651:G:H4' | 13:2R:39:PRO:HG2 | 2.00 | 0.43 |
| 1:2A:2028:U:H2' | 1:2A:2029:G:O4' | 2.18 | 0.43 |
| 1:2A:2199:A:H3' | 1:2A:2200:C:H6 | 1.83 | 0.43 |
| 3:2D:112:GLN:O | 3:2D:115:GLN:HG2 | 2.18 | 0.43 |
| 4:2E:48:GLN:HA | 4:2E:80:GLU:HA | 2.01 | 0.43 |
| 8:2I:54:GLN:HA | 8:2I:57:ARG:HB2 | 2.00 | 0.43 |
| 13:2R:67:LEU:HD23 | 13:2R:67:LEU:HA | 1.88 | 0.43 |
| 16:2U:52:ARG:O | 16:2U:56:ASP:N | 2.47 | 0.43 |
| 30:28:17:THR:HG1 | 30:28:21:LYS:H | 1.67 | 0.43 |
| 33:2b:174:VAL:O | 33:2b:178:ARG:HG2 | 2.18 | 0.43 |
| 36:2e:74:GLY:O | 36:2e:115:VAL:HA | 2.18 | 0.43 |
| 43:2l:53:ARG:HB2 | 43:2l:93:LEU:HD11 | 2.01 | 0.43 |
| 1:1A:880:G:H8 | 1:1A:880:G:OP2 | 2.01 | 0.42 |
| 1:1A:996:A:OP2 | 16:1U:93:LYS:NZ | 2.46 | 0.42 |
| 1:1A:1141:U:H4' | 1:1A:1142(A):A:O4' | 2.19 | 0.42 |
| 3:1D:30:GLU:HB3 | 3:1D:33:LEU:HD12 | 2.01 | 0.42 |
| 4:1E:31:CYS:HB3 | 4:1E:49:LEU:HG | 2.01 | 0.42 |
| 5:1F:8:GLN:HE22 | 5:1F:21:ALA:HB2 | 1.84 | 0.42 |
| 5:1F:64:ILE:HG21 | 5:1F:78:ILE:HG23 | 2.01 | 0.42 |
| 7:1H:40:GLU:OE2 | 7:1H:60:ARG:NH2 | 2.49 | 0.42 |
| 7:1H:159:GLU:HG3 | 7:1H:169:VAL:HG11 | 2.01 | 0.42 |
| 10:1O:25:LEU:HD23 | 10:1O:25:LEU:HA | 1.78 | 0.42 |
| 16:1U:85:LYS:HE3 | 16:1U:116:ALA:O | 2.18 | 0.42 |
| 17:1V:14:VAL:HB | 17:1V:96:ILE:HG13 | 2.00 | 0.42 |
| 21:1Z:125:LEU:HG | 21:1Z:164:ALA:HB3 | 2.01 | 0.42 |
| 32:1a:567:G:H2' | 32:1a:568:G:O4' | 2.19 | 0.42 |
| 32:1a:766:A:C8 | 32:1a:814:A:N6 | 2.87 | 0.42 |
| 32:1a:779:C:H5" | 42:1k:122:LYS:HG3 | 2.01 | 0.42 |
| 32:1a:864:A:N1 | 32:1a:917:G:O2' | 2.47 | 0.42 |
| 32:1a:1025:U:C2 | 32:1a:1036:G:O6 | 2.72 | 0.42 |
| 32:1a:1239:A:H62 | 32:1a:1299:A:H62 | 1.66 | 0.42 |
| 33:1b:16:HIS:HB3 | 33:1b:210:SER:HB2 | 2.00 | 0.42 |
| 36:1e:41:VAL:HG22 | 36:1e:113:ALA:HA | 2.00 | 0.42 |
| 40:1i:81:ILE:O | 40:1i:85:LEU:HG | 2.19 | 0.42 |
| 43:1l:36:VAL:HG12 | 43:1l:82:VAL:HG22 | 2.01 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 48:1q:58:GLU:O | 48:1q:74:LEU:N | 2.51 | 0.42 |
| 1:2A:228:A:C4 | 1:2A:230:U:H1' | 2.53 | 0.42 |
| 1:2A:414:C:H2' | 1:2A:415:A:H8 | 1.84 | 0.42 |
| 1:2A:601:C:O2' | 1:2A:605:C:H5" | 2.19 | 0.42 |
| 1:2A:945:A:C4 | 1:2A:2448:A:C2 | 3.07 | 0.42 |
| 1:2A:1674:G:H1' | 1:2A:1676:A:N6 | 2.34 | 0.42 |
| 1:2A:2074:U:H2' | 1:2A:2075:U:C6 | 2.54 | 0.42 |
| 1:2A:2125:G:H1' | 1:2A:2173:A:N6 | 2.34 | 0.42 |
| 1:2A:2351:G:H8 | 1:2A:2351:G:O5' | 2.02 | 0.42 |
| 1:2A:2801(A):A:H1' | 1:2A:2895:U:O2' | 2.19 | 0.42 |
| 1:2A:2820:A:HO2' | 1:2A:2821:A:P | 2.40 | 0.42 |
| 5:2F:29:ASN:HB3 | 5:2F:112:MET:HE1 | 1.99 | 0.42 |
| 6:2G:142:PRO:HB2 | 26:24:31:ILE:HG21 | 2.00 | 0.42 |
| 22:20:70:GLN:HG2 | 22:20:72:ARG:HG3 | 2.00 | 0.42 |
| 32:2a:45:U:H2' | 32:2a:46:G:H8 | 1.82 | 0.42 |
| 32:2a:657:G:N2 | 46:2o:22:THR:OG1 | 2.47 | 0.42 |
| 32:2a:685:G:N2 | 32:2a:686:U:O4 | 2.52 | 0.42 |
| 32:2a:922:G:O2' | 32:2a:1398:A:N1 | 2.49 | 0.42 |
| 32:2a:1247:U:H1' | 32:2a:1291:G:N2 | 2.33 | 0.42 |
| 32:2a:1347:G:N2 | 32:2a:1373:G:H2' | 2.33 | 0.42 |
| 35:2d:159:ARG:O | 35:2d:163:GLU:N | 2.51 | 0.42 |
| 40:2i:128:ARG:NE | 54:2x:32:5MC:OP2 | 2.52 | 0.42 |
| 1:1A:11:G:H2' | 1:1A:12:U:H5" | 2.00 | 0.42 |
| 1:1A:121:G:H4' | 1:1A:149:A:H5' | 2.01 | 0.42 |
| 1:1A:1074:G:C6 | 1:1A:1075:C:H1' | 2.54 | 0.42 |
| 1:1A:1213:A:H1' | 1:1A:1238:G:N3 | 2.35 | 0.42 |
| 1:1A:1816:G:H8 | 3:1D:62:TYR:CZ | 2.36 | 0.42 |
| 1:1A:1996:C:H5 | 10:1O:32:TYR:OH | 2.01 | 0.42 |
| 1:1A:2128:C:N3 | 1:1A:2160:G:N2 | 2.51 | 0.42 |
| 1:1A:2881:C:O2' | 13:1R:96:ARG:HA | 2.19 | 0.42 |
| 2:1B:75:G:H22 | 21:1Z:73:GLN:NE2 | 2.17 | 0.42 |
| 6:1G:56:ALA:HB2 | 6:1G:153:ARG:NE | 2.34 | 0.42 |
| 18:1W:11:ARG:NH1 | 18:1W:99:ARG:O | 2.52 | 0.42 |
| 32:1a:116:A:H61 | 32:1a:313:A:H1' | 1.84 | 0.42 |
| 32:1a:129:U:H5' | 48:1q:3:LYS:NZ | 2.32 | 0.42 |
| 32:1a:245:C:C2 | 32:1a:284:G:C2 | 3.07 | 0.42 |
| 32:1a:508:C:OP1 | 35:1d:209:ARG:NH2 | 2.45 | 0.42 |
| 32:1a:721:G:H4' | 32:1a:722:A:O4' | 2.19 | 0.42 |
| 32:1a:1146:A:H2' | 32:1a:1147:C:O4' | 2.19 | 0.42 |
| 33:1b:185:ILE:HG22 | 33:1b:199:TYR:HD2 | 1.83 | 0.42 |
| 36:1e:53:LEU:H | 36:1e:53:LEU:HD12 | 1.83 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 38:1g:150:ALA:HA | 42:1k:59:TYR:HB3 | 2.01 | 0.42 |
| 1:2A:31:C:H5" | 1:2A:1239:G:OP1 | 2.20 | 0.42 |
| 1:2A:681:G:H2' | 1:2A:682:G:O4' | 2.19 | 0.42 |
| 1:2A:863:A:H2' | 1:2A:864:G:H8 | 1.83 | 0.42 |
| 1:2A:1766:U:H2' | 1:2A:1767:C:H6 | 1.83 | 0.42 |
| 1:2A:2144:U:H1' | 1:2A:2148:G:H22 | 1.84 | 0.42 |
| 1:2A:2840:C:H2' | 1:2A:2841:C:C6 | 2.54 | 0.42 |
| 10:2O:106:LEU:HD23 | 10:2O:106:LEU:HA | 1.89 | 0.42 |
| 12:2Q:54:MET:H | 12:2Q:54:MET:HG2 | 1.58 | 0.42 |
| 12:2Q:132:VAL:HB | 21:2Z:81:ARG:HH21 | 1.83 | 0.42 |
| 16:2U:44:ASN:HD21 | 17:2V:75:PHE:HB3 | 1.85 | 0.42 |
| 25:23:7:LYS:HE3 | 25:23:32:GLN:HA | 2.01 | 0.42 |
| 32:2a:59:A:H1' | 32:2a:354:G:N2 | 2.34 | 0.42 |
| 32:2a:559:A:H4' | 32:2a:560:U:H5" | 2.01 | 0.42 |
| 32:2a:741:G:H2' | 32:2a:742:G:O4' | 2.19 | 0.42 |
| 32:2a:976:G:N2 | 32:2a:1363:C:OP2 | 2.52 | 0.42 |
| 33:2b:210:SER:O | 33:2b:214:ILE:HD12 | 2.18 | 0.42 |
| 34:2c:180:ALA:HB1 | 34:2c:203:PHE:CE1 | 2.53 | 0.42 |
| 35:2d:107:ARG:C | 35:2d:109:GLY:H | 2.28 | 0.42 |
| 36:2e:33:VAL:HG13 | 36:2e:112:LEU:HD12 | 1.99 | 0.42 |
| 39:2h:7:ALA:HB2 | 39:2h:85:ARG:HG3 | 1.99 | 0.42 |
| 39:2h:28:ALA:HB3 | 39:2h:57:PRO:HB2 | 2.00 | 0.42 |
| 44:2m:14:ARG:HA | 44:2m:43:THR:O | 2.19 | 0.42 |
| 51:2t:39:LYS:HE2 | 51:2t:39:LYS:HB2 | 1.89 | 0.42 |
| 1:1A:82:G:N1 | 1:1A:103:A:OP2 | 2.47 | 0.42 |
| 1:1A:263:C:H2' | 1:1A:264:C:O4' | 2.19 | 0.42 |
| 1:1A:554:U:O2' | 1:1A:555:U:H5' | 2.20 | 0.42 |
| 1:1A:904:C:H2' | 1:1A:905:U:C6 | 2.53 | 0.42 |
| 1:1A:1353:A:O4' | 1:1A:1569:A:H2 | 2.03 | 0.42 |
| 1:1A:1364:G:N2 | 1:1A:1367:A:OP2 | 2.36 | 0.42 |
| 1:1A:1372:U:H2' | 1:1A:1373:A:O4' | 2.19 | 0.42 |
| 5:1F:117:ARG:HD3 | 5:1F:117:ARG:HA | 1.77 | 0.42 |
| 12:1Q:29:PHE:HB2 | 12:1Q:105:GLU:OE1 | 2.18 | 0.42 |
| 12:1Q:85:LYS:HD3 | 22:10:7:LEU:HD22 | 2.01 | 0.42 |
| 19:1X:50:LYS:N | 19:1X:87:GLN:OE1 | 2.46 | 0.42 |
| 21:1Z:1:MET:HA | 21:1Z:2:GLU:HA | 1.88 | 0.42 |
| 21:1Z:54:HIS:CG | 21:1Z:101:PRO:HG3 | 2.54 | 0.42 |
| 32:1a:1136:U:H5" | 32:1a:1137:C:C6 | 2.55 | 0.42 |
| 32:1a:1144:G:H21 | 32:1a:1146:A:H62 | 1.67 | 0.42 |
| 32:1a:1241:G:OP1 | 38:1g:35:LYS:NZ | 2.52 | 0.42 |
| 32:1a:1316:G:N2 | 32:1a:1318:A:H3' | 2.35 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:2A:143:G:C2 | 1:2A:143(A):C:C2 | 3.07 | 0.42 |
| 1:2A:222:A:H3' | 1:2A:421:U:H5' | 2.01 | 0.42 |
| 1:2A:338:G:H2' | 1:2A:339:U:H6 | 1.83 | 0.42 |
| 1:2A:686:G:H21 | 1:2A:788:A:H61 | 1.65 | 0.42 |
| 1:2A:900:A:C3' | 1:2A:901:A:H8 | 2.32 | 0.42 |
| 1:2A:997:G:H5" | 16:2U:92:ARG:HH12 | 1.83 | 0.42 |
| 1:2A:1012:U:O4 | 9:2N:28:THR:HG21 | 2.19 | 0.42 |
| 1:2A:1157:G:C6 | 1:2A:1158:C:C4 | 3.07 | 0.42 |
| 1:2A:2040:C:H2' | 1:2A:2041:U:O4' | 2.18 | 0.42 |
| 1:2A:2237:G:H5" | 1:2A:2238:G:OP1 | 2.19 | 0.42 |
| 1:2A:2382:G:H21 | 30:28:42:ARG:NH2 | 2.16 | 0.42 |
| 2:2B:48:A:H4' | 14:2S:95:HIS:CD2 | 2.43 | 0.42 |
| 5:2F:176:LEU:HD23 | 5:2F:176:LEU:HA | 1.74 | 0.42 |
| 5:2F:178:PRO:HB2 | 5:2F:201:VAL:HG21 | 2.01 | 0.42 |
| 11:2P:88:LEU:HD11 | 11:2P:114:ILE:HD12 | 2.00 | 0.42 |
| 21:2Z:99:TYR:HA | 21:2Z:124:ILE:O | 2.19 | 0.42 |
| 32:2a:229:U:H2' | 32:2a:230:G:O4' | 2.19 | 0.42 |
| 32:2a:391:G:C6 | 32:2a:392:G:C5 | 3.07 | 0.42 |
| 36:2e:143:ARG:HE | 39:2h:77:GLU:CD | 2.26 | 0.42 |
| 42:2k:21:ILE:HG12 | 42:2k:30:VAL:HG12 | 2.01 | 0.42 |
| 42:2k:33:THR:HA | 42:2k:39:PRO:HA | 2.00 | 0.42 |
| 46:2o:87:ILE:HG22 | 46:2o:88:ARG:N | 2.30 | 0.42 |
| 50:2s:36:ARG:O | 50:2s:71:LEU:HB3 | 2.18 | 0.42 |
| 1:1A:27:G:C2 | 1:1A:512:G:N3 | 2.87 | 0.42 |
| 1:1A:266:G:N2 | 1:1A:427:U:H1' | 2.34 | 0.42 |
| 1:1A:271(G):C:H2' | 1:1A:271(H):G:H8 | 1.85 | 0.42 |
| 1:1A:464:U:H2' | 1:1A:465:G:O4' | 2.19 | 0.42 |
| 1:1A:589:C:H2' | 1:1A:590:A:C8 | 2.54 | 0.42 |
| 1:1A:868:U:C4 | 1:1A:869:G:N7 | 2.87 | 0.42 |
| 1:1A:957:A:H4' | 12:1Q:74:TYR:OH | 2.18 | 0.42 |
| 1:1A:1424:G:H2' | 1:1A:1425:G:O4' | 2.19 | 0.42 |
| 1:1A:1509(B):A:H2' | 1:1A:1510:G:O4' | 2.20 | 0.42 |
| 1:1A:1593:G:H2' | 1:1A:1594:G:C8 | 2.53 | 0.42 |
| 1:1A:2723:C:OP1 | 13:1R:3:HIS:ND1 | 2.48 | 0.42 |
| 3:1D:249:PRO:HD2 | 3:1D:250:TRP:CZ3 | 2.54 | 0.42 |
| 7:1H:11:VAL:HG13 | 7:1H:15:VAL:CG2 | 2.49 | 0.42 |
| 8:1I:123:LEU:HD12 | 8:1I:123:LEU:HA | 1.95 | 0.42 |
| 11:1P:64:LYS:O | 30:18:30:ARG:NH2 | 2.51 | 0.42 |
| 21:1Z:48:PHE:CE1 | 21:1Z:71:VAL:HG11 | 2.55 | 0.42 |
| 21:1Z:158:PRO:O | 21:1Z:161:VAL:HG22 | 2.20 | 0.42 |
| 24:12:2:LYS:O | 24:12:6:VAL:HG23 | 2.20 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 25:13:6:VAL:HG12 | 25:13:54:VAL:CG2 | 2.48 | 0.42 |
| 32:1a:9:G:OP2 | 36:1e:121:LYS:NZ | 2.32 | 0.42 |
| 32:1a:502:G:C6 | 32:1a:503:C:C4 | 3.07 | 0.42 |
| 32:1a:688:G:H5' | 42:1k:46:GLY:C | 2.44 | 0.42 |
| 32:1a:1359:C:OP1 | 45:1n:22:THR:OG1 | 2.31 | 0.42 |
| 36:1e:74:GLY:HA3 | 36:1e:116:THR:HG22 | 2.01 | 0.42 |
| 44:1m:3:ARG:HG3 | 44:1m:4:ILE:N | 2.34 | 0.42 |
| 54:1x:63:G:H2' | 54:1x:64:G:H8 | 1.84 | 0.42 |
| 1:2A:272(E):G:C2 | 1:2A:364:C:C2 | 3.08 | 0.42 |
| 1:2A:578:A:OP2 | 59:2A:3967:HOH:O | 2.21 | 0.42 |
| 1:2A:932:G:H4' | 1:2A:933:A:O5' | 2.19 | 0.42 |
| 1:2A:1403:C:O5' | 1:2A:1471:A:H1' | 2.18 | 0.42 |
| 1:2A:1464:C:H2' | 1:2A:1465:G:C8 | 2.54 | 0.42 |
| 1:2A:2184:G:C2' | 1:2A:2185:C:H5' | 2.49 | 0.42 |
| 5:2F:57:VAL:HG13 | 5:2F:59:TYR:H | 1.84 | 0.42 |
| 6:2G:36:LYS:HG3 | 6:2G:160:VAL:HB | 2.02 | 0.42 |
| 9:2N:42:TRP:O | 16:2U:64:ARG:NE | 2.48 | 0.42 |
| 13:2R:94:TYR:C | 13:2R:117:VAL:HG23 | 2.44 | 0.42 |
| 14:2S:66:ALA:O | 14:2S:69:VAL:HG13 | 2.20 | 0.42 |
| 21:2Z:150:LEU:HD23 | 21:2Z:154:ASP:OD2 | 2.19 | 0.42 |
| 26:24:15:ILE:O | 26:24:33:VAL:HG23 | 2.20 | 0.42 |
| 32:2a:130:A:H5' | 48:2q:63:ARG:HE | 1.85 | 0.42 |
| 32:2a:501:C:OP1 | 43:2l:124:LYS:HD2 | 2.19 | 0.42 |
| 32:2a:600:C:H2' | 32:2a:601:C:H6 | 1.84 | 0.42 |
| 32:2a:724:G:H2' | 32:2a:725:G:H8 | 1.85 | 0.42 |
| 32:2a:1095:U:OP1 | 32:2a:1108:G:N2 | 2.52 | 0.42 |
| 32:2a:1252:A:H2' | 32:2a:1253:G:O4' | 2.20 | 0.42 |
| 32:2a:1403:C:C2 | 32:2a:1404:5MC:HM52 | 2.55 | 0.42 |
| 32:2a:1457:G:H5" | 51:2t:35:THR:HG21 | 2.01 | 0.42 |
| 33:2b:109:SER:O | 33:2b:112:VAL:HB | 2.18 | 0.42 |
| 34:2c:122:GLU:HA | 34:2c:125:GLU:CD | 2.44 | 0.42 |
| 38:2g:15:ASP:OD1 | 38:2g:20:ASP:N | 2.52 | 0.42 |
| 41:2j:12:ASP:HB3 | 41:2j:15:THR:HG23 | 2.02 | 0.42 |
| 43:2l:93:LEU:HD23 | 43:2l:93:LEU:HA | 1.86 | 0.42 |
| 50:2s:50:ALA:HA | 50:2s:58:VAL:O | 2.19 | 0.42 |
| 54:2x:50:U:H2' | 54:2x:51:C:C6 | 2.55 | 0.42 |
| 1:1A:335:C:H4' | 20:1Y:73:ARG:HD2 | 2.02 | 0.42 |
| 1:1A:340:A:H2' | 1:1A:341:G:O4' | 2.20 | 0.42 |
| 1:1A:1011:G:OP1 | 16:1U:77:SER:OG | 2.36 | 0.42 |
| 1:1A:1358:G:O2' | 1:1A:1373:A:N6 | 2.47 | 0.42 |
| 1:1A:1371:G:N7 | 59:1A:4421:HOH:O | 2.37 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1A:1406:U:H2' | 1:1A:1407:C:C6 | 2.54 | 0.42 |
| 1:1A:2040:C:H2' | 1:1A:2041:U:O4' | 2.20 | 0.42 |
| 1:1A:2636:U:H2' | 1:1A:2637:U:H6 | 1.84 | 0.42 |
| 14:1S:61:ASN:ND2 | 14:1S:64:GLU:HG3 | 2.33 | 0.42 |
| 19:1X:12:VAL:HG21 | 19:1X:27:THR:HG22 | 2.00 | 0.42 |
| 21:1Z:54:HIS:ND1 | 21:1Z:101:PRO:HG3 | 2.34 | 0.42 |
| 32:1a:1004:A:H5' | 32:1a:1024:G:H1 | 1.84 | 0.42 |
| 32:1a:1030(C):G:H2' | 32:1a:1030(D):A:C8 | 2.54 | 0.42 |
| 32:1a:1293:G:H2' | 32:1a:1294:G:C8 | 2.54 | 0.42 |
| 33:1b:28:PHE:CD2 | 33:1b:190:THR:HA | 2.55 | 0.42 |
| 36:1e:78:HIS:HE1 | 36:1e:143:ARG:N | 2.12 | 0.42 |
| 37:1f:76:ALA:O | 37:1f:80:ARG:HG3 | 2.20 | 0.42 |
| 47:1p:43:LYS:HG2 | 47:1p:48:TRP:CD2 | 2.54 | 0.42 |
| 1:2A:38:A:H2' | 1:2A:39:C:C6 | 2.55 | 0.42 |
| 1:2A:90:U:H1' | 1:2A:92:A:C8 | 2.54 | 0.42 |
| 1:2A:459:U:H4' | 29:27:40:TRP:CZ3 | 2.54 | 0.42 |
| 1:2A:649:G:C6 | 1:2A:650:C:C4 | 3.07 | 0.42 |
| 1:2A:722:A:H2' | 1:2A:723:G:O4' | 2.19 | 0.42 |
| 1:2A:860:U:H1' | 1:2A:2268:A:H5' | 2.01 | 0.42 |
| 1:2A:912:C:P | 12:2Q:8:LYS:HZ3 | 2.41 | 0.42 |
| 1:2A:1475:G:C2 | 1:2A:1517:G:C2 | 3.08 | 0.42 |
| 1:2A:2027:G:H2' | 1:2A:2028:U:O4' | 2.19 | 0.42 |
| 1:2A:2128:C:H2' | 1:2A:2129:C:O4' | 2.20 | 0.42 |
| 1:2A:2690:C:OP1 | 13:2R:17:ARG:NH2 | 2.52 | 0.42 |
| 1:2A:2881:C:H2' | 1:2A:2882:A:O4' | 2.19 | 0.42 |
| 2:2B:12:C:O2 | 22:20:74:ARG:NH2 | 2.52 | 0.42 |
| 2:2B:50:G:OP1 | 14:2S:63:THR:N | 2.51 | 0.42 |
| 3:2D:70:TRP:HB3 | 3:2D:190:TYR:CE2 | 2.55 | 0.42 |
| 3:2D:136:ILE:HG22 | 3:2D:140:THR:OG1 | 2.19 | 0.42 |
| 6:2G:47:LYS:HG3 | 6:2G:48:GLU:H | 1.84 | 0.42 |
| 6:2G:151:ALA:HB3 | 6:2G:153:ARG:NH1 | 2.35 | 0.42 |
| 7:2H:38:SER:HB3 | 7:2H:41:MET:HG2 | 2.01 | 0.42 |
| 19:2X:24:GLY:O | 19:2X:83:VAL:HG22 | 2.19 | 0.42 |
| 32:2a:373:A:H61 | 32:2a:391:G:H1' | 1.85 | 0.42 |
| 32:2a:941:G:H2' | 32:2a:942:G:O4' | 2.19 | 0.42 |
| 32:2a:1158:C:O2' | 33:2b:133:LYS:HE2 | 2.19 | 0.42 |
| 33:2b:149:LEU:HA | 33:2b:152:PHE:HB3 | 2.02 | 0.42 |
| 33:2b:178:ARG:HH12 | 39:2h:68:ARG:NH2 | 2.16 | 0.42 |
| 34:2c:206:GLU:H | 34:2c:206:GLU:HG3 | 1.74 | 0.42 |
| 37:2f:2:ARG:HD2 | 37:2f:69:GLU:HB3 | 2.02 | 0.42 |
| 39:2h:86:ILE:HG21 | 39:2h:133:LEU:HD23 | 2.00 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:2j:6:ILE:HB | 41:2j:72:VAL:HG22 | 2.01 | 0.42 |
| 51:2t:92:LEU:HD23 | 51:2t:92:LEU:HA | 1.71 | 0.42 |
| 1:1A:557:U:H2' | 1:1A:558:G:H8 | 1.84 | 0.42 |
| 1:1A:571:A:O2' | 17:1V:78:LYS:HE2 | 2.20 | 0.42 |
| 1:1A:729:G:O5' | 3:1D:208:LYS:NZ | 2.52 | 0.42 |
| 1:1A:1051:G:H4' | 1:1A:2752:C:H4' | 2.00 | 0.42 |
| 1:1A:1095:A:C8 | 1:1A:1096:A:C8 | 3.08 | 0.42 |
| 1:1A:1923:U:H2' | 1:1A:1924:C:C6 | 2.54 | 0.42 |
| 1:1A:2118:U:O4 | 1:1A:2149:G:H1' | 2.19 | 0.42 |
| 1:1A:2393:A:H5" | 11:1P:63:PRO:HB3 | 2.02 | 0.42 |
| 1:1A:2690:C:N4 | 1:1A:2713:A:H1' | 2.35 | 0.42 |
| 1:1A:2821:A:H2' | 1:1A:2822:G:C8 | 2.55 | 0.42 |
| 28:16:34:LEU:N | 28:16:51:GLU:HG2 | 2.34 | 0.42 |
| 29:17:23:ARG:NH2 | 59:17:203:HOH:O | 2.51 | 0.42 |
| 30:18:46:ARG:HE | 30:18:46:ARG:HB3 | 1.73 | 0.42 |
| 32:1a:171:A:H2' | 32:1a:172:A:C8 | 2.54 | 0.42 |
| 32:1a:509:A:O2' | 32:1a:510:A:OP1 | 2.35 | 0.42 |
| 32:1a:564:C:OP1 | 43:1l:15:ARG:NE | 2.41 | 0.42 |
| 32:1a:738:C:H2' | 32:1a:739:C:H6 | 1.84 | 0.42 |
| 32:1a:1025:U:O2 | 32:1a:1036:G:C6 | 2.71 | 0.42 |
| 32:1a:1053:G:N7 | 32:1a:1200:C:H5' | 2.33 | 0.42 |
| 32:1a:1279:A:O2' | 32:1a:1281:U:OP2 | 2.26 | 0.42 |
| 33:1b:162:ILE:O | 33:1b:185:ILE:HG12 | 2.19 | 0.42 |
| 34:1c:15:THR:C | 34:1c:16:ARG:HG2 | 2.45 | 0.42 |
| 34:1c:23:TYR:HA | 41:1j:11:PHE:CE2 | 2.54 | 0.42 |
| 41:1j:55:LYS:HE2 | 41:1j:56:HIS:CE1 | 2.55 | 0.42 |
| 50:1s:44:MET:O | 50:1s:47:HIS:HB2 | 2.20 | 0.42 |
| 54:1x:58:A:H4' | 54:1x:59:A:OP1 | 2.20 | 0.42 |
| 1:2A:198:C:H4' | 1:2A:2243:U:O2' | 2.19 | 0.42 |
| 1:2A:522:G:C2 | 1:2A:523:C:C2 | 3.07 | 0.42 |
| 1:2A:748:G:C8 | 18:2W:89:ALA:HB1 | 2.55 | 0.42 |
| 1:2A:1301:A:O2' | 1:2A:1302:A:H3' | 2.18 | 0.42 |
| 2:2B:6:C:H42 | 2:2B:115:G:H1 | 1.66 | 0.42 |
| 6:2G:18:GLU:O | 6:2G:22:ARG:HB2 | 2.20 | 0.42 |
| 10:2O:78:ARG:HH22 | 15:2T:75:ILE:HD11 | 1.85 | 0.42 |
| 13:2R:66:VAL:HG12 | 13:2R:70:LEU:HD12 | 2.01 | 0.42 |
| 14:2S:36:TYR:CD2 | 14:2S:36:TYR:N | 2.87 | 0.42 |
| 17:2V:20:LEU:HG | 17:2V:22:VAL:HG13 | 2.00 | 0.42 |
| 20:2Y:11:ASP:O | 20:2Y:27:VAL:HG23 | 2.19 | 0.42 |
| 29:27:46:VAL:HG13 | 29:27:48:LYS:NZ | 2.34 | 0.42 |
| 32:2a:142:G:H2' | 32:2a:143:A:H8 | 1.84 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 32:2a:293:G:H5' | 32:2a:610:G:C2 | 2.54 | 0.42 |
| 32:2a:430:A:OP2 | 35:2d:8:VAL:HG12 | 2.18 | 0.42 |
| 32:2a:662:G:O2' | 32:2a:836:G:O5' | 2.37 | 0.42 |
| 32:2a:872:A:C4 | 32:2a:874:G:N7 | 2.87 | 0.42 |
| 32:2a:902:G:H2' | 32:2a:903:G:H8 | 1.83 | 0.42 |
| 32:2a:1060:C:C5' | 41:2j:51:ARG:HG2 | 2.48 | 0.42 |
| 32:2a:1217:C:H2' | 32:2a:1218:C:O4' | 2.20 | 0.42 |
| 35:2d:105:VAL:HG13 | 35:2d:110:PHE:HB2 | 2.00 | 0.42 |
| 38:2g:51:GLN:O | 38:2g:55:GLY:HA2 | 2.19 | 0.42 |
| 40:2i:8:GLY:HA3 | 40:2i:76:ALA:O | 2.18 | 0.42 |
| 44:2m:97:PRO:HA | 44:2m:110:ARG:HD3 | 2.02 | 0.42 |
| 1:1A:1607:C:H4' | 1:1A:1608:A:O5' | 2.19 | 0.42 |
| 1:1A:1635:G:C6 | 1:1A:1636:C:C4 | 3.07 | 0.42 |
| 1:1A:1680:U:O2 | 1:1A:1763:G:H3' | 2.19 | 0.42 |
| 1:1A:1919:A:O3' | 32:1a:1517:G:H1' | 2.20 | 0.42 |
| 1:1A:2093:G:C6 | 1:1A:2225:A:C8 | 3.07 | 0.42 |
| 1:1A:2115:G:H8 | 1:1A:2115:G:O5' | 2.02 | 0.42 |
| 1:1A:2391:G:O6 | 1:1A:2425:A:H8 | 2.02 | 0.42 |
| 1:1A:2464:C:H1' | 59:1A:5146:HOH:O | 2.20 | 0.42 |
| 2:1B:33:G:C2 | 2:1B:50:G:C2 | 3.08 | 0.42 |
| 2:1B:41:U:OP1 | 2:1B:42:C:H5 | 2.02 | 0.42 |
| 11:1P:81:GLN:NE2 | 11:1P:105:LEU:O | 2.51 | 0.42 |
| 20:1Y:9:LYS:HA | 20:1Y:10:GLY:HA2 | 1.56 | 0.42 |
| 21:1Z:151:HIS:HB3 | 21:1Z:169:GLU:O | 2.19 | 0.42 |
| 32:1a:510:A:N3 | 32:1a:543:C:H1' | 2.34 | 0.42 |
| 32:1a:708:C:OP1 | 42:1k:85:ARG:NH2 | 2.51 | 0.42 |
| 32:1a:859:A:H2' | 32:1a:860:A:O4' | 2.20 | 0.42 |
| 32:1a:1367:C:O2' | 41:1j:48:THR:HG21 | 2.20 | 0.42 |
| 32:1a:1434:A:H2' | 32:1a:1435:G:O4' | 2.19 | 0.42 |
| 33:1b:127:ILE:HG13 | 33:1b:130:ARG:NH2 | 2.35 | 0.42 |
| 38:1g:23:VAL:HG13 | 38:1g:43:PHE:CZ | 2.54 | 0.42 |
| 40:1i:33:PHE:HD2 | 40:1i:34:ASN:HD22 | 1.68 | 0.42 |
| 45:1n:29:ARG:NH2 | 45:1n:42:ILE:HD11 | 2.34 | 0.42 |
| 46:1o:39:LEU:HD22 | 46:1o:43:LEU:HG | 2.02 | 0.42 |
| 54:1x:63:G:H2' | 54:1x:64:G:C8 | 2.54 | 0.42 |
| 1:2A:96:G:H4' | 24:22:48:HIS:CD2 | 2.55 | 0.42 |
| 1:2A:569:U:C4 | 1:2A:570:G:C6 | 3.08 | 0.42 |
| 1:2A:817:C:H2' | 1:2A:818:G:O4' | 2.20 | 0.42 |
| 1:2A:1000:A:C6 | 1:2A:1001:A:N1 | 2.88 | 0.42 |
| 1:2A:1115:G:C2 | 1:2A:1116:C:C2 | 3.08 | 0.42 |
| 1:2A:1233:C:H2' | 1:2A:1234:U:H6 | 1.85 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:2A:1848:A:C4 | 1:2A:1849:G:C8 | 3.07 | 0.42 |
| 1:2A:1853:A:N3 | 1:2A:2233:U:O2' | 2.35 | 0.42 |
| 1:2A:2379:G:H2' | 1:2A:2380:C:C6 | 2.55 | 0.42 |
| 1:2A:2755:C:HO2' | 1:2A:2756:U:H6 | 1.67 | 0.42 |
| 6:2G:146:TYR:HB3 | 44:2m:11:ARG:NH2 | 2.32 | 0.42 |
| 7:2H:83:TYR:CE2 | 7:2H:138:LYS:HB2 | 2.54 | 0.42 |
| 12:2Q:29:PHE:HB2 | 12:2Q:105:GLU:OE1 | 2.19 | 0.42 |
| 17:2V:14:VAL:HA | 17:2V:18:LEU:HD23 | 2.01 | 0.42 |
| 32:2a:585:G:O2' | 32:2a:879:C:OP1 | 2.33 | 0.42 |
| 57:2a:3210:V7A:OAY | 57:2a:3210:V7A:OAX | 2.36 | 0.42 |
| 36:2e:94:ALA:HB1 | 36:2e:98:THR:HG21 | 2.00 | 0.42 |
| 38:2g:133:GLY:O | 38:2g:137:LYS:HD3 | 2.20 | 0.42 |
| 46:2o:54:ARG:HG2 | 46:2o:58:MET:HE2 | 2.02 | 0.42 |
| 51:2t:76:ALA:HA | 51:2t:79:ARG:NH1 | 2.34 | 0.42 |
| 1:1A:93:G:H2' | 1:1A:94:C:C6 | 2.55 | 0.42 |
| 1:1A:530:G:H4' | 1:1A:531:C:OP1 | 2.20 | 0.42 |
| 1:1A:1107:G:O2' | 1:1A:1108:U:H5' | 2.20 | 0.42 |
| 1:1A:1920:4OC:HM22 | 1:1A:1921:G:O4' | 2.19 | 0.42 |
| 1:1A:2102:U:H2' | 1:1A:2103:C:C6 | 2.55 | 0.42 |
| 1:1A:2820:A:N3 | 1:1A:2820:A:H2' | 2.35 | 0.42 |
| 2:1B:66:A:H61 | 2:1B:109:C:C5' | 2.27 | 0.42 |
| 5:1F:176:LEU:HD13 | 5:1F:181:LEU:HA | 2.01 | 0.42 |
| 6:1G:102:PHE:HA | 6:1G:105:LYS:HE2 | 2.02 | 0.42 |
| 14:1S:87:PHE:HZ | 14:1S:98:VAL:HG12 | 1.85 | 0.42 |
| 16:1U:21:ALA:HB2 | 16:1U:35:ALA:HB1 | 2.00 | 0.42 |
| 17:1V:22:VAL:HG23 | 17:1V:23:GLU:O | 2.20 | 0.42 |
| 20:1Y:35:TYR:CE2 | 20:1Y:69:ALA:HB3 | 2.54 | 0.42 |
| 25:13:12:PRO:O | 25:13:20:LYS:HE3 | 2.19 | 0.42 |
| 32:1a:344:A:O5' | 32:1a:345:C:H5 | 2.03 | 0.42 |
| 32:1a:553:A:H2' | 32:1a:554:C:O4' | 2.20 | 0.42 |
| 32:1a:1355:G:H2' | 32:1a:1356:G:C8 | 2.55 | 0.42 |
| 32:1a:1430:C:H2' | 32:1a:1431:C:O4' | 2.20 | 0.42 |
| 32:1a:1465:C:H2' | 32:1a:1466:C:O4' | 2.19 | 0.42 |
| 34:1c:34:LEU:HD21 | 34:1c:38:ARG:NE | 2.33 | 0.42 |
| 43:1l:24:VAL:HB | 43:1l:27:LEU:HD12 | 2.01 | 0.42 |
| 43:1l:39:VAL:HG21 | 43:1l:57:LYS:HE3 | 2.02 | 0.42 |
| 54:1x:61:C:H2' | 54:1x:62:C:H6 | 1.84 | 0.42 |
| 1:2A:353:G:H2' | 1:2A:354:G:C8 | 2.55 | 0.42 |
| 1:2A:923:C:H2' | 1:2A:924:C:H6 | 1.83 | 0.42 |
| 1:2A:959:A:C6 | 1:2A:960:A:C6 | 3.07 | 0.42 |
| 1:2A:1448:G:H2' | 1:2A:1449:A:C8 | 2.55 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:2A:1525:G:H2' | 1:2A:1526:G:C8 | 2.55 | 0.42 |
| 1:2A:1827:C:H5' | 1:2A:1971:A:H4' | 2.02 | 0.42 |
| 1:2A:2023:G:H5' | 1:2A:2617:C:H4' | 2.00 | 0.42 |
| 1:2A:2086:U:H2' | 1:2A:2087:G:H8 | 1.80 | 0.42 |
| 1:2A:2515:C:H2' | 1:2A:2516:G:C8 | 2.55 | 0.42 |
| 8:2I:72:LEU:HG | 8:2I:140:LEU:HB2 | 2.02 | 0.42 |
| 32:2a:399:G:H2' | 32:2a:400:C:C6 | 2.54 | 0.42 |
| 32:2a:401:C:H2' | 32:2a:402:G:H8 | 1.83 | 0.42 |
| 32:2a:512:U:H2' | 32:2a:513:C:C6 | 2.54 | 0.42 |
| 32:2a:1151:A:H5" | 41:2j:42:THR:H | 1.84 | 0.42 |
| 32:2a:1480:G:H2' | 32:2a:1481:U:O4' | 2.19 | 0.42 |
| 36:2e:41:VAL:HG23 | 36:2e:67:VAL:CG1 | 2.50 | 0.42 |
| 41:2j:8:LEU:HD23 | 41:2j:8:LEU:H | 1.83 | 0.42 |
| 43:2l:42:THR:HG22 | 43:2l:54:LYS:HG3 | 2.02 | 0.42 |
| 54:2x:36:U:H2' | 54:2x:37:A:O4' | 2.20 | 0.42 |
| 1:1A:278:A:H2' | 1:1A:279:C:C6 | 2.55 | 0.42 |
| 1:1A:284:U:H2' | 1:1A:285:C:C6 | 2.55 | 0.42 |
| 1:1A:649:G:H2' | 1:1A:650:C:C6 | 2.55 | 0.42 |
| 1:1A:796:C:H2' | 1:1A:797:C:C6 | 2.55 | 0.42 |
| 1:1A:1138:G:N3 | 9:1N:106:MET:HE2 | 2.35 | 0.42 |
| 1:1A:1359:A:H2' | 1:1A:1360:A:H5' | 2.01 | 0.42 |
| 1:1A:1651:G:H2' | 1:1A:1652:A:O4' | 2.20 | 0.42 |
| 1:1A:1669:A:O4' | 10:1O:5:GLN:HG3 | 2.20 | 0.42 |
| 1:1A:1721:G:H1' | 1:1A:1741:A:H61 | 1.85 | 0.42 |
| 1:1A:2626:C:H2' | 1:1A:2627:G:O4' | 2.20 | 0.42 |
| 1:1A:2649:U:H2' | 1:1A:2650:U:C6 | 2.54 | 0.42 |
| 2:1B:96:U:H2' | 2:1B:97:G:C8 | 2.55 | 0.42 |
| 15:1T:2:ASN:O | 15:1T:6:LEU:HD13 | 2.20 | 0.42 |
| 22:10:4:LYS:NZ | 59:10:203:HOH:O | 2.51 | 0.42 |
| 26:14:1:MET:HB3 | 26:14:6:HIS:CD2 | 2.55 | 0.42 |
| 26:14:40:HIS:O | 26:14:43:TYR:N | 2.50 | 0.42 |
| 28:16:8:LYS:HG2 | 30:18:34:TRP:CG | 2.54 | 0.42 |
| 28:16:14:THR:HG21 | 28:16:48:VAL:HG13 | 2.02 | 0.42 |
| 32:1a:437:U:H5' | 35:1d:155:LEU:CD1 | 2.50 | 0.42 |
| 32:1a:707:C:H5" | 42:1k:85:ARG:HH12 | 1.85 | 0.42 |
| 32:1a:749:C:H2' | 32:1a:750:G:H8 | 1.85 | 0.42 |
| 32:1a:942:G:H21 | 40:1i:124:GLN:NE2 | 2.17 | 0.42 |
| 32:1a:1268:A:O3' | 52:1u:19:GLY:HA2 | 2.20 | 0.42 |
| 33:1b:71:VAL:N | 33:1b:163:PHE:O | 2.48 | 0.42 |
| 40:1i:3:GLN:HE21 | 40:1i:20:ARG:NH1 | 2.18 | 0.42 |
| 1:2A:534:U:H2' | 1:2A:535:C:C6 | 2.55 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:2A:705:A:H2' | 1:2A:706:A:O4' | 2.20 | 0.42 |
| 1:2A:718:A:H3' | 1:2A:719:C:C6 | 2.54 | 0.42 |
| 1:2A:886:C:H2' | 1:2A:887:A:H1' | 2.02 | 0.42 |
| 1:2A:1019:U:O2' | 1:2A:1021:A:H2 | 2.03 | 0.42 |
| 1:2A:1248:G:C5 | 16:2U:3:ARG:HB2 | 2.55 | 0.42 |
| 1:2A:1346:G:C5 | 1:2A:1347:G:N7 | 2.88 | 0.42 |
| 1:2A:1417:C:H2' | 1:2A:1418:G:O4' | 2.20 | 0.42 |
| 1:2A:1598:C:H2' | 1:2A:1599:C:H6 | 1.85 | 0.42 |
| 1:2A:1658:C:OP1 | 59:2A:3969:HOH:O | 2.22 | 0.42 |
| 1:2A:2184:G:H2' | 1:2A:2185:C:H5' | 2.02 | 0.42 |
| 10:2O:12:ASP:CG | 10:2O:14:THR:HG23 | 2.44 | 0.42 |
| 10:2O:43:VAL:HG23 | 10:2O:56:ASP:O | 2.20 | 0.42 |
| 17:2V:85:LYS:NZ | 17:2V:85:LYS:HB3 | 2.35 | 0.42 |
| 21:2Z:60:GLU:H | 21:2Z:60:GLU:HG2 | 1.58 | 0.42 |
| 26:24:1:MET:HB3 | 26:24:6:HIS:CD2 | 2.54 | 0.42 |
| 32:2a:297:G:N2 | 32:2a:300:A:OP2 | 2.53 | 0.42 |
| 32:2a:311:C:H2' | 32:2a:312:C:O4' | 2.20 | 0.42 |
| 32:2a:523:A:H61 | 43:2l:92:0TD:CG | 2.32 | 0.42 |
| 32:2a:636:U:H2' | 32:2a:637:G:C8 | 2.55 | 0.42 |
| 32:2a:640:A:N3 | 39:2h:115:SER:HB3 | 2.35 | 0.42 |
| 32:2a:792:A:H4' | 32:2a:793:U:C5' | 2.49 | 0.42 |
| 32:2a:962:C:H2' | 32:2a:963:G:O4' | 2.19 | 0.42 |
| 32:2a:1032:G:H2' | 32:2a:1033:G:C8 | 2.55 | 0.42 |
| 32:2a:1168:A:H3' | 32:2a:1169:A:H8 | 1.85 | 0.42 |
| 32:2a:1346:A:N7 | 38:2g:10:ARG:NH1 | 2.68 | 0.42 |
| 34:2c:36:ASP:O | 34:2c:40:ARG:HG3 | 2.19 | 0.42 |
| 38:2g:65:ALA:O | 38:2g:69:VAL:HG23 | 2.20 | 0.42 |
| 44:2m:105:THR:HG22 | 44:2m:106:ASN:H | 1.84 | 0.42 |
| 1:1A:466:A:N3 | 1:1A:683:C:H1' | 2.34 | 0.42 |
| 1:1A:540:C:H2' | 1:1A:541:C:C6 | 2.55 | 0.42 |
| 1:1A:581:C:H2' | 1:1A:582:G:H8 | 1.85 | 0.42 |
| 1:1A:603:A:O4' | 1:1A:655:A:N6 | 2.53 | 0.42 |
| 1:1A:714:U:O2' | 1:1A:716:A:N7 | 2.45 | 0.42 |
| 1:1A:865:C:N3 | 1:1A:908:C:N4 | 2.68 | 0.42 |
| 1:1A:1011:G:H4' | 16:1U:75:ASN:ND2 | 2.34 | 0.42 |
| 1:1A:1878:G:H2' | 1:1A:1879:C:C6 | 2.55 | 0.42 |
| 1:1A:2075:U:H2' | 1:1A:2238:G:N2 | 2.34 | 0.42 |
| 1:1A:2143:C:H3' | 1:1A:2144:U:H5" | 2.01 | 0.42 |
| 1:1A:2320:A:H2' | 1:1A:2320:A:N3 | 2.35 | 0.42 |
| 1:1A:2869:G:H2' | 1:1A:2870:C:O4' | 2.20 | 0.42 |
| 2:1B:89:G:H2' | 2:1B:90:A:C8 | 2.54 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:1D:37:LEU:HD22 | 3:1D:87:ASN:ND2 | 2.34 | 0.42 |
| 7:1H:3:ARG:HE | 7:1H:54:ARG:HH12 | 1.68 | 0.42 |
| 8:1I:26:ALA:HA | 8:1I:30:LEU:HB2 | 2.02 | 0.42 |
| 9:1N:47:ALA:HB2 | 9:1N:112:LEU:HD11 | 2.01 | 0.42 |
| 11:1P:37:GLY:C | 11:1P:38:GLN:O | 2.62 | 0.42 |
| 11:1P:63:PRO:HB2 | 30:18:30:ARG:NH2 | 2.35 | 0.42 |
| 12:1Q:36:ALA:HB2 | 12:1Q:103:MET:SD | 2.60 | 0.42 |
| 21:1Z:137:ILE:CG2 | 21:1Z:155:LEU:HG | 2.50 | 0.42 |
| 32:1a:345:C:H4' | 32:1a:346:G:H5" | 2.02 | 0.42 |
| 32:1a:790:A:N1 | 32:1a:1497:G:H5" | 2.35 | 0.42 |
| 32:1a:980:C:H1' | 45:1n:19:ARG:HA | 2.02 | 0.42 |
| 32:1a:1114:C:H42 | 32:1a:1186:G:H1 | 1.67 | 0.42 |
| 32:1a:1137:C:H5" | 32:1a:1138:G:O5' | 2.20 | 0.42 |
| 32:1a:1226:C:H4' | 50:1s:80:TYR:OH | 2.20 | 0.42 |
| 32:1a:1343:G:H1' | 40:1i:121:ARG:NH1 | 2.35 | 0.42 |
| 33:1b:178:ARG:NH2 | 39:1h:74:PRO:HB3 | 2.35 | 0.42 |
| 36:1e:100:VAL:O | 36:1e:107:ARG:NH1 | 2.51 | 0.42 |
| 42:1k:48:ILE:O | 42:1k:50:TYR:N | 2.53 | 0.42 |
| 43:1l:33:ARG:HD2 | 43:1l:62:SER:HB3 | 2.02 | 0.42 |
| 1:2A:720:C:H2' | 1:2A:721:C:C6 | 2.54 | 0.42 |
| 1:2A:729:G:H2' | 1:2A:1775:U:O2 | 2.20 | 0.42 |
| 1:2A:887:A:H4' | 1:2A:888:C:C5 | 2.55 | 0.42 |
| 1:2A:993:G:OP1 | 16:2U:50:ARG:HD2 | 2.20 | 0.42 |
| 1:2A:1114:G:H2' | 1:2A:1115:G:H8 | 1.85 | 0.42 |
| 1:2A:2106:G:H2' | 1:2A:2107:C:O4' | 2.19 | 0.42 |
| 1:2A:2199:A:H3' | 1:2A:2200:C:C6 | 2.55 | 0.42 |
| 1:2A:2328:A:H2' | 1:2A:2329:G:C8 | 2.55 | 0.42 |
| 1:2A:2406:U:C4 | 11:2P:72:PRO:HD2 | 2.55 | 0.42 |
| 1:2A:2489:G:C6 | 1:2A:2490:G:C6 | 3.08 | 0.42 |
| 2:2B:4:C:H42 | 2:2B:117:G:H1 | 1.67 | 0.42 |
| 2:2B:103:G:H21 | 21:2Z:73:GLN:NE2 | 2.18 | 0.42 |
| 4:2E:96:PHE:O | 4:2E:175:VAL:HG21 | 2.20 | 0.42 |
| 4:2E:175:VAL:O | 4:2E:177:PRO:HD3 | 2.20 | 0.42 |
| 22:20:21:LEU:HD21 | 22:20:41:ARG:CZ | 2.50 | 0.42 |
| 32:2a:958:A:N6 | 50:2s:77:THR:O | 2.53 | 0.42 |
| 32:2a:991:U:C4 | 32:2a:1212:U:H1' | 2.55 | 0.42 |
| 32:2a:1047:G:H5" | 45:2n:4:LYS:HD3 | 2.02 | 0.42 |
| 32:2a:1255:G:P | 41:2j:45:ARG:HH21 | 2.43 | 0.42 |
| 32:2a:1371:G:C6 | 32:2a:1372:U:C4 | 3.08 | 0.42 |
| 35:2d:163:GLU:C | 35:2d:165:MET:H | 2.27 | 0.42 |
| 47:2p:19:ILE:N | 47:2p:37:GLY:O | 2.53 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1A:330:A:N7 | 1:1A:1210:A:O2' | 2.33 | 0.41 |
| 1:1A:887:A:OP1 | 1:1A:888:C:H5 | 2.03 | 0.41 |
| 1:1A:2038:G:H2' | 1:1A:2039:C:O4' | 2.20 | 0.41 |
| 1:1A:2439:A:H5' | 1:1A:2439:A:C8 | 2.55 | 0.41 |
| 1:1A:2563:U:H1' | 1:1A:2566:A:C6 | 2.56 | 0.41 |
| 1:1A:2577:A:O4' | 27:15:3:LYS:HB2 | 2.19 | 0.41 |
| 3:1D:26:LYS:HE2 | 3:1D:28:GLU:O | 2.21 | 0.41 |
| 7:1H:23:ARG:HE | 7:1H:23:ARG:HB2 | 1.61 | 0.41 |
| 10:1O:68:GLU:HB3 | 10:1O:78:ARG:HB2 | 2.01 | 0.41 |
| 16:1U:17:ILE:HD12 | 16:1U:32:PHE:CE1 | 2.55 | 0.41 |
| 18:1W:25:ARG:NH2 | 18:1W:74:ALA:O | 2.52 | 0.41 |
| 32:1a:501:C:H2' | 32:1a:502:G:C8 | 2.55 | 0.41 |
| 32:1a:684:A:H2' | 32:1a:685:G:C8 | 2.55 | 0.41 |
| 32:1a:922:G:C6 | 32:1a:923:A:C6 | 3.08 | 0.41 |
| 32:1a:1263:C:H2' | 32:1a:1264:C:C6 | 2.55 | 0.41 |
| 32:1a:1302:U:H5 | 44:1m:17:VAL:HG21 | 1.84 | 0.41 |
| 33:1b:19:HIS:HA | 33:1b:39:ILE:HG21 | 2.01 | 0.41 |
| 34:1c:69:HIS:HA | 34:1c:104:GLN:HB3 | 2.02 | 0.41 |
| 38:1g:65:ALA:HB3 | 38:1g:124:LEU:HD23 | 2.00 | 0.41 |
| 47:1p:8:ARG:HB2 | 47:1p:17:TYR:CE1 | 2.55 | 0.41 |
| 51:1t:50:GLU:HG3 | 51:1t:100:ILE:HG12 | 2.02 | 0.41 |
| 1:2A:948:G:N1 | 1:2A:970:C:O2 | 2.53 | 0.41 |
| 1:2A:1268:A:C2 | 1:2A:2013:A:C4 | 3.07 | 0.41 |
| 1:2A:1493:C:N4 | 1:2A:2206:G:O2' | 2.49 | 0.41 |
| 1:2A:1608:A:H1' | 1:2A:1610:A:OP2 | 2.20 | 0.41 |
| 1:2A:1654:A:O4' | 1:2A:2823:A:H5' | 2.20 | 0.41 |
| 1:2A:2051:A:H5' | 1:2A:2578:G:O4' | 2.20 | 0.41 |
| 1:2A:2131:G:H4' | 1:2A:2132:U:H3' | 2.01 | 0.41 |
| 1:2A:2377:A:H2' | 1:2A:2378:A:C8 | 2.55 | 0.41 |
| 1:2A:2391:G:O2' | 1:2A:2422:A:N7 | 2.53 | 0.41 |
| 6:2G:138:GLN:OE1 | 6:2G:138:GLN:N | 2.53 | 0.41 |
| 7:2H:123:PHE:CD1 | 7:2H:133:VAL:HG22 | 2.55 | 0.41 |
| 9:2N:34:LEU:O | 9:2N:49:GLY:HA3 | 2.19 | 0.41 |
| 12:2Q:63:LYS:HD3 | 12:2Q:65:PHE:CZ | 2.55 | 0.41 |
| 16:2U:44:ASN:ND2 | 17:2V:75:PHE:HB3 | 2.35 | 0.41 |
| 26:24:58:ARG:HE | 50:2s:68:GLY:HA3 | 1.85 | 0.41 |
| 32:2a:226:G:H2' | 32:2a:227:G:H8 | 1.85 | 0.41 |
| 32:2a:266:G:H2' | 32:2a:266:G:N3 | 2.34 | 0.41 |
| 1:1A:568:U:O5' | 1:1A:945:A:N6 | 2.52 | 0.41 |
| 1:1A:1248:G:P | 5:1F:92:PRO:HG3 | 2.60 | 0.41 |
| 1:1A:1287:A:C6 | 1:1A:1288:U:N3 | 2.88 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1A:1334:G:C6 | 1:1A:1335:U:C4 | 3.08 | 0.41 |
| 1:1A:2206:G:OP2 | 1:1A:2206:G:H4' | 2.20 | 0.41 |
| 1:1A:2360:A:H8 | 1:1A:2360:A:O5' | 2.04 | 0.41 |
| 3:1D:166:GLN:NE2 | 32:1a:713:G:OP1 | 2.48 | 0.41 |
| 8:1I:2:LYS:HA | 8:1I:19:VAL:O | 2.20 | 0.41 |
| 8:1I:38:LEU:HD23 | 8:1I:38:LEU:H | 1.85 | 0.41 |
| 9:1N:67:LEU:HD12 | 9:1N:67:LEU:HA | 1.72 | 0.41 |
| 18:1W:18:ARG:HG2 | 18:1W:76:VAL:HB | 2.02 | 0.41 |
| 20:1Y:1:MET:HB2 | 20:1Y:2:ARG:H | 1.68 | 0.41 |
| 20:1Y:68:HIS:HB3 | 20:1Y:71:LYS:HG3 | 2.02 | 0.41 |
| 21:1Z:101:PRO:O | 21:1Z:102:LEU:HD12 | 2.20 | 0.41 |
| 32:1a:269:C:H2' | 32:1a:270:A:C8 | 2.55 | 0.41 |
| 32:1a:689:C:OP2 | 42:1k:55:LYS:NZ | 2.45 | 0.41 |
| 32:1a:742:G:H4' | 46:1o:58:MET:HE1 | 2.01 | 0.41 |
| 32:1a:1152:A:H5' | 41:1j:13:HIS:CG | 2.55 | 0.41 |
| 32:1a:1370:G:C2 | 32:1a:1371:G:C8 | 3.09 | 0.41 |
| 33:1b:12:GLU:HB2 | 33:1b:213:LEU:HD11 | 2.01 | 0.41 |
| 33:1b:76:GLN:O | 33:1b:208:ILE:HG22 | 2.20 | 0.41 |
| 34:1c:6:HIS:CD2 | 34:1c:8:ILE:HG12 | 2.56 | 0.41 |
| 35:1d:65:ARG:O | 35:1d:68:TYR:N | 2.52 | 0.41 |
| 36:1e:105:VAL:HB | 36:1e:106:PRO:HD3 | 2.03 | 0.41 |
| 39:1h:30:ARG:O | 39:1h:34:GLU:HG2 | 2.20 | 0.41 |
| 39:1h:86:ILE:HG21 | 39:1h:133:LEU:HD13 | 2.02 | 0.41 |
| 41:1j:21:GLN:O | 41:1j:25:GLU:HG2 | 2.19 | 0.41 |
| 43:1l:77:LEU:HD23 | 43:1l:77:LEU:HA | 1.84 | 0.41 |
| 44:1m:86:CYS:HB2 | 50:1s:73:GLU:HB3 | 2.02 | 0.41 |
| 1:2A:153:C:H2' | 1:2A:154:G:H8 | 1.85 | 0.41 |
| 1:2A:523:C:H5" | 1:2A:540:C:O2' | 2.20 | 0.41 |
| 1:2A:528:A:C2 | 1:2A:2043:C:H4' | 2.54 | 0.41 |
| 1:2A:882:G:H2' | 1:2A:883:G:H8 | 1.85 | 0.41 |
| 1:2A:1022:G:H1 | 1:2A:1142(A):A:H2 | 1.68 | 0.41 |
| 1:2A:1161:C:H2' | 1:2A:1162:G:H8 | 1.85 | 0.41 |
| 1:2A:1218:C:H42 | 1:2A:1231:G:H1 | 1.68 | 0.41 |
| 1:2A:1759:A:H1' | 1:2A:2711:A:C2 | 2.55 | 0.41 |
| 1:2A:2142:C:H2' | 1:2A:2143:C:C6 | 2.55 | 0.41 |
| 1:2A:2322:A:H2' | 1:2A:2323:G:O4' | 2.20 | 0.41 |
| 1:2A:2406:U:H6 | 1:2A:2406:U:H2' | 1.70 | 0.41 |
| 1:2A:2511:U:O2' | 4:2E:138:PRO:O | 2.34 | 0.41 |
| 1:2A:2577:A:OP2 | 27:25:3:LYS:NZ | 2.51 | 0.41 |
| 1:2A:2781:A:H5" | 1:2A:2782:G:H5' | 2.00 | 0.41 |
| 1:2A:2831:G:O2' | 1:2A:2883:A:H2' | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 8:2I:1:MET:HE1 | 8:2I:27:ARG:HH12 | 1.84 | 0.41 |
| 8:2I:29:TYR:HD2 | 8:2I:30:LEU:HD23 | 1.84 | 0.41 |
| 14:2S:30:ARG:HG3 | 14:2S:97:ARG:CZ | 2.50 | 0.41 |
| 21:2Z:105:VAL:N | 21:2Z:139:VAL:O | 2.36 | 0.41 |
| 22:20:24:LYS:N | 22:20:37:LEU:O | 2.47 | 0.41 |
| 25:23:16:PRO:HB2 | 25:23:18:ASP:OD1 | 2.21 | 0.41 |
| 32:2a:542:G:H5' | 35:2d:41:GLY:HA3 | 2.02 | 0.41 |
| 32:2a:715:A:H2' | 32:2a:716:A:C8 | 2.55 | 0.41 |
| 33:2b:188:ALA:O | 33:2b:202:PRO:HA | 2.19 | 0.41 |
| 40:2i:4:TYR:O | 40:2i:19:LEU:N | 2.45 | 0.41 |
| 44:2m:91:ARG:HD2 | 44:2m:96:LEU:HB2 | 2.01 | 0.41 |
| 45:2n:32:SER:O | 45:2n:32:SER:OG | 2.33 | 0.41 |
| 46:2o:28:GLN:HE21 | 46:2o:28:GLN:HB3 | 1.62 | 0.41 |
| 47:2p:3:LYS:O | 47:2p:21:VAL:HA | 2.20 | 0.41 |
| 1:1A:129:C:H2' | 1:1A:130:C:H6 | 1.85 | 0.41 |
| 1:1A:1022:G:C5 | 1:1A:1140:C:C4 | 3.07 | 0.41 |
| 1:1A:1056:G:C2' | 1:1A:1103:A:H61 | 2.34 | 0.41 |
| 1:1A:1230:C:H2' | 1:1A:1231:G:H8 | 1.85 | 0.41 |
| 1:1A:1826:G:H4' | 3:1D:242:ARG:CZ | 2.50 | 0.41 |
| 1:1A:2875:C:H2' | 1:1A:2876:G:O4' | 2.20 | 0.41 |
| 5:1F:53:THR:HG23 | 5:1F:55:GLY:H | 1.85 | 0.41 |
| 8:1I:100:ALA:O | 8:1I:104:GLN:HB2 | 2.21 | 0.41 |
| 11:1P:101:VAL:HG23 | 11:1P:106:LEU:O | 2.20 | 0.41 |
| 13:1R:56:LYS:NZ | 13:1R:90:ARG:O | 2.54 | 0.41 |
| 14:1S:92:TYR:CB | 14:1S:98:VAL:HG21 | 2.51 | 0.41 |
| 16:1U:97:ASP:OD1 | 16:1U:101:ARG:HD2 | 2.19 | 0.41 |
| 26:14:53:GLU:HB2 | 26:14:55:ARG:O | 2.19 | 0.41 |
| 31:19:32:HIS:O | 31:19:34:GLN:HG3 | 2.19 | 0.41 |
| 32:1a:375:U:O3' | 47:1p:6:LEU:HB2 | 2.20 | 0.41 |
| 32:1a:510:A:H8 | 59:1a:1931:HOH:O | 2.02 | 0.41 |
| 32:1a:1084:G:N2 | 59:1a:1941:HOH:O | 2.35 | 0.41 |
| 32:1a:1090:U:H2' | 32:1a:1091:U:C6 | 2.55 | 0.41 |
| 32:1a:1168:A:P | 32:1a:1168:A:H8 | 2.42 | 0.41 |
| 32:1a:1194:U:H2' | 32:1a:1195:C:C6 | 2.56 | 0.41 |
| 38:1g:28:ASN:HD22 | 38:1g:28:ASN:HA | 1.70 | 0.41 |
| 38:1g:97:GLN:HG2 | 38:1g:101:LEU:HD11 | 2.03 | 0.41 |
| 1:2A:272(E):G:C6 | 1:2A:272(F):C:C4 | 3.08 | 0.41 |
| 1:2A:750:A:C4 | 1:2A:753:C:H1' | 2.56 | 0.41 |
| 1:2A:851:U:H5' | 25:23:49:LYS:HD2 | 2.03 | 0.41 |
| 1:2A:1158:C:C2' | 1:2A:1159:U:H5' | 2.51 | 0.41 |
| 1:2A:1206:G:C6 | 1:2A:1207:C:C4 | 3.08 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:2A:2014:A:H2' | 1:2A:2015:A:C8 | 2.55 | 0.41 |
| 1:2A:2497:A:H5" | 59:2A:4033:HOH:O | 2.19 | 0.41 |
| 1:2A:2547:U:H2' | 1:2A:2548:G:C8 | 2.55 | 0.41 |
| 1:2A:2633:G:H2' | 1:2A:2634:G:O4' | 2.19 | 0.41 |
| 1:2A:2849:U:O4 | 15:2T:23:ARG:NH2 | 2.52 | 0.41 |
| 6:2G:122:PRO:HB3 | 6:2G:170:ARG:HH21 | 1.84 | 0.41 |
| 11:2P:49:ARG:O | 30:28:57:ARG:NH2 | 2.43 | 0.41 |
| 14:2S:26:LEU:HD22 | 14:2S:87:PHE:CE1 | 2.55 | 0.41 |
| 20:2Y:20:TYR:HB3 | 20:2Y:23:ARG:HG3 | 2.01 | 0.41 |
| 32:2a:46:G:HO2' | 32:2a:365:U:H1' | 1.84 | 0.41 |
| 32:2a:102:G:H2' | 32:2a:103:C:H6 | 1.84 | 0.41 |
| 32:2a:376:G:OP2 | 47:2p:67:THR:HG21 | 2.20 | 0.41 |
| 32:2a:920:U:H2' | 32:2a:921:U:C6 | 2.55 | 0.41 |
| 32:2a:1112:C:N3 | 34:2c:178:LEU:HD12 | 2.36 | 0.41 |
| 32:2a:1188:A:H2' | 32:2a:1189:C:O4' | 2.20 | 0.41 |
| 34:2c:12:LEU:HA | 34:2c:16:ARG:O | 2.20 | 0.41 |
| 35:2d:38:TYR:CD2 | 35:2d:38:TYR:N | 2.87 | 0.41 |
| 37:2f:11:ASN:HB3 | 37:2f:14:LEU:HG | 2.02 | 0.41 |
| 39:2h:56:LYS:HD3 | 39:2h:56:LYS:HA | 1.83 | 0.41 |
| 46:2o:7:GLU:OE1 | 46:2o:38:ARG:NH2 | 2.54 | 0.41 |
| 47:2p:59:TRP:HB3 | 47:2p:64:ALA:CB | 2.50 | 0.41 |
| 48:2q:22:LEU:HD13 | 48:2q:41:LYS:HG2 | 2.02 | 0.41 |
| 49:2r:37:VAL:HB | 49:2r:78:LEU:HB3 | 2.02 | 0.41 |
| 54:2x:19:G:C4 | 54:2x:57:A:C2 | 3.09 | 0.41 |
| 1:1A:196:A:H2' | 1:1A:196:A:N3 | 2.35 | 0.41 |
| 1:1A:583:G:OP2 | 16:1U:10:ARG:HD2 | 2.21 | 0.41 |
| 1:1A:784:A:C8 | 1:1A:792:G:C5 | 3.08 | 0.41 |
| 1:1A:819:A:C4 | 1:1A:1189:A:C2 | 3.08 | 0.41 |
| 1:1A:1025:G:O2' | 59:1A:4231:HOH:O | 2.05 | 0.41 |
| 1:1A:1356:G:N2 | 1:1A:1376:C:C2 | 2.89 | 0.41 |
| 1:1A:1448:G:H4' | 1:1A:1542:A:OP1 | 2.21 | 0.41 |
| 1:1A:1721:G:H1' | 1:1A:1741:A:N6 | 2.35 | 0.41 |
| 1:1A:1815:A:OP1 | 1:1A:1815:A:H8 | 2.03 | 0.41 |
| 1:1A:1843:C:H2' | 1:1A:1844:C:C6 | 2.54 | 0.41 |
| 1:1A:2378:A:H2' | 14:1S:21:THR:HG21 | 2.02 | 0.41 |
| 1:1A:2443:C:H2' | 1:1A:2444:G:C8 | 2.55 | 0.41 |
| 1:1A:2712:U:OP1 | 1:1A:2714:G:H4' | 2.21 | 0.41 |
| 14:1S:72:ALA:O | 14:1S:76:LYS:HG3 | 2.21 | 0.41 |
| 26:14:57:GLU:HA | 26:14:58:ARG:HA | 1.79 | 0.41 |
| 32:1a:46:G:O2' | 32:1a:365:U:H1' | 2.19 | 0.41 |
| 32:1a:143:A:H2 | 32:1a:220:G:H1 | 1.66 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 32:1a:363:A:C5 | 43:1l:31:PRO:HD2 | 2.56 | 0.41 |
| 32:1a:401:C:P | 35:1d:73:ARG:HH21 | 2.42 | 0.41 |
| 33:1b:171:ALA:HA | 33:1b:174:VAL:HG22 | 2.01 | 0.41 |
| 33:1b:178:ARG:NH1 | 33:1b:198:ASP:OD1 | 2.42 | 0.41 |
| 35:1d:88:VAL:O | 35:1d:92:VAL:HG23 | 2.19 | 0.41 |
| 35:1d:173:TRP:CE2 | 35:1d:189:PRO:HG3 | 2.55 | 0.41 |
| 36:1e:31:LEU:HD23 | 36:1e:31:LEU:HA | 1.68 | 0.41 |
| 36:1e:110:LEU:HD13 | 36:1e:118:ILE:HD13 | 2.02 | 0.41 |
| 43:1l:28:LYS:HE3 | 43:1l:64:TYR:HE2 | 1.85 | 0.41 |
| 1:2A:317:G:C2 | 1:2A:318:C:C2 | 3.08 | 0.41 |
| 1:2A:642:G:H21 | 1:2A:646:A:H2 | 1.69 | 0.41 |
| 1:2A:709:U:H2' | 1:2A:710:G:C8 | 2.55 | 0.41 |
| 1:2A:898:C:H2' | 1:2A:899:A:H5' | 2.00 | 0.41 |
| 1:2A:1028:A:H61 | 1:2A:1125:G:H2' | 1.83 | 0.41 |
| 1:2A:1514:U:H2' | 1:2A:1515:G:C8 | 2.55 | 0.41 |
| 1:2A:1788:C:H2' | 1:2A:1789:A:O4' | 2.21 | 0.41 |
| 1:2A:1810:A:H2' | 1:2A:1811:G:O4' | 2.21 | 0.41 |
| 1:2A:2578:G:H1' | 59:2A:4268:HOH:O | 2.20 | 0.41 |
| 1:2A:2688:U:H1' | 1:2A:2721:A:N6 | 2.36 | 0.41 |
| 5:2F:130:ALA:H | 5:2F:142:TRP:CD1 | 2.38 | 0.41 |
| 6:2G:5:VAL:HG23 | 6:2G:8:LYS:HB3 | 2.01 | 0.41 |
| 7:2H:121:ILE:HD11 | 7:2H:140:LYS:HD2 | 2.02 | 0.41 |
| 12:2Q:50:ALA:HB1 | 12:2Q:121:ALA:HB1 | 2.02 | 0.41 |
| 20:2Y:19:LYS:HE2 | 20:2Y:20:TYR:CE2 | 2.55 | 0.41 |
| 32:2a:41:G:H2' | 32:2a:42:G:C8 | 2.55 | 0.41 |
| 32:2a:57:G:H2' | 32:2a:58:C:C6 | 2.55 | 0.41 |
| 32:2a:186:C:H5' | 51:2t:78:ALA:HB1 | 2.03 | 0.41 |
| 32:2a:293:G:C6 | 32:2a:294:U:C4 | 3.09 | 0.41 |
| 32:2a:779:C:H2' | 32:2a:780:A:O4' | 2.20 | 0.41 |
| 32:2a:826:C:H2' | 32:2a:827:U:C6 | 2.56 | 0.41 |
| 32:2a:838:G:H2' | 32:2a:839:U:H2' | 2.02 | 0.41 |
| 57:2a:3210:V7A:OBE | 57:2a:3210:V7A:OBI | 2.34 | 0.41 |
| 1:1A:272(C):G:H2' | 1:1A:272(D):G:O4' | 2.20 | 0.41 |
| 1:1A:370:G:O5' | 1:1A:423:A:N6 | 2.53 | 0.41 |
| 1:1A:952:G:C6 | 1:1A:953:A:N7 | 2.88 | 0.41 |
| 1:1A:1039:G:H1 | 1:1A:1116:C:H42 | 1.66 | 0.41 |
| 1:1A:1668:A:H4' | 1:1A:1669:A:O5' | 2.20 | 0.41 |
| 1:1A:1968:G:OP2 | 59:1A:4299:HOH:O | 2.22 | 0.41 |
| 1:1A:2171:A:O2' | 1:1A:2172:U:H5" | 2.20 | 0.41 |
| 2:1B:78:A:H2' | 2:1B:79:C:O4' | 2.20 | 0.41 |
| 8:1I:81:VAL:O | 8:1I:146:ALA:HA | 2.19 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 15:1T:96:ARG:HG2 | 15:1T:98:LYS:O | 2.19 | 0.41 |
| 32:1a:303:A:H2' | 32:1a:304:U:O4' | 2.21 | 0.41 |
| 32:1a:835:U:OP1 | 49:1r:64:ARG:NH1 | 2.32 | 0.41 |
| 32:1a:947:G:H2' | 32:1a:948:C:C6 | 2.56 | 0.41 |
| 32:1a:1431:C:H2' | 32:1a:1432:G:O4' | 2.20 | 0.41 |
| 32:1a:1512:U:H2' | 32:1a:1513:A:C8 | 2.56 | 0.41 |
| 34:1c:123:GLN:O | 34:1c:128:PHE:HB2 | 2.21 | 0.41 |
| 35:1d:166:LYS:NZ | 35:1d:166:LYS:HB2 | 2.36 | 0.41 |
| 36:1e:83:GLU:HA | 36:1e:87:SER:O | 2.20 | 0.41 |
| 48:1q:28:PRO:HA | 48:1q:35:VAL:HA | 2.03 | 0.41 |
| 48:1q:66:SER:HB3 | 48:1q:69:LYS:HB2 | 2.03 | 0.41 |
| 50:1s:12:ASP:HB3 | 50:1s:14:HIS:CE1 | 2.54 | 0.41 |
| 1:2A:615:G:OP2 | 5:2F:43:LYS:NZ | 2.44 | 0.41 |
| 1:2A:810:U:OP1 | 59:2A:3968:HOH:O | 2.22 | 0.41 |
| 1:2A:1257:C:O5' | 1:2A:1257:C:H6 | 2.03 | 0.41 |
| 1:2A:1580:A:H5' | 1:2A:1581:G:OP2 | 2.21 | 0.41 |
| 1:2A:1788:C:C2 | 1:2A:1789:A:C8 | 3.09 | 0.41 |
| 1:2A:1812:A:H2' | 1:2A:1813:G:H8 | 1.84 | 0.41 |
| 1:2A:2484:G:C2 | 1:2A:2485:G:C8 | 3.09 | 0.41 |
| 1:2A:2572:A:N7 | 4:2E:145:LYS:HB2 | 2.35 | 0.41 |
| 1:2A:2739:U:O2 | 1:2A:2766:G:N2 | 2.53 | 0.41 |
| 1:2A:2836:U:C4 | 1:2A:2883:A:N6 | 2.89 | 0.41 |
| 3:2D:275:LYS:HD2 | 3:2D:276:LYS:HG3 | 2.02 | 0.41 |
| 4:2E:105:THR:HG23 | 4:2E:166:THR:OG1 | 2.20 | 0.41 |
| 5:2F:37:VAL:HG22 | 5:2F:183:VAL:HG23 | 2.02 | 0.41 |
| 6:2G:7:LEU:HD13 | 6:2G:104:GLU:HA | 2.02 | 0.41 |
| 8:2I:114:LEU:HB2 | 8:2I:130:TYR:HD1 | 1.85 | 0.41 |
| 10:2O:78:ARG:NE | 15:2T:73:GLU:OE1 | 2.50 | 0.41 |
| 14:2S:92:TYR:HB3 | 14:2S:98:VAL:HG21 | 2.03 | 0.41 |
| 25:23:3:ARG:NH2 | 25:23:36:VAL:HG11 | 2.36 | 0.41 |
| 32:2a:335:C:H2' | 32:2a:336:C:C6 | 2.56 | 0.41 |
| 32:2a:369:C:N4 | 32:2a:392:G:H1 | 2.14 | 0.41 |
| 32:2a:422:C:H4' | 32:2a:423:G:C4 | 2.55 | 0.41 |
| 32:2a:737:A:H1' | 37:2f:73:ASN:ND2 | 2.32 | 0.41 |
| 32:2a:755:G:OP2 | 46:2o:65:ARG:HD2 | 2.20 | 0.41 |
| 32:2a:1062:U:H2' | 32:2a:1063:C:C5 | 2.55 | 0.41 |
| 32:2a:1095:U:C4 | 32:2a:1096:C:C4 | 3.08 | 0.41 |
| 32:2a:1177:G:C6 | 32:2a:1178:G:C4 | 3.09 | 0.41 |
| 32:2a:1271:G:H2' | 32:2a:1272:G:H5" | 2.02 | 0.41 |
| 32:2a:1304:G:C6 | 32:2a:1305:G:N1 | 2.87 | 0.41 |
| 43:2l:58:VAL:O | 43:2l:65:GLU:HA | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 46:2o:5:LYS:H | 46:2o:5:LYS:HG2 | 1.58 | 0.41 |
| 46:2o:39:LEU:HD13 | 46:2o:56:LEU:HB2 | 2.01 | 0.41 |
| 1:1A:90:U:H1' | 1:1A:92:A:C8 | 2.55 | 0.41 |
| 1:1A:197:A:N6 | 1:1A:2430:A:O2' | 2.53 | 0.41 |
| 1:1A:274:G:H2' | 1:1A:274:G:N3 | 2.35 | 0.41 |
| 1:1A:419:C:H2' | 1:1A:420:C:O4' | 2.20 | 0.41 |
| 1:1A:576:U:H2' | 1:1A:577:G:C8 | 2.56 | 0.41 |
| 1:1A:1062:G:C5 | 1:1A:1088:A:H2' | 2.55 | 0.41 |
| 1:1A:1692:U:O2' | 1:1A:1693:U:H2' | 2.21 | 0.41 |
| 1:1A:2323:G:C6 | 1:1A:2324:C:C4 | 3.08 | 0.41 |
| 1:1A:2693:A:H2' | 1:1A:2694:G:C8 | 2.56 | 0.41 |
| 1:1A:2851:A:H2' | 1:1A:2852:G:O4' | 2.20 | 0.41 |
| 6:1G:41:GLN:NE2 | 6:1G:154:GLY:O | 2.32 | 0.41 |
| 8:1I:3:VAL:HG12 | 8:1I:38:LEU:HA | 2.01 | 0.41 |
| 10:1O:14:THR:HG21 | 10:1O:86:ILE:HB | 2.02 | 0.41 |
| 32:1a:60:A:N3 | 32:1a:61:G:H1' | 2.36 | 0.41 |
| 32:1a:261:U:O2' | 32:1a:263:A:N7 | 2.48 | 0.41 |
| 32:1a:1003:G:N3 | 32:1a:1004:A:H2 | 2.19 | 0.41 |
| 32:1a:1016:A:H2' | 32:1a:1017:G:O4' | 2.21 | 0.41 |
| 32:1a:1380:U:C4 | 38:1g:3:ARG:HG3 | 2.55 | 0.41 |
| 35:1d:178:VAL:HG12 | 35:1d:179:GLU:H | 1.85 | 0.41 |
| 39:1h:112:LEU:HB3 | 39:1h:133:LEU:HA | 2.02 | 0.41 |
| 42:1k:65:ALA:HB3 | 42:1k:97:ALA:HB3 | 2.02 | 0.41 |
| 49:1r:25:THR:CG2 | 49:1r:42:ARG:HH12 | 2.33 | 0.41 |
| 51:1t:13:LEU:O | 51:1t:17:ARG:HG3 | 2.20 | 0.41 |
| 51:1t:66:ALA:C | 51:1t:68:LYS:H | 2.29 | 0.41 |
| 51:1t:83:ARG:HA | 51:1t:86:ARG:NH1 | 2.31 | 0.41 |
| 1:2A:243:U:OP1 | 30:28:6:THR:OG1 | 2.31 | 0.41 |
| 1:2A:342:G:H2' | 1:2A:343:C:C6 | 2.54 | 0.41 |
| 1:2A:812:C:H5" | 1:2A:1250:G:O2' | 2.20 | 0.41 |
| 1:2A:873:G:N2 | 1:2A:905:U:C2 | 2.88 | 0.41 |
| 1:2A:1252:G:C2 | 1:2A:1253:A:C2 | 3.09 | 0.41 |
| 1:2A:1269:A:N7 | 59:2A:4053:HOH:O | 2.37 | 0.41 |
| 1:2A:2558:C:H2' | 1:2A:2559:C:O4' | 2.21 | 0.41 |
| 1:2A:2692:C:H5" | 1:2A:2870:C:O2' | 2.21 | 0.41 |
| 2:2B:17:C:N4 | 2:2B:109:C:C2 | 2.89 | 0.41 |
| 8:2I:131:LYS:CB | 8:2I:137:PRO:HA | 2.50 | 0.41 |
| 23:21:7:ILE:HG23 | 23:21:98:LEU:HD11 | 2.02 | 0.41 |
| 27:25:20:ARG:HG2 | 27:25:23:HIS:ND1 | 2.34 | 0.41 |
| 32:2a:674:G:N2 | 32:2a:717:C:O2 | 2.54 | 0.41 |
| 32:2a:868:C:H2' | 32:2a:869:G:O4' | 2.21 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 32:2a:909:A:H2' | 32:2a:910:C:O4' | 2.20 | 0.41 |
| 32:2a:1277:C:O2' | 32:2a:1278:U:O5' | 2.39 | 0.41 |
| 32:2a:1322:C:OP1 | 50:2s:78:ARG:NH1 | 2.52 | 0.41 |
| 32:2a:1513:A:H2' | 32:2a:1514:C:C6 | 2.55 | 0.41 |
| 41:2j:5:ARG:HA | 41:2j:73:ASP:OD1 | 2.21 | 0.41 |
| 41:2j:47:PHE:CZ | 45:2n:37:PHE:HE2 | 2.38 | 0.41 |
| 1:1A:57:C:H2' | 1:1A:58:G:O4' | 2.21 | 0.41 |
| 1:1A:445:C:O2' | 1:1A:446:G:H5' | 2.19 | 0.41 |
| 1:1A:527:C:N3 | 1:1A:2779:U:H2' | 2.36 | 0.41 |
| 1:1A:1182:A:H2' | 1:1A:1183:G:C8 | 2.56 | 0.41 |
| 1:1A:1235:G:C6 | 1:1A:1236:G:N1 | 2.89 | 0.41 |
| 1:1A:1530:C:H2' | 1:1A:1531:C:H6 | 1.86 | 0.41 |
| 1:1A:1800:C:OP2 | 3:1D:183:ARG:NH2 | 2.53 | 0.41 |
| 1:1A:2032:G:OP2 | 1:1A:2454:G:O2' | 2.32 | 0.41 |
| 1:1A:2443:C:H2' | 1:1A:2444:G:H8 | 1.86 | 0.41 |
| 1:1A:2542:A:H4' | 1:1A:2543:G:H8 | 1.85 | 0.41 |
| 6:1G:143:GLU:HG3 | 26:14:31:ILE:HD11 | 2.03 | 0.41 |
| 6:1G:179:PRO:HB2 | 26:14:42:PHE:CE2 | 2.56 | 0.41 |
| 11:1P:2:LYS:HG3 | 11:1P:4:SER:H | 1.86 | 0.41 |
| 11:1P:122:PRO:O | 11:1P:123:LEU:HD23 | 2.21 | 0.41 |
| 12:1Q:7:MET:HE2 | 12:1Q:7:MET:HB3 | 1.92 | 0.41 |
| 13:1R:12:ARG:HG2 | 13:1R:16:HIS:CE1 | 2.56 | 0.41 |
| 32:1a:39:G:C6 | 32:1a:40:C:C4 | 3.09 | 0.41 |
| 32:1a:189:G:C6 | 32:1a:189(L):G:N1 | 2.89 | 0.41 |
| 32:1a:545:C:H2' | 32:1a:546:G:O4' | 2.21 | 0.41 |
| 32:1a:577:G:H2' | 32:1a:578:C:H6 | 1.85 | 0.41 |
| 32:1a:996:A:H2' | 32:1a:997:U:O4' | 2.21 | 0.41 |
| 32:1a:1091:U:H2' | 32:1a:1093:A:OP2 | 2.20 | 0.41 |
| 32:1a:1152:A:H2' | 32:1a:1153:C:H6 | 1.86 | 0.41 |
| 32:1a:1304:G:C5 | 32:1a:1305:G:C6 | 3.09 | 0.41 |
| 32:1a:1519:MA6:N7 | 32:1a:1520:G:H1' | 2.35 | 0.41 |
| 33:1b:174:VAL:O | 33:1b:178:ARG:HG3 | 2.20 | 0.41 |
| 34:1c:32:LEU:HG | 34:1c:59:ARG:NH1 | 2.36 | 0.41 |
| 35:1d:202:LEU:HD23 | 35:1d:202:LEU:HA | 1.77 | 0.41 |
| 39:1h:20:TYR:HA | 39:1h:65:TYR:CZ | 2.55 | 0.41 |
| 40:1i:43:ALA:HA | 40:1i:74:ILE:HD13 | 2.02 | 0.41 |
| 1:2A:407:G:H2' | 1:2A:408:G:C8 | 2.56 | 0.41 |
| 1:2A:812:C:H2' | 1:2A:813:U:H6 | 1.85 | 0.41 |
| 1:2A:1357:U:H2' | 1:2A:1358:G:O4' | 2.21 | 0.41 |
| 1:2A:1368:G:OP1 | 29:27:28:ARG:NH2 | 2.53 | 0.41 |
| 1:2A:1453:U:O2' | 1:2A:1455:G:N7 | 2.51 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:2A:1773:A:C5 | 1:2A:1829:A:H1' | 2.56 | 0.41 |
| 1:2A:1897:G:H2' | 1:2A:1898:U:C6 | 2.55 | 0.41 |
| 1:2A:2114:A:H2' | 1:2A:2114:A:N3 | 2.36 | 0.41 |
| 3:2D:231:HIS:CD2 | 3:2D:249:PRO:HG3 | 2.56 | 0.41 |
| 4:2E:1:MET:HB3 | 4:2E:83:ASP:O | 2.21 | 0.41 |
| 11:2P:47:ASP:CG | 11:2P:49:ARG:HE | 2.29 | 0.41 |
| 12:2Q:36:ALA:HB2 | 12:2Q:103:MET:SD | 2.60 | 0.41 |
| 16:2U:36:ARG:HG2 | 16:2U:40:PHE:CZ | 2.56 | 0.41 |
| 18:2W:55:ALA:O | 18:2W:59:VAL:HG23 | 2.20 | 0.41 |
| 32:2a:62:U:H2' | 32:2a:63:C:C6 | 2.55 | 0.41 |
| 32:2a:559:A:OP1 | 36:2e:126:ARG:NH2 | 2.54 | 0.41 |
| 32:2a:935:A:H2' | 32:2a:936:C:C6 | 2.56 | 0.41 |
| 32:2a:1084:G:OP1 | 32:2a:1086:U:C2 | 2.74 | 0.41 |
| 34:2c:123:GLN:O | 34:2c:128:PHE:HB2 | 2.21 | 0.41 |
| 35:2d:191:ARG:HE | 35:2d:200:GLU:CD | 2.29 | 0.41 |
| 36:2e:110:LEU:HD13 | 36:2e:118:ILE:HG21 | 2.03 | 0.41 |
| 44:2m:67:GLU:HB3 | 44:2m:68:GLY:H | 1.67 | 0.41 |
| 1:1A:53:A:H2' | 1:1A:54:G:O4' | 2.21 | 0.41 |
| 1:1A:226:G:H21 | 1:1A:228:A:H62 | 1.68 | 0.41 |
| 1:1A:376:C:H2' | 1:1A:377:C:H6 | 1.86 | 0.41 |
| 1:1A:637:A:H4' | 1:1A:638:G:O5' | 2.21 | 0.41 |
| 1:1A:686:G:OP2 | 1:1A:686:G:H4' | 2.20 | 0.41 |
| 1:1A:838:C:H2' | 1:1A:839:U:H6 | 1.85 | 0.41 |
| 1:1A:1358:G:N2 | 1:1A:1372:U:C5 | 2.88 | 0.41 |
| 1:1A:1541:G:H3' | 1:1A:1542:A:H2' | 2.01 | 0.41 |
| 1:1A:1594:G:H2' | 1:1A:1595:G:O4' | 2.20 | 0.41 |
| 1:1A:1653:G:O3' | 13:1R:2:ARG:HB2 | 2.20 | 0.41 |
| 1:1A:2167:U:O2 | 1:1A:2167:U:H2' | 2.20 | 0.41 |
| 1:1A:2405:G:O2' | 1:1A:2406:U:OP1 | 2.30 | 0.41 |
| 1:1A:2804:C:H2' | 1:1A:2805:G:O4' | 2.20 | 0.41 |
| 11:1P:100:LEU:HD12 | 11:1P:112:LEU:HD22 | 2.02 | 0.41 |
| 32:1a:160:A:H1' | 32:1a:344:A:C5 | 2.55 | 0.41 |
| 32:1a:530:G:O6 | 53:1v:21:C:H1' | 2.20 | 0.41 |
| 32:1a:600:C:H4' | 39:1h:128:GLY:O | 2.21 | 0.41 |
| 32:1a:738:C:OP2 | 37:1f:92:LYS:NZ | 2.35 | 0.41 |
| 32:1a:1413:A:C2 | 32:1a:1488:G:C2 | 3.09 | 0.41 |
| 39:1h:29:SER:HB3 | 39:1h:32:LYS:HD3 | 2.03 | 0.41 |
| 45:1n:26:ARG:HD3 | 45:1n:43:CYS:SG | 2.60 | 0.41 |
| 48:1q:4:LYS:HG3 | 48:1q:6:LEU:CD1 | 2.51 | 0.41 |
| 1:2A:222:A:H5" | 1:2A:421:U:OP1 | 2.21 | 0.41 |
| 1:2A:262:A:N3 | 1:2A:430:G:O2' | 2.41 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:2A:651:G:OP1 | 30:28:17:THR:HB | 2.20 | 0.41 |
| 1:2A:784:A:C8 | 1:2A:792:G:C5 | 3.09 | 0.41 |
| 1:2A:804:A:H2' | 1:2A:806:C:C4 | 2.56 | 0.41 |
| 1:2A:1030:G:OP2 | 12:2Q:128:LYS:NZ | 2.53 | 0.41 |
| 1:2A:1354:A:H2' | 1:2A:1355:G:O4' | 2.21 | 0.41 |
| 1:2A:1563:G:H2' | 1:2A:1564:C:O4' | 2.20 | 0.41 |
| 1:2A:1942:5MC:OP2 | 1:2A:1943:U:O2' | 2.31 | 0.41 |
| 1:2A:1993:U:H4' | 4:2E:128:SER:OG | 2.21 | 0.41 |
| 1:2A:2133:G:O2' | 1:2A:2157:G:N2 | 2.53 | 0.41 |
| 1:2A:2494:G:O2' | 12:2Q:80:GLU:HA | 2.21 | 0.41 |
| 2:2B:43:C:H5" | 26:24:1:MET:HG2 | 2.02 | 0.41 |
| 3:2D:132:PRO:O | 3:2D:136:ILE:HG13 | 2.20 | 0.41 |
| 4:2E:59:VAL:HG13 | 4:2E:63:LEU:HB2 | 2.03 | 0.41 |
| 5:2F:102:PRO:HB2 | 5:2F:105:VAL:HG23 | 2.01 | 0.41 |
| 21:2Z:45:ASP:OD1 | 21:2Z:49:ARG:HD3 | 2.21 | 0.41 |
| 30:28:28:GLY:O | 30:28:36:LYS:NZ | 2.38 | 0.41 |
| 30:28:30:ARG:HD3 | 30:28:30:ARG:HA | 1.95 | 0.41 |
| 32:2a:27:G:H2' | 32:2a:28:G:C8 | 2.56 | 0.41 |
| 32:2a:309:G:H2' | 32:2a:310:G:C8 | 2.53 | 0.41 |
| 32:2a:376:G:O3' | 47:2p:5:ARG:HD2 | 2.20 | 0.41 |
| 32:2a:601:C:H2' | 32:2a:602:A:H8 | 1.86 | 0.41 |
| 32:2a:790:A:C6 | 32:2a:791:G:C6 | 3.09 | 0.41 |
| 32:2a:932:C:H5" | 38:2g:4:ARG:CZ | 2.50 | 0.41 |
| 32:2a:983:A:H2 | 32:2a:984:C:C6 | 2.38 | 0.41 |
| 32:2a:1121:U:C2' | 32:2a:1122:U:H5' | 2.51 | 0.41 |
| 32:2a:1154:G:H2' | 32:2a:1155:G:H8 | 1.86 | 0.41 |
| 32:2a:1186:G:H4' | 40:2i:110:GLU:OE2 | 2.20 | 0.41 |
| 32:2a:1191:A:H5" | 34:2c:4:LYS:HE3 | 2.03 | 0.41 |
| 40:2i:8:GLY:HA2 | 40:2i:79:LEU:HB3 | 2.03 | 0.41 |
| 46:2o:29:VAL:HG13 | 46:2o:63:ARG:HG3 | 2.03 | 0.41 |
| 1:1A:272(H):C:N4 | 1:1A:272(I):U:O4 | 2.54 | 0.41 |
| 1:1A:459:U:H4' | 29:17:40:TRP:CZ3 | 2.56 | 0.41 |
| 1:1A:1035:U:H2' | 1:1A:1036:G:C8 | 2.56 | 0.41 |
| 1:1A:1324:G:C4 | 1:1A:1328:G:O6 | 2.74 | 0.41 |
| 1:1A:1368:G:C2 | 1:1A:1369:G:C8 | 3.08 | 0.41 |
| 1:1A:1517:G:C6 | 1:1A:1518:U:C4 | 3.08 | 0.41 |
| 1:1A:1702:G:H2' | 1:1A:1703:G:O4' | 2.21 | 0.41 |
| 1:1A:1952:A:C5 | 1:1A:1953:A:C6 | 3.09 | 0.41 |
| 1:1A:2251:OMG:HM23 | 1:1A:2251:OMG:H1' | 1.90 | 0.41 |
| 1:1A:2308:G:O2' | 1:1A:2310:A:N7 | 2.46 | 0.41 |
| 1:1A:2370:G:C6 | 1:1A:2371:G:C6 | 3.08 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1A:2788:C:OP1 | 4:1E:61:ARG:NH2 | 2.53 | 0.41 |
| 3:1D:70:TRP:HB3 | 3:1D:190:TYR:CZ | 2.55 | 0.41 |
| 3:1D:145:VAL:HG12 | 3:1D:146:GLU:O | 2.21 | 0.41 |
| 3:1D:202:LYS:NZ | 32:1a:774:G:OP1 | 2.52 | 0.41 |
| 3:1D:223:GLY:HA3 | 3:1D:231:HIS:CE1 | 2.56 | 0.41 |
| 4:1E:12:THR:HG22 | 4:1E:13:ARG:H | 1.86 | 0.41 |
| 5:1F:34:TRP:HE3 | 5:1F:35:GLU:HG2 | 1.82 | 0.41 |
| 6:1G:97:ASP:O | 6:1G:101:ILE:HG13 | 2.21 | 0.41 |
| 7:1H:84:SER:HA | 7:1H:133:VAL:O | 2.21 | 0.41 |
| 10:1O:10:VAL:HG13 | 10:1O:17:ARG:O | 2.21 | 0.41 |
| 11:1P:75:ILE:H | 11:1P:75:ILE:HD12 | 1.85 | 0.41 |
| 14:1S:11:LYS:HG3 | 14:1S:91:PRO:HD3 | 2.03 | 0.41 |
| 18:1W:7:ALA:HB2 | 18:1W:50:VAL:HG22 | 2.03 | 0.41 |
| 18:1W:80:PRO:O | 18:1W:100:THR:OG1 | 2.37 | 0.41 |
| 21:1Z:125:LEU:HB3 | 21:1Z:165:VAL:HG12 | 2.02 | 0.41 |
| 29:17:33:ARG:NH2 | 59:17:202:HOH:O | 2.46 | 0.41 |
| 32:1a:78:G:C6 | 32:1a:91:C:N4 | 2.89 | 0.41 |
| 32:1a:182:U:OP2 | 59:1a:1918:HOH:O | 2.21 | 0.41 |
| 32:1a:255:G:H2' | 32:1a:256:U:H6 | 1.85 | 0.41 |
| 32:1a:431:A:H2' | 32:1a:432:A:O4' | 2.21 | 0.41 |
| 32:1a:499:A:O3' | 32:1a:500:G:H8 | 2.04 | 0.41 |
| 32:1a:593:G:H2' | 32:1a:594:G:O4' | 2.21 | 0.41 |
| 32:1a:624:C:O3' | 47:1p:10:GLY:HA2 | 2.20 | 0.41 |
| 32:1a:826:C:H2' | 32:1a:827:U:C6 | 2.56 | 0.41 |
| 32:1a:991:U:C5 | 32:1a:1212:U:H1' | 2.56 | 0.41 |
| 32:1a:996:A:H8 | 32:1a:996:A:O5' | 2.04 | 0.41 |
| 32:1a:1020:U:O2 | 32:1a:1020:U:H2' | 2.20 | 0.41 |
| 32:1a:1151:A:O2' | 32:1a:1152:A:H8 | 2.02 | 0.41 |
| 32:1a:1220:G:H2' | 32:1a:1221:G:C8 | 2.56 | 0.41 |
| 32:1a:1367:C:OP1 | 40:1i:115:GLY:N | 2.48 | 0.41 |
| 33:1b:60:ASP:O | 33:1b:64:ARG:HD2 | 2.21 | 0.41 |
| 33:1b:93:VAL:HG21 | 33:1b:97:TRP:CD1 | 2.55 | 0.41 |
| 34:1c:58:GLU:HB2 | 34:1c:65:ALA:HB3 | 2.03 | 0.41 |
| 35:1d:173:TRP:C | 35:1d:186:LEU:HB2 | 2.46 | 0.41 |
| 36:1e:27:ARG:NH1 | 36:1e:27:ARG:HB2 | 2.36 | 0.41 |
| 38:1g:15:ASP:OD1 | 38:1g:19:GLY:N | 2.54 | 0.41 |
| 38:1g:18:TYR:CE1 | 38:1g:59:LEU:HB2 | 2.55 | 0.41 |
| 39:1h:26:VAL:C | 39:1h:58:TYR:HD1 | 2.29 | 0.41 |
| 41:1j:61:GLU:OE2 | 45:1n:49:HIS:NE2 | 2.54 | 0.41 |
| 43:1l:55:VAL:HB | 43:1l:67:THR:HG23 | 2.02 | 0.41 |
| 44:1m:78:ILE:HG22 | 44:1m:82:MET:HE2 | 2.01 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 48:1q:4:LYS:HG3 | 48:1q:6:LEU:HD13 | 2.03 | 0.41 |
| 51:1t:22:ARG:C | 51:1t:26:ASN:HD22 | 2.29 | 0.41 |
| 1:2A:186:G:H2' | 1:2A:187:G:H8 | 1.84 | 0.41 |
| 1:2A:193:U:O3' | 1:2A:803:U:H4' | 2.20 | 0.41 |
| 1:2A:298:G:H5" | 1:2A:299:A:OP1 | 2.20 | 0.41 |
| 1:2A:414:C:H5" | 1:2A:1879:C:O2' | 2.21 | 0.41 |
| 1:2A:479:A:O2' | 1:2A:481:G:H5' | 2.21 | 0.41 |
| 1:2A:494:G:H5' | 18:2W:8:ARG:HD3 | 2.03 | 0.41 |
| 1:2A:500:G:N2 | 1:2A:502:A:H3' | 2.36 | 0.41 |
| 1:2A:529:A:C5 | 1:2A:2042:A:C2 | 3.09 | 0.41 |
| 1:2A:729:G:C5 | 3:2D:208:LYS:HB2 | 2.56 | 0.41 |
| 1:2A:956:G:H2' | 1:2A:957:A:H2' | 2.03 | 0.41 |
| 1:2A:956:G:N2 | 1:2A:959:A:H3' | 2.35 | 0.41 |
| 1:2A:1312:U:OP2 | 19:2X:63:LYS:HD3 | 2.20 | 0.41 |
| 1:2A:1459:G:H2' | 1:2A:1461:G:OP2 | 2.21 | 0.41 |
| 1:2A:1491:G:H2' | 1:2A:1492:G:C8 | 2.56 | 0.41 |
| 1:2A:1518:U:H2' | 1:2A:1519:G:O4' | 2.20 | 0.41 |
| 1:2A:2134:A:H1' | 1:2A:2158:A:N1 | 2.35 | 0.41 |
| 1:2A:2207:G:H3' | 1:2A:2208:A:H5" | 2.02 | 0.41 |
| 1:2A:2462:U:H1' | 1:2A:2491:U:O4 | 2.21 | 0.41 |
| 1:2A:2478:A:C2 | 1:2A:2529:G:H2' | 2.56 | 0.41 |
| 1:2A:2607:G:H2' | 1:2A:2608:G:O4' | 2.20 | 0.41 |
| 1:2A:2792:G:H2' | 1:2A:2792:G:N3 | 2.36 | 0.41 |
| 1:2A:2872:G:O2' | 1:2A:2873:A:H5' | 2.21 | 0.41 |
| 1:2A:2880:C:O3' | 13:2R:90:ARG:NH1 | 2.54 | 0.41 |
| 2:2B:17:C:N4 | 2:2B:109:C:N3 | 2.69 | 0.41 |
| 2:2B:32:C:H2' | 2:2B:33:G:O4' | 2.21 | 0.41 |
| 2:2B:95:C:H2' | 2:2B:96:U:C6 | 2.56 | 0.41 |
| 4:2E:16:ARG:NH1 | 4:2E:173:VAL:HG13 | 2.35 | 0.41 |
| 4:2E:38:THR:OG1 | 4:2E:41:LYS:N | 2.42 | 0.41 |
| 5:2F:116:ASP:O | 5:2F:120:GLU:HG2 | 2.21 | 0.41 |
| 10:2O:2:ILE:HD11 | 10:2O:82:ASN:HB3 | 2.03 | 0.41 |
| 12:2Q:132:VAL:HB | 21:2Z:81:ARG:NH2 | 2.36 | 0.41 |
| 21:2Z:35:ARG:HD2 | 21:2Z:35:ARG:HA | 1.72 | 0.41 |
| 21:2Z:43:GLU:O | 21:2Z:47:VAL:HG12 | 2.21 | 0.41 |
| 21:2Z:54:HIS:HB3 | 21:2Z:101:PRO:HG3 | 2.02 | 0.41 |
| 21:2Z:98:MET:HE2 | 21:2Z:98:MET:HB2 | 1.95 | 0.41 |
| 26:24:60:GLN:O | 26:24:62:ARG:NH2 | 2.54 | 0.41 |
| 29:27:9:ARG:HB3 | 29:27:46:VAL:HG23 | 2.03 | 0.41 |
| 29:27:12:ARG:NH2 | 29:27:44:PRO:HB3 | 2.35 | 0.41 |
| 29:27:26:GLY:O | 29:27:30:VAL:HG23 | 2.21 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 32:2a:189(D):C:H2' | 32:2a:189(E):U:O4' | 2.20 | 0.41 |
| 32:2a:631:G:H2' | 32:2a:632:A:C8 | 2.55 | 0.41 |
| 32:2a:841:U:OP1 | 32:2a:841:U:H6 | 2.04 | 0.41 |
| 32:2a:983:A:H3' | 32:2a:983:A:N3 | 2.35 | 0.41 |
| 32:2a:1122:U:C4 | 32:2a:1123:A:N7 | 2.87 | 0.41 |
| 32:2a:1265:G:C6 | 32:2a:1266:G:C6 | 3.09 | 0.41 |
| 33:2b:43:ASP:OD2 | 33:2b:46:LYS:N | 2.54 | 0.41 |
| 33:2b:98:LEU:HD12 | 33:2b:98:LEU:HA | 1.93 | 0.41 |
| 33:2b:160:ASP:OD1 | 33:2b:160:ASP:N | 2.54 | 0.41 |
| 34:2c:6:HIS:CG | 45:2n:49:HIS:HB3 | 2.55 | 0.41 |
| 35:2d:33:MET:HB2 | 58:2d:303:SF4:S2 | 2.61 | 0.41 |
| 35:2d:155:LEU:O | 35:2d:159:ARG:HG2 | 2.20 | 0.41 |
| 36:2e:9:LYS:HB2 | 36:2e:112:LEU:HD11 | 2.03 | 0.41 |
| 36:2e:57:LYS:HE3 | 36:2e:57:LYS:HB2 | 1.72 | 0.41 |
| 38:2g:69:VAL:HG21 | 38:2g:104:LEU:HD21 | 2.02 | 0.41 |
| 45:2n:7:ILE:HD12 | 45:2n:11:LYS:HE3 | 2.03 | 0.41 |
| 1:1A:64:A:C4 | 19:1X:66:LEU:HD13 | 2.56 | 0.41 |
| 1:1A:306:U:H2' | 1:1A:307:G:O4' | 2.21 | 0.41 |
| 1:1A:817:C:H4' | 1:1A:932:G:C5 | 2.56 | 0.41 |
| 1:1A:1274:A:N3 | 1:1A:1297:C:H1' | 2.36 | 0.41 |
| 1:1A:1405:U:H2' | 1:1A:1406:U:C6 | 2.56 | 0.41 |
| 1:1A:1688:U:O2 | 1:1A:1700:A:H5' | 2.21 | 0.41 |
| 1:1A:2296:U:OP2 | 14:1S:9:ARG:NH2 | 2.54 | 0.41 |
| 1:1A:2563:U:O2 | 1:1A:2565:A:H8 | 2.04 | 0.41 |
| 1:1A:2632:A:O2' | 1:1A:2811:G:O2' | 2.23 | 0.41 |
| 2:1B:2:C:H2' | 2:1B:3:C:H6 | 1.86 | 0.41 |
| 3:1D:35:LYS:HD3 | 3:1D:64:ILE:HD11 | 2.03 | 0.41 |
| 5:1F:197:ASP:OD1 | 5:1F:197:ASP:N | 2.54 | 0.41 |
| 10:1O:52:VAL:HG12 | 10:1O:94:ARG:NH2 | 2.36 | 0.41 |
| 11:1P:82:GLY:HA2 | 11:1P:113:LYS:O | 2.20 | 0.41 |
| 14:1S:87:PHE:CZ | 14:1S:98:VAL:HG12 | 2.55 | 0.41 |
| 17:1V:71:LEU:HD23 | 17:1V:71:LEU:HA | 1.92 | 0.41 |
| 19:1X:64:LYS:HD3 | 19:1X:64:LYS:HA | 1.87 | 0.41 |
| 30:18:54:GLU:O | 30:18:58:ILE:HD12 | 2.21 | 0.41 |
| 32:1a:10:A:H2' | 32:1a:11:G:H8 | 1.85 | 0.41 |
| 32:1a:503:C:H2' | 32:1a:504:C:H6 | 1.86 | 0.41 |
| 32:1a:607:A:H2' | 32:1a:608:A:H8 | 1.85 | 0.41 |
| 32:1a:674:G:H2' | 32:1a:675:A:C8 | 2.56 | 0.41 |
| 32:1a:880:C:P | 43:1l:8:ASN:HD22 | 2.43 | 0.41 |
| 32:1a:1206:G:C6 | 32:1a:1207:2MG:C5 | 3.08 | 0.41 |
| 32:1a:1298:C:C4 | 38:1g:114:ARG:HD3 | 2.55 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 32:1a:1329:A:P | 44:1m:28:ALA:HB3 | 2.61 | 0.41 |
| 33:1b:151:GLY:HA2 | 33:1b:154:LEU:HD13 | 2.03 | 0.41 |
| 34:1c:115:LEU:HD12 | 34:1c:115:LEU:HA | 1.85 | 0.41 |
| 39:1h:82:HIS:NE2 | 39:1h:84:ARG:HG2 | 2.35 | 0.41 |
| 51:1t:76:ALA:HA | 51:1t:79:ARG:NH1 | 2.36 | 0.41 |
| 1:2A:523:C:H2' | 1:2A:524:U:O4' | 2.21 | 0.41 |
| 1:2A:1658:C:OP1 | 4:2E:135:HIS:NE2 | 2.52 | 0.41 |
| 1:2A:1908:C:O2 | 54:2x:12:G:H4' | 2.21 | 0.41 |
| 7:2H:144:VAL:O | 7:2H:148:ILE:HG13 | 2.21 | 0.41 |
| 32:2a:15:G:C4 | 32:2a:16:A:C8 | 3.08 | 0.41 |
| 32:2a:359:U:H2' | 32:2a:360:A:C8 | 2.56 | 0.41 |
| 32:2a:389:A:C5 | 32:2a:390:C:H1' | 2.56 | 0.41 |
| 32:2a:654:G:H2' | 32:2a:655:A:O4' | 2.21 | 0.41 |
| 32:2a:668:G:H2' | 32:2a:669:U:C6 | 2.56 | 0.41 |
| 32:2a:839:U:H3' | 32:2a:840:C:C6 | 2.56 | 0.41 |
| 32:2a:1077:G:N1 | 32:2a:1080:A:OP2 | 2.49 | 0.41 |
| 33:2b:69:LEU:HD12 | 33:2b:69:LEU:HA | 1.90 | 0.41 |
| 37:2f:63:TYR:O | 37:2f:65:VAL:HG13 | 2.20 | 0.41 |
| 38:2g:77:SER:OG | 38:2g:86:GLN:NE2 | 2.54 | 0.41 |
| 46:2o:31:LEU:HA | 46:2o:31:LEU:HD23 | 1.76 | 0.41 |
| 50:2s:36:ARG:NH2 | 50:2s:72:GLY:O | 2.54 | 0.41 |
| 1:1A:84:A:C5' | 20:1Y:8:LYS:HG2 | 2.50 | 0.40 |
| 1:1A:184:C:H1' | 1:1A:217:G:H1' | 2.03 | 0.40 |
| 1:1A:363(B):G:C4 | 1:1A:363(C):G:C8 | 3.09 | 0.40 |
| 1:1A:611:C:H42 | 1:1A:616:G:H1 | 1.68 | 0.40 |
| 1:1A:664:C:H2' | 1:1A:665:C:H6 | 1.85 | 0.40 |
| 1:1A:1011:G:H4' | 16:1U:75:ASN:HD22 | 1.86 | 0.40 |
| 1:1A:1020:A:N1 | 1:1A:1141:U:O2' | 2.47 | 0.40 |
| 1:1A:1101:U:H2' | 1:1A:1102:C:O4' | 2.21 | 0.40 |
| 1:1A:1266:G:H3' | 59:1A:5127:HOH:O | 2.21 | 0.40 |
| 1:1A:1805:U:H2' | 1:1A:1806:C:C6 | 2.56 | 0.40 |
| 1:1A:1818:U:H2' | 3:1D:157:ARG:HG3 | 2.02 | 0.40 |
| 1:1A:2065:C:H2' | 1:1A:2066:C:C6 | 2.55 | 0.40 |
| 1:1A:2470:G:OP1 | 12:1Q:56:ARG:NH2 | 2.54 | 0.40 |
| 7:1H:117:PRO:HA | 7:1H:118:PRO:HD3 | 1.96 | 0.40 |
| 18:1W:82:LEU:HD22 | 18:1W:84:ARG:HH22 | 1.86 | 0.40 |
| 19:1X:56:THR:HB | 19:1X:77:LYS:HE2 | 2.02 | 0.40 |
| 32:1a:79:G:C6 | 32:1a:90:U:N3 | 2.90 | 0.40 |
| 32:1a:189:G:C6 | 32:1a:189(L):G:C6 | 3.09 | 0.40 |
| 32:1a:880:C:OP1 | 43:1l:8:ASN:ND2 | 2.54 | 0.40 |
| 32:1a:1137:C:H4' | 32:1a:1138:G:C2 | 2.56 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 32:1a:1367:C:H2' | 32:1a:1368:G:O4' | 2.21 | 0.40 |
| 32:1a:1469:G:H2' | 32:1a:1470:G:C8 | 2.56 | 0.40 |
| 35:1d:119:GLN:HE21 | 35:1d:123:HIS:CD2 | 2.40 | 0.40 |
| 37:1f:70:ASP:OD1 | 37:1f:70:ASP:N | 2.47 | 0.40 |
| 1:2A:324:A:N6 | 1:2A:338:G:O2' | 2.52 | 0.40 |
| 1:2A:652:C:O2' | 1:2A:652(A):A:H5' | 2.20 | 0.40 |
| 1:2A:652(D):C:N4 | 1:2A:652(U):G:H1 | 2.17 | 0.40 |
| 1:2A:1037:G:H2' | 1:2A:1038:C:O4' | 2.21 | 0.40 |
| 1:2A:1288:U:C2 | 1:2A:1327:C:C2 | 3.10 | 0.40 |
| 1:2A:1416:G:O2' | 1:2A:1417:C:OP2 | 2.32 | 0.40 |
| 1:2A:1581:G:H2' | 1:2A:1582:C:O4' | 2.21 | 0.40 |
| 1:2A:2312:U:H5' | 6:2G:88:ILE:HD11 | 2.02 | 0.40 |
| 1:2A:2332:U:O2' | 1:2A:2335:A:N3 | 2.54 | 0.40 |
| 1:2A:2629:A:H1' | 1:2A:2630:G:H5" | 2.03 | 0.40 |
| 2:2B:33:G:C6 | 2:2B:34:U:C4 | 3.09 | 0.40 |
| 8:2I:102:SER:HB3 | 8:2I:108:THR:OG1 | 2.21 | 0.40 |
| 18:2W:11:ARG:HD2 | 18:2W:11:ARG:HA | 1.83 | 0.40 |
| 18:2W:14:PRO:HA | 18:2W:17:VAL:HG23 | 2.02 | 0.40 |
| 19:2X:47:PHE:O | 19:2X:49:VAL:HG13 | 2.21 | 0.40 |
| 30:28:52:LYS:N | 30:28:53:PRO:HD2 | 2.36 | 0.40 |
| 32:2a:142:G:H1 | 32:2a:221:C:H42 | 1.69 | 0.40 |
| 32:2a:405:U:OP1 | 32:2a:406:G:O2' | 2.31 | 0.40 |
| 32:2a:736:C:H2' | 32:2a:737:A:H8 | 1.84 | 0.40 |
| 32:2a:737:A:H5' | 37:2f:90:VAL:O | 2.22 | 0.40 |
| 32:2a:823:G:H1 | 32:2a:877:C:N4 | 2.12 | 0.40 |
| 32:2a:1124:G:C2 | 32:2a:1127:G:N2 | 2.89 | 0.40 |
| 32:2a:1305:G:C2 | 32:2a:1331:G:H1' | 2.56 | 0.40 |
| 33:2b:91:PRO:HG3 | 33:2b:154:LEU:HD22 | 2.02 | 0.40 |
| 33:2b:192:SER:O | 33:2b:194:PRO:HD3 | 2.20 | 0.40 |
| 34:2c:30:ARG:HG3 | 34:2c:31:HIS:ND1 | 2.36 | 0.40 |
| 44:2m:29:ARG:HH11 | 44:2m:64:TRP:CD1 | 2.38 | 0.40 |
| 1:1A:69:C:O2 | 1:1A:73:A:O2' | 2.31 | 0.40 |
| 1:1A:226:G:N2 | 1:1A:228:A:H62 | 2.19 | 0.40 |
| 1:1A:1260:G:H2' | 1:1A:1261:C:O4' | 2.21 | 0.40 |
| 1:1A:1367:A:C5 | 1:1A:1368:G:H1' | 2.56 | 0.40 |
| 1:1A:1815:A:OP2 | 3:1D:54:ARG:NH2 | 2.54 | 0.40 |
| 1:1A:2135:A:N6 | 1:1A:2156:G:O2' | 2.54 | 0.40 |
| 1:1A:2136:C:C4 | 1:1A:2155:G:N1 | 2.89 | 0.40 |
| 1:1A:2193:G:H2' | 1:1A:2194:G:C8 | 2.56 | 0.40 |
| 1:1A:2406:U:H2' | 1:1A:2406:U:H6 | 1.65 | 0.40 |
| 1:1A:2721:A:H2' | 1:1A:2722:G:O4' | 2.21 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 14:1S:94:TYR:CE2 | 14:1S:99:LYS:HG3 | 2.57 | 0.40 |
| 18:1W:18:ARG:CG | 18:1W:76:VAL:HB | 2.51 | 0.40 |
| 19:1X:31:HIS:CD2 | 19:1X:33:LYS:H | 2.39 | 0.40 |
| 21:1Z:150:LEU:HA | 21:1Z:150:LEU:HD12 | 1.81 | 0.40 |
| 32:1a:49:U:C2 | 32:1a:361:G:N2 | 2.89 | 0.40 |
| 32:1a:430:A:OP2 | 35:1d:8:VAL:HG12 | 2.21 | 0.40 |
| 32:1a:598:U:H4' | 39:1h:94:TYR:CD2 | 2.56 | 0.40 |
| 32:1a:757:U:O2' | 32:1a:879:C:O2 | 2.35 | 0.40 |
| 32:1a:1118:C:H1' | 32:1a:1179:A:C4 | 2.55 | 0.40 |
| 32:1a:1121:U:H2' | 32:1a:1122:U:H6 | 1.85 | 0.40 |
| 33:1b:24:TRP:CD1 | 33:1b:24:TRP:H | 2.38 | 0.40 |
| 35:1d:182:LYS:HE3 | 35:1d:182:LYS:HB2 | 1.70 | 0.40 |
| 42:1k:103:LEU:HD23 | 42:1k:103:LEU:HA | 1.93 | 0.40 |
| 43:1l:60:LEU:HD12 | 43:1l:64:TYR:HB2 | 2.04 | 0.40 |
| 51:1t:74:LYS:HA | 51:1t:74:LYS:HD2 | 1.90 | 0.40 |
| 1:2A:205:G:O6 | 23:21:39:LYS:NZ | 2.45 | 0.40 |
| 1:2A:299:A:N1 | 1:2A:322:A:O2' | 2.46 | 0.40 |
| 1:2A:864:G:OP2 | 12:2Q:22:LYS:HE2 | 2.21 | 0.40 |
| 1:2A:956:G:O2' | 1:2A:959:A:N7 | 2.53 | 0.40 |
| 1:2A:966:G:C6 | 1:2A:967:C:N4 | 2.89 | 0.40 |
| 1:2A:2488:A:O5' | 1:2A:2488:A:H8 | 2.04 | 0.40 |
| 1:2A:2843:G:H1 | 1:2A:2874:C:N4 | 2.18 | 0.40 |
| 6:2G:107:LEU:HD21 | 6:2G:178:PHE:CE1 | 2.55 | 0.40 |
| 10:2O:19:ILE:HG22 | 10:2O:43:VAL:HA | 2.03 | 0.40 |
| 11:2P:75:ILE:HD12 | 11:2P:75:ILE:H | 1.86 | 0.40 |
| 20:2Y:17:SER:HA | 20:2Y:21:LYS:HB3 | 2.03 | 0.40 |
| 28:26:11:LEU:HB3 | 28:26:49:HIS:HB3 | 2.03 | 0.40 |
| 29:27:40:TRP:HE3 | 29:27:41:ARG:HH21 | 1.69 | 0.40 |
| 32:2a:46:G:O2' | 32:2a:365:U:H1' | 2.21 | 0.40 |
| 32:2a:142:G:H2' | 32:2a:143:A:C8 | 2.57 | 0.40 |
| 32:2a:445:G:H2' | 32:2a:446:G:H8 | 1.85 | 0.40 |
| 32:2a:583:A:H2' | 32:2a:584:G:O4' | 2.21 | 0.40 |
| 32:2a:811:C:H4' | 32:2a:900:A:N6 | 2.37 | 0.40 |
| 32:2a:1286:A:H2' | 32:2a:1287:A:H5' | 2.02 | 0.40 |
| 32:2a:1387:G:H2' | 32:2a:1388:C:H6 | 1.87 | 0.40 |
| 33:2b:185:ILE:HB | 33:2b:199:TYR:HB2 | 2.03 | 0.40 |
| 49:2r:70:ILE:O | 49:2r:74:ARG:HG3 | 2.20 | 0.40 |
| 51:2t:43:LEU:HD23 | 51:2t:43:LEU:HA | 1.97 | 0.40 |
| 1:1A:84:A:N1 | 1:1A:98:G:O2' | 2.51 | 0.40 |
| 1:1A:657:U:H2' | 1:1A:658:C:H6 | 1.86 | 0.40 |
| 1:1A:662:G:H5' | 11:1P:14:LYS:O | 2.21 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1A:876:C:H2' | 1:1A:877:U:O4' | 2.21 | 0.40 |
| 1:1A:1027:A:C6 | 1:1A:1126:A:C4 | 3.09 | 0.40 |
| 1:1A:1598:C:H2' | 1:1A:1599:C:C6 | 2.54 | 0.40 |
| 1:1A:2168:G:N1 | 1:1A:2171:A:C8 | 2.89 | 0.40 |
| 1:1A:2283:C:H2' | 1:1A:2284:C:O4' | 2.22 | 0.40 |
| 3:1D:145:VAL:HG11 | 3:1D:175:LEU:HD11 | 2.03 | 0.40 |
| 9:1N:67:LEU:O | 9:1N:88:GLU:HG3 | 2.21 | 0.40 |
| 10:1O:104:ARG:NH2 | 15:1T:43:GLN:OE1 | 2.50 | 0.40 |
| 12:1Q:65:PHE:HB2 | 12:1Q:105:GLU:HB2 | 2.03 | 0.40 |
| 13:1R:67:LEU:HG | 13:1R:76:VAL:HG11 | 2.03 | 0.40 |
| 14:1S:11:LYS:O | 14:1S:15:ARG:HG3 | 2.21 | 0.40 |
| 23:11:18:ILE:HG12 | 23:11:37:ILE:CG2 | 2.49 | 0.40 |
| 23:11:23:LYS:HB3 | 23:11:29:GLY:HA3 | 2.02 | 0.40 |
| 30:18:14:VAL:HG11 | 30:18:58:ILE:HG21 | 2.03 | 0.40 |
| 32:1a:142:G:H2' | 32:1a:143:A:H8 | 1.86 | 0.40 |
| 32:1a:604:G:C6 | 32:1a:605:U:C4 | 3.09 | 0.40 |
| 32:1a:626:U:C2 | 32:1a:627:G:C8 | 3.10 | 0.40 |
| 32:1a:964:A:O2' | 41:1j:55:LYS:HD2 | 2.21 | 0.40 |
| 32:1a:1220:G:O3' | 50:1s:36:ARG:HD3 | 2.21 | 0.40 |
| 33:1b:223:ILE:HD12 | 33:1b:229:VAL:HA | 2.03 | 0.40 |
| 35:1d:107:ARG:HA | 35:1d:107:ARG:HD2 | 1.87 | 0.40 |
| 35:1d:128:VAL:HG12 | 35:1d:129:ASN:HD22 | 1.86 | 0.40 |
| 35:1d:173:TRP:CE3 | 35:1d:174:LEU:HG | 2.55 | 0.40 |
| 38:1g:18:TYR:CD1 | 38:1g:59:LEU:HD13 | 2.56 | 0.40 |
| 40:1i:111:ARG:HH22 | 41:1j:62:HIS:HE2 | 1.70 | 0.40 |
| 47:1p:28:ARG:HE | 47:1p:29:ASP:CG | 2.30 | 0.40 |
| 48:1q:48:GLU:HB2 | 48:1q:50:LYS:HG3 | 2.03 | 0.40 |
| 1:2A:77:C:H5" | 24:22:10:LEU:HD21 | 2.04 | 0.40 |
| 1:2A:320:A:H4' | 1:2A:322:A:C8 | 2.56 | 0.40 |
| 1:2A:805:G:O4' | 11:2P:38:GLN:HG3 | 2.21 | 0.40 |
| 1:2A:840:C:H2' | 1:2A:841:A:C8 | 2.56 | 0.40 |
| 1:2A:858:U:O2 | 1:2A:2268:A:H2' | 2.22 | 0.40 |
| 1:2A:1001:A:C8 | 1:2A:1002:G:C8 | 3.09 | 0.40 |
| 1:2A:1131:G:H8 | 1:2A:2025:C:H4' | 1.86 | 0.40 |
| 1:2A:2018:G:H2' | 1:2A:2019:A:O4' | 2.21 | 0.40 |
| 1:2A:2163:C:H5' | 1:2A:2172:U:H5" | 2.03 | 0.40 |
| 1:2A:2271:G:OP1 | 22:20:18:ALA:HB1 | 2.22 | 0.40 |
| 5:2F:110:LEU:HA | 5:2F:183:VAL:HG12 | 2.03 | 0.40 |
| 5:2F:178:PRO:HB2 | 5:2F:201:VAL:CG2 | 2.51 | 0.40 |
| 6:2G:115:ARG:NH1 | 6:2G:115:ARG:HB2 | 2.36 | 0.40 |
| 7:2H:12:PRO:O | 7:2H:15:VAL:HG22 | 2.22 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 10:2O:73:ASP:OD2 | 15:2T:32:TYR:OH | 2.36 | 0.40 |
| 22:20:21:LEU:HD21 | 22:20:41:ARG:NH2 | 2.37 | 0.40 |
| 32:2a:6:G:H1 | 36:2e:98:THR:CG2 | 2.34 | 0.40 |
| 32:2a:66:G:H8 | 32:2a:66:G:OP1 | 2.04 | 0.40 |
| 32:2a:443:C:H2' | 32:2a:444:C:H6 | 1.86 | 0.40 |
| 32:2a:484:G:C8 | 32:2a:486:U:C2 | 3.09 | 0.40 |
| 32:2a:683:G:C6 | 32:2a:684:A:C5 | 3.09 | 0.40 |
| 32:2a:942:G:C2 | 32:2a:1342:C:C2 | 3.09 | 0.40 |
| 32:2a:1126:U:H3 | 41:2j:40:LEU:HD21 | 1.85 | 0.40 |
| 32:2a:1133:G:N2 | 32:2a:1142:G:C4 | 2.89 | 0.40 |
| 40:2i:77:ILE:O | 40:2i:81:ILE:HG12 | 2.22 | 0.40 |
| 44:2m:33:ALA:HB2 | 44:2m:64:TRP:CH2 | 2.49 | 0.40 |
| 1:1A:149:A:C6 | 1:1A:150:C:N3 | 2.90 | 0.40 |
| 1:1A:1249:U:O4 | 11:1P:18:ARG:HD2 | 2.22 | 0.40 |
| 1:1A:1529:G:H2' | 1:1A:1530:C:C6 | 2.56 | 0.40 |
| 1:1A:2552:2MU:C2 | 1:1A:2554:U:H5' | 2.52 | 0.40 |
| 1:1A:2783:G:C2 | 1:1A:2784:C:C2 | 3.09 | 0.40 |
| 1:1A:2791:C:H2' | 1:1A:2792:G:H8 | 1.87 | 0.40 |
| 1:1A:2810:A:H2' | 1:1A:2811:G:O4' | 2.21 | 0.40 |
| 3:1D:118:VAL:HG22 | 3:1D:119:ALA:H | 1.85 | 0.40 |
| 3:1D:159:ALA:HB1 | 3:1D:198:ASN:O | 2.21 | 0.40 |
| 5:1F:7:TYR:O | 5:1F:21:ALA:HA | 2.21 | 0.40 |
| 7:1H:7:LEU:HA | 7:1H:8:PRO:HD3 | 1.97 | 0.40 |
| 11:1P:124:LYS:HA | 11:1P:144:GLU:O | 2.22 | 0.40 |
| 12:1Q:39:PRO:HA | 12:1Q:97:VAL:O | 2.21 | 0.40 |
| 14:1S:89:ARG:O | 14:1S:90:GLY:C | 2.65 | 0.40 |
| 19:1X:94:GLY:N | 19:1X:95:LEU:HB2 | 2.37 | 0.40 |
| 32:1a:22:G:H4' | 32:1a:885:G:C8 | 2.57 | 0.40 |
| 32:1a:310:G:H5" | 47:1p:31:LYS:HB2 | 2.04 | 0.40 |
| 32:1a:676:A:H2' | 32:1a:677:U:C6 | 2.56 | 0.40 |
| 32:1a:1120:G:C6 | 32:1a:1121:U:C4 | 3.09 | 0.40 |
| 36:1e:72:GLN:O | 36:1e:75:THR:HG22 | 2.22 | 0.40 |
| 38:1g:45:ASP:O | 38:1g:49:ILE:HG13 | 2.22 | 0.40 |
| 51:1t:41:ILE:HG23 | 51:1t:91:LEU:HD21 | 2.03 | 0.40 |
| 1:2A:24:G:H2' | 1:2A:25:U:O4' | 2.22 | 0.40 |
| 1:2A:25:U:C4 | 1:2A:26:G:C6 | 3.10 | 0.40 |
| 1:2A:676:A:H1' | 1:2A:2443:C:H1' | 2.03 | 0.40 |
| 1:2A:797:C:C2 | 1:2A:798:G:C8 | 3.09 | 0.40 |
| 1:2A:1812:A:H2' | 1:2A:1813:G:C8 | 2.56 | 0.40 |
| 1:2A:1864:U:OP1 | 1:2A:2410:G:O2' | 2.36 | 0.40 |
| 1:2A:1910:G:H22 | 1:2A:1920:4OC:C2 | 2.33 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:2A:2110:G:OP1 | 1:2A:2118:U:N3 | 2.54 | 0.40 |
| 1:2A:2286:A:H4' | 1:2A:2287:A:O4' | 2.21 | 0.40 |
| 1:2A:2292:C:H4' | 1:2A:2375:G:H4' | 2.03 | 0.40 |
| 1:2A:2362:G:OP1 | 30:28:44:LYS:NZ | 2.47 | 0.40 |
| 1:2A:2386:C:H2' | 1:2A:2387:U:C6 | 2.56 | 0.40 |
| 1:2A:2525:G:C2 | 1:2A:2539:C:C2 | 3.09 | 0.40 |
| 1:2A:2562:U:H4' | 10:2O:25:LEU:HD21 | 2.03 | 0.40 |
| 5:2F:111:ALA:HB2 | 5:2F:206:ILE:HG21 | 2.04 | 0.40 |
| 6:2G:64:THR:HG21 | 6:2G:92:VAL:HG11 | 2.04 | 0.40 |
| 10:2O:70:LYS:HB3 | 10:2O:70:LYS:HE2 | 1.59 | 0.40 |
| 17:2V:55:ALA:HA | 17:2V:100:ARG:HB2 | 2.04 | 0.40 |
| 22:20:46:LYS:N | 22:20:77:ARG:O | 2.48 | 0.40 |
| 24:22:35:LEU:HD21 | 24:22:49:LYS:HB2 | 2.04 | 0.40 |
| 32:2a:296:U:O2' | 32:2a:556:C:O2 | 2.34 | 0.40 |
| 32:2a:401:C:H2' | 32:2a:402:G:C8 | 2.55 | 0.40 |
| 32:2a:414:A:H2' | 32:2a:415:A:C8 | 2.57 | 0.40 |
| 32:2a:437:U:O2' | 35:2d:125:HIS:HE1 | 2.05 | 0.40 |
| 32:2a:543:C:O2' | 32:2a:544:G:H5' | 2.22 | 0.40 |
| 32:2a:559:A:H5" | 32:2a:560:U:H3' | 2.02 | 0.40 |
| 32:2a:957:U:O2 | 32:2a:959:A:H8 | 2.04 | 0.40 |
| 32:2a:1388:C:H2' | 32:2a:1389:C:O4' | 2.22 | 0.40 |
| 35:2d:108:LEU:HA | 35:2d:108:LEU:HD12 | 1.91 | 0.40 |
| 44:2m:68:GLY:O | 44:2m:72:ALA:N | 2.37 | 0.40 |
| 51:2t:89:ARG:NH2 | 51:2t:103:GLY:HA3 | 2.37 | 0.40 |
| 1:1A:41:C:H2' | 1:1A:42:G:O4' | 2.22 | 0.40 |
| 1:1A:630:G:OP1 | 30:18:47:LYS:NZ | 2.46 | 0.40 |
| 1:1A:963:U:H1' | 1:1A:2250:G:O6 | 2.21 | 0.40 |
| 1:1A:1784:A:H4' | 1:1A:1785:A:O5' | 2.22 | 0.40 |
| 1:1A:1818:U:O4 | 3:1D:154:LYS:HD2 | 2.22 | 0.40 |
| 1:1A:1972:A:H2' | 1:1A:1973:G:C8 | 2.57 | 0.40 |
| 1:1A:2365:G:H5" | 59:1A:4250:HOH:O | 2.21 | 0.40 |
| 2:1B:79:C:H2' | 2:1B:80:U:O4' | 2.22 | 0.40 |
| 4:1E:34:VAL:HB | 4:1E:48:GLN:HE21 | 1.86 | 0.40 |
| 5:1F:74:ARG:H | 5:1F:74:ARG:HG3 | 1.47 | 0.40 |
| 5:1F:161:GLU:HG2 | 5:1F:164:ARG:NH2 | 2.37 | 0.40 |
| 6:1G:73:ALA:HB3 | 6:1G:85:GLY:H | 1.85 | 0.40 |
| 10:1O:7:TYR:CZ | 10:1O:44:LYS:HG3 | 2.56 | 0.40 |
| 11:1P:38:GLN:O | 11:1P:40:SER:N | 2.47 | 0.40 |
| 12:1Q:54:MET:HG2 | 12:1Q:117:ALA:HB1 | 2.04 | 0.40 |
| 13:1R:63:ARG:HA | 13:1R:80:PHE:CZ | 2.57 | 0.40 |
| 25:13:8:LEU:HG | 25:13:31:LEU:CD2 | 2.51 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 26:14:54:GLY:N | 26:14:55:ARG:HA | 2.36 | 0.40 |
| 30:18:42:ARG:HD2 | 59:18:201:HOH:O | 2.21 | 0.40 |
| 32:1a:107:G:C2 | 32:1a:108:G:H1' | 2.57 | 0.40 |
| 32:1a:658:G:H2' | 32:1a:659:U:H6 | 1.87 | 0.40 |
| 32:1a:925:G:H1 | 32:1a:1391:U:H3 | 1.69 | 0.40 |
| 32:1a:1104:G:H4' | 33:1b:111:ARG:CZ | 2.51 | 0.40 |
| 32:1a:1183:A:O2' | 32:1a:1184:G:H5" | 2.22 | 0.40 |
| 32:1a:1391:U:H2' | 32:1a:1392:G:H8 | 1.83 | 0.40 |
| 33:1b:21:ARG:CB | 33:1b:39:ILE:HA | 2.50 | 0.40 |
| 38:1g:57:GLU:HA | 38:1g:58:PRO:HD3 | 1.99 | 0.40 |
| 38:1g:69:VAL:HG12 | 38:1g:69:VAL:O | 2.21 | 0.40 |
| 38:1g:113:GLU:H | 38:1g:113:GLU:HG2 | 1.58 | 0.40 |
| 44:1m:50:GLU:O | 44:1m:54:VAL:HG22 | 2.22 | 0.40 |
| 1:2A:252:G:OP1 | 11:2P:50:ARG:NH1 | 2.51 | 0.40 |
| 1:2A:634:C:H2' | 1:2A:635:C:C6 | 2.56 | 0.40 |
| 1:2A:747:U:O2 | 1:2A:2014:A:H1' | 2.22 | 0.40 |
| 1:2A:1422:G:H1' | 1:2A:1496:A:N1 | 2.37 | 0.40 |
| 1:2A:1422:G:C6 | 1:2A:1423:G:C5 | 3.10 | 0.40 |
| 1:2A:1557:C:H2' | 1:2A:1558:A:C2 | 2.57 | 0.40 |
| 1:2A:1789:A:H2' | 1:2A:1790:C:O4' | 2.22 | 0.40 |
| 1:2A:1801:G:OP2 | 3:2D:154:LYS:NZ | 2.47 | 0.40 |
| 1:2A:1814:G:H5" | 3:2D:54:ARG:NH2 | 2.35 | 0.40 |
| 1:2A:2611:U:H3' | 1:2A:2611:U:OP2 | 2.21 | 0.40 |
| 3:2D:147:LEU:HD13 | 3:2D:155:LEU:HD21 | 2.04 | 0.40 |
| 6:2G:150:ASP:OD1 | 6:2G:150:ASP:N | 2.54 | 0.40 |
| 7:2H:117:PRO:HA | 7:2H:118:PRO:HD3 | 1.89 | 0.40 |
| 21:2Z:14:LYS:HE2 | 21:2Z:14:LYS:HB3 | 1.85 | 0.40 |
| 32:2a:6:G:C4 | 36:2e:119:LEU:HD11 | 2.56 | 0.40 |
| 32:2a:194:C:H2' | 32:2a:195:A:H5" | 2.03 | 0.40 |
| 32:2a:404:U:H2' | 32:2a:405:U:H6 | 1.85 | 0.40 |
| 32:2a:512:U:H2' | 32:2a:513:C:H6 | 1.86 | 0.40 |
| 32:2a:565:U:OP2 | 32:2a:566:G:O2' | 2.36 | 0.40 |
| 32:2a:671:G:H1 | 32:2a:735:C:H42 | 1.69 | 0.40 |
| 32:2a:1325:C:H5" | 52:2u:17:THR:HG21 | 2.04 | 0.40 |
| 32:2a:1342:C:O2' | 40:2i:124:GLN:HA | 2.21 | 0.40 |
| 32:2a:1417:G:C6 | 32:2a:1482:G:C6 | 3.09 | 0.40 |
| 47:2p:52:ASP:CG | 47:2p:55:ARG:HG2 | 2.47 | 0.40 |

All (12) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 32:1a:55:A:C5 | 8:2I:89:TYR:CZ[2_655] | 1.80 | 0.40 |
| 32:1a:55:A:C4 | 8:2I:89:TYR:CZ[2_655] | 1.82 | 0.38 |
| 32:1a:55:A:C4 | 8:2I:89:TYR:CE2[2_655] | 1.95 | 0.25 |
| 32:1a:55:A:C5 | 8:2I:89:TYR:CE2[2_655] | 1.98 | 0.22 |
| 32:1a:55:A:C8 | 8:2I:89:TYR:CE1[2_655] | 2.01 | 0.19 |
| 32:1a:55:A:N7 | 8:2I:89:TYR:CE1[2_655] | 2.02 | 0.18 |
| 32:1a:55:A:N7 | 8:2I:89:TYR:CZ[2_655] | 2.05 | 0.15 |
| 32:1a:55:A:C5 | 8:2I:89:TYR:CE1[2_655] | 2.05 | 0.15 |
| 32:1a:55:A:N9 | 8:2I:89:TYR:CZ[2_655] | 2.07 | 0.13 |
| 32:1a:55:A:N9 | 8:2I:89:TYR:CE1[2_655] | 2.08 | 0.12 |
| 32:1a:55:A:C4 | 8:2I:89:TYR:CE1[2_655] | 2.09 | 0.11 |
| 32:1a:55:A:N1 | 8:2I:89:TYR:CD2[2_655] | 2.17 | 0.03 |

## 5.3 Torsion angles (i)

### 5.3.1 Protein backbone (i)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| 3 | 1D | 273/276 (99%) | 255 (93%) | 18 (7%) | 0 | 100 100 |
| 3 | 2D | 273/276 (99%) | 251 (92%) | 21 (8%) | 1 (0%) | 30 60 |
| 4 | 1E | 202/206 (98%) | 188 (93%) | 12 (6%) | 2 (1%) | 12 38 |
| 4 | 2E | 202/206 (98%) | 187 (93%) | 13 (6%) | 2 (1%) | 12 38 |
| 5 | 1F | 201/210 (96%) | 194 (96%) | 4 (2%) | 3 (2%) | 8 28 |
| 5 | 2F | 201/210 (96%) | 188 (94%) | 12 (6%) | 1 (0%) | 24 55 |
| 6 | 1G | 179/182 (98%) | 162 (90%) | 13 (7%) | 4 (2%) | 5 19 |
| 6 | 2G | 179/182 (98%) | 148 (83%) | 24 (13%) | 7 (4%) | 2 8 |
| 7 | 1H | 172/180 (96%) | 158 (92%) | 14 (8%) | 0 | 100 100 |
| 7 | 2H | 172/180 (96%) | 151 (88%) | 17 (10%) | 4 (2%) | 5 18 |
| 8 | 1I | 144/148 (97%) | 126 (88%) | 16 (11%) | 2 (1%) | 9 30 |
| 8 | 2I | 144/148 (97%) | 112 (78%) | 26 (18%) | 6 (4%) | 2 7 |
| 9 | 1N | 138/140 (99%) | 135 (98%) | 2 (1%) | 1 (1%) | 18 47 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| 9 | 2N | 138/140 (99%) | 131 (95%) | 6 (4%) | 1 (1%) | 18 47 |
| 10 | 1O | 120/122 (98%) | 108 (90%) | 11 (9%) | 1 (1%) | 16 44 |
| 10 | 2O | 120/122 (98%) | 107 (89%) | 12 (10%) | 1 (1%) | 16 44 |
| 11 | 1P | 147/150 (98%) | 134 (91%) | 10 (7%) | 3 (2%) | 6 21 |
| 11 | 2P | 147/150 (98%) | 133 (90%) | 12 (8%) | 2 (1%) | 9 30 |
| 12 | 1Q | 139/141 (99%) | 128 (92%) | 10 (7%) | 1 (1%) | 18 47 |
| 12 | 2Q | 139/141 (99%) | 124 (89%) | 15 (11%) | 0 | 100 100 |
| 13 | 1R | 116/118 (98%) | 108 (93%) | 8 (7%) | 0 | 100 100 |
| 13 | 2R | 116/118 (98%) | 108 (93%) | 7 (6%) | 1 (1%) | 14 41 |
| 14 | 1S | 108/112 (96%) | 96 (89%) | 11 (10%) | 1 (1%) | 14 41 |
| 14 | 2S | 108/112 (96%) | 101 (94%) | 4 (4%) | 3 (3%) | 4 14 |
| 15 | 1T | 129/146 (88%) | 121 (94%) | 7 (5%) | 1 (1%) | 16 44 |
| 15 | 2T | 129/146 (88%) | 121 (94%) | 8 (6%) | 0 | 100 100 |
| 16 | 1U | 114/118 (97%) | 112 (98%) | 2 (2%) | 0 | 100 100 |
| 16 | 2U | 114/118 (97%) | 112 (98%) | 2 (2%) | 0 | 100 100 |
| 17 | 1V | 99/101 (98%) | 90 (91%) | 8 (8%) | 1 (1%) | 12 38 |
| 17 | 2V | 99/101 (98%) | 93 (94%) | 6 (6%) | 0 | 100 100 |
| 18 | 1W | 110/113 (97%) | 106 (96%) | 3 (3%) | 1 (1%) | 14 41 |
| 18 | 2W | 110/113 (97%) | 108 (98%) | 2 (2%) | 0 | 100 100 |
| 19 | 1X | 93/96 (97%) | 85 (91%) | 6 (6%) | 2 (2%) | 5 19 |
| 19 | 2X | 93/96 (97%) | 87 (94%) | 5 (5%) | 1 (1%) | 11 36 |
| 20 | 1Y | 105/110 (96%) | 101 (96%) | 4 (4%) | 0 | 100 100 |
| 20 | 2Y | 105/110 (96%) | 93 (89%) | 11 (10%) | 1 (1%) | 12 38 |
| 21 | 1Z | 148/206 (72%) | 130 (88%) | 16 (11%) | 2 (1%) | 9 30 |
| 21 | 2Z | 156/206 (76%) | 128 (82%) | 24 (15%) | 4 (3%) | 4 15 |
| 22 | 10 | 81/85 (95%) | 76 (94%) | 4 (5%) | 1 (1%) | 10 34 |
| 22 | 20 | 81/85 (95%) | 76 (94%) | 4 (5%) | 1 (1%) | 10 34 |
| 23 | 11 | 95/98 (97%) | 91 (96%) | 2 (2%) | 2 (2%) | 5 20 |
| 23 | 21 | 95/98 (97%) | 91 (96%) | 4 (4%) | 0 | 100 100 |
| 24 | 12 | 68/72 (94%) | 67 (98%) | 1 (2%) | 0 | 100 100 |
| 24 | 22 | 68/72 (94%) | 60 (88%) | 8 (12%) | 0 | 100 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| 25 | 13 | 57/60 (95%) | 54 (95%) | 3 (5%) | 0 | 100 100 |
| 25 | 23 | 57/60 (95%) | 52 (91%) | 4 (7%) | 1 (2%) | 6 23 |
| 26 | 14 | 67/71 (94%) | 56 (84%) | 7 (10%) | 4 (6%) | 1 3 |
| 26 | 24 | 67/71 (94%) | 53 (79%) | 13 (19%) | 1 (2%) | 8 28 |
| 27 | 15 | 57/60 (95%) | 55 (96%) | 2 (4%) | 0 | 100 100 |
| 27 | 25 | 57/60 (95%) | 55 (96%) | 2 (4%) | 0 | 100 100 |
| 28 | 16 | 51/54 (94%) | 49 (96%) | 2 (4%) | 0 | 100 100 |
| 28 | 26 | 51/54 (94%) | 47 (92%) | 4 (8%) | 0 | 100 100 |
| 29 | 17 | 46/49 (94%) | 46 (100%) | 0 | 0 | 100 100 |
| 29 | 27 | 46/49 (94%) | 46 (100%) | 0 | 0 | 100 100 |
| 30 | 18 | 62/65 (95%) | 59 (95%) | 3 (5%) | 0 | 100 100 |
| 30 | 28 | 62/65 (95%) | 58 (94%) | 4 (6%) | 0 | 100 100 |
| 31 | 19 | 35/37 (95%) | 35 (100%) | 0 | 0 | 100 100 |
| 31 | 29 | 35/37 (95%) | 30 (86%) | 4 (11%) | 1 (3%) | 3 13 |
| 33 | 1b | 229/256 (90%) | 193 (84%) | 29 (13%) | 7 (3%) | 3 12 |
| 33 | 2b | 229/256 (90%) | 199 (87%) | 21 (9%) | 9 (4%) | 2 8 |
| 34 | 1c | 204/239 (85%) | 179 (88%) | 24 (12%) | 1 (0%) | 24 55 |
| 34 | 2c | 204/239 (85%) | 179 (88%) | 22 (11%) | 3 (2%) | 8 28 |
| 35 | 1d | 206/209 (99%) | 184 (89%) | 21 (10%) | 1 (0%) | 24 55 |
| 35 | 2d | 206/209 (99%) | 191 (93%) | 15 (7%) | 0 | 100 100 |
| 36 | 1e | 146/162 (90%) | 128 (88%) | 16 (11%) | 2 (1%) | 9 30 |
| 36 | 2e | 146/162 (90%) | 126 (86%) | 18 (12%) | 2 (1%) | 9 30 |
| 37 | 1f | 98/101 (97%) | 89 (91%) | 9 (9%) | 0 | 100 100 |
| 37 | 2f | 98/101 (97%) | 91 (93%) | 7 (7%) | 0 | 100 100 |
| 38 | 1g | 153/156 (98%) | 134 (88%) | 17 (11%) | 2 (1%) | 9 31 |
| 38 | 2g | 153/156 (98%) | 132 (86%) | 18 (12%) | 3 (2%) | 6 21 |
| 39 | 1h | 135/138 (98%) | 125 (93%) | 10 (7%) | 0 | 100 100 |
| 39 | 2h | 135/138 (98%) | 124 (92%) | 11 (8%) | 0 | 100 100 |
| 40 | 1i | 125/128 (98%) | 106 (85%) | 17 (14%) | 2 (2%) | 7 27 |
| 40 | 2i | 125/128 (98%) | 106 (85%) | 18 (14%) | 1 (1%) | 16 44 |
| 41 | 1j | 95/105 (90%) | 77 (81%) | 13 (14%) | 5 (5%) | 1 5 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| 41 | 2j | 94/105 (90%) | 82 (87%) | 8 (8%) | 4 (4%) | 2 7 |
| 42 | 1k | 112/129 (87%) | 101 (90%) | 7 (6%) | 4 (4%) | 2 10 |
| 42 | 2k | 112/129 (87%) | 99 (88%) | 11 (10%) | 2 (2%) | 6 23 |
| 43 | 1l | 119/132 (90%) | 107 (90%) | 12 (10%) | 0 | 100 100 |
| 43 | 2l | 119/132 (90%) | 105 (88%) | 14 (12%) | 0 | 100 100 |
| 44 | 1m | 120/126 (95%) | 107 (89%) | 11 (9%) | 2 (2%) | 7 25 |
| 44 | 2m | 119/126 (94%) | 105 (88%) | 11 (9%) | 3 (2%) | 4 16 |
| 45 | 1n | 58/61 (95%) | 52 (90%) | 6 (10%) | 0 | 100 100 |
| 45 | 2n | 58/61 (95%) | 54 (93%) | 3 (5%) | 1 (2%) | 7 25 |
| 46 | 1o | 86/89 (97%) | 81 (94%) | 5 (6%) | 0 | 100 100 |
| 46 | 2o | 86/89 (97%) | 78 (91%) | 8 (9%) | 0 | 100 100 |
| 47 | 1p | 80/88 (91%) | 68 (85%) | 9 (11%) | 3 (4%) | 2 9 |
| 47 | 2p | 80/88 (91%) | 71 (89%) | 9 (11%) | 0 | 100 100 |
| 48 | 1q | 97/105 (92%) | 87 (90%) | 10 (10%) | 0 | 100 100 |
| 48 | 2q | 97/105 (92%) | 86 (89%) | 10 (10%) | 1 (1%) | 12 38 |
| 49 | 1r | 66/88 (75%) | 58 (88%) | 7 (11%) | 1 (2%) | 8 28 |
| 49 | 2r | 66/88 (75%) | 65 (98%) | 1 (2%) | 0 | 100 100 |
| 50 | 1s | 81/93 (87%) | 67 (83%) | 13 (16%) | 1 (1%) | 10 34 |
| 50 | 2s | 81/93 (87%) | 71 (88%) | 8 (10%) | 2 (2%) | 4 16 |
| 51 | 1t | 94/106 (89%) | 82 (87%) | 7 (7%) | 5 (5%) | 1 5 |
| 51 | 2t | 94/106 (89%) | 82 (87%) | 7 (7%) | 5 (5%) | 1 5 |
| 52 | 1u | 21/27 (78%) | 18 (86%) | 2 (10%) | 1 (5%) | 2 6 |
| 52 | 2u | 21/27 (78%) | 17 (81%) | 4 (19%) | 0 | 100 100 |
| All | All | 11368/12128 (94%) | 10282 (90%) | 942 (8%) | 144 (1%) | 9 31 |

All (144) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 4 | 1E | 71 | GLY |
| 5 | 1F | 130 | ALA |
| 11 | 1P | 36 | LYS |
| 11 | 1P | 38 | GLN |
| 12 | 1Q | 27 | VAL |
| 14 | 1S | 94 | TYR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 26 | 14 | 62 | ARG |
| 33 | 1b | 17 | PHE |
| 33 | 1b | 125 | PRO |
| 38 | 1g | 80 | VAL |
| 40 | 1i | 54 | ASP |
| 44 | 1m | 67 | GLU |
| 44 | 1m | 106 | ASN |
| 5 | 2F | 130 | ALA |
| 7 | 2H | 126 | PRO |
| 8 | 2I | 127 | VAL |
| 10 | 2O | 5 | GLN |
| 11 | 2P | 45 | LEU |
| 33 | 2b | 16 | HIS |
| 33 | 2b | 123 | ALA |
| 40 | 2i | 54 | ASP |
| 42 | 2k | 105 | VAL |
| 50 | 2s | 12 | ASP |
| 51 | 2t | 10 | LEU |
| 5 | 1F | 168 | ARG |
| 6 | 1G | 43 | LEU |
| 18 | 1W | 40 | ASN |
| 21 | 1Z | 52 | SER |
| 23 | 11 | 3 | LYS |
| 26 | 14 | 45 | GLY |
| 26 | 14 | 49 | PHE |
| 34 | 1c | 129 | ALA |
| 36 | 1e | 85 | GLY |
| 41 | 1j | 56 | HIS |
| 41 | 1j | 79 | ARG |
| 42 | 1k | 49 | GLY |
| 42 | 1k | 107 | SER |
| 4 | 2E | 71 | GLY |
| 6 | 2G | 45 | GLU |
| 6 | 2G | 51 | ARG |
| 8 | 2I | 108 | THR |
| 8 | 2I | 115 | ALA |
| 11 | 2P | 38 | GLN |
| 14 | 2S | 96 | GLY |
| 19 | 2X | 94 | GLY |
| 21 | 2Z | 65 | GLN |
| 21 | 2Z | 66 | SER |
| 26 | 24 | 45 | GLY |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 33 | 2b | 126 | GLU |
| 36 | 2e | 21 | ALA |
| 36 | 2e | 85 | GLY |
| 42 | 2k | 49 | GLY |
| 44 | 2m | 67 | GLU |
| 48 | 2q | 68 | ARG |
| 4 | 1E | 52 | LEU |
| 6 | 1G | 44 | GLY |
| 17 | 1V | 43 | GLU |
| 19 | 1X | 94 | GLY |
| 26 | 14 | 53 | GLU |
| 33 | 1b | 124 | SER |
| 38 | 1g | 4 | ARG |
| 42 | 1k | 91 | ARG |
| 47 | 1p | 28 | ARG |
| 47 | 1p | 81 | ARG |
| 50 | 1s | 12 | ASP |
| 51 | 1t | 102 | GLY |
| 52 | 1u | 5 | ASP |
| 6 | 2G | 117 | PHE |
| 8 | 2I | 135 | GLU |
| 9 | 2N | 2 | LYS |
| 14 | 2S | 94 | TYR |
| 21 | 2Z | 52 | SER |
| 31 | 29 | 21 | GLY |
| 33 | 2b | 78 | GLN |
| 33 | 2b | 105 | PHE |
| 51 | 2t | 9 | ASN |
| 51 | 2t | 95 | ALA |
| 6 | 1G | 47 | LYS |
| 23 | 11 | 84 | GLY |
| 33 | 1b | 231 | GLU |
| 40 | 1i | 42 | ARG |
| 42 | 1k | 106 | LYS |
| 49 | 1r | 33 | ASP |
| 51 | 1t | 47 | GLY |
| 51 | 1t | 95 | ALA |
| 51 | 1t | 100 | ILE |
| 4 | 2E | 52 | LEU |
| 7 | 2H | 47 | GLU |
| 7 | 2H | 55 | PRO |
| 7 | 2H | 92 | ILE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 8 | 2I | 94 | ALA |
| 14 | 2S | 84 | GLN |
| 34 | 2c | 129 | ALA |
| 34 | 2c | 181 | ASN |
| 38 | 2g | 7 | ALA |
| 38 | 2g | 80 | VAL |
| 41 | 2j | 29 | ARG |
| 41 | 2j | 78 | ASN |
| 45 | 2n | 14 | PRO |
| 5 | 1F | 122 | LYS |
| 6 | 1G | 49 | ASP |
| 8 | 1I | 33 | ARG |
| 8 | 1I | 42 | SER |
| 9 | 1N | 2 | LYS |
| 10 | 1O | 5 | GLN |
| 21 | 1Z | 137 | ILE |
| 22 | 10 | 4 | LYS |
| 33 | 1b | 22 | LYS |
| 47 | 1p | 63 | GLY |
| 51 | 1t | 96 | GLY |
| 8 | 2I | 10 | GLU |
| 33 | 2b | 17 | PHE |
| 33 | 2b | 20 | GLU |
| 33 | 2b | 209 | ARG |
| 38 | 2g | 4 | ARG |
| 11 | 1P | 93 | GLY |
| 19 | 1X | 2 | LYS |
| 33 | 1b | 207 | ALA |
| 41 | 1j | 75 | ILE |
| 41 | 1j | 78 | ASN |
| 6 | 2G | 3 | LEU |
| 6 | 2G | 44 | GLY |
| 20 | 2Y | 21 | LYS |
| 21 | 2Z | 93 | ASP |
| 22 | 20 | 4 | LYS |
| 33 | 2b | 231 | GLU |
| 41 | 2j | 39 | PRO |
| 44 | 2m | 5 | ALA |
| 44 | 2m | 90 | LEU |
| 50 | 2s | 33 | THR |
| 51 | 2t | 47 | GLY |
| 15 | 1T | 37 | GLY |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 33 | 1b | 229 | VAL |
| 41 | 1j | 77 | PRO |
| 51 | 2t | 102 | GLY |
| 36 | 1e | 22 | GLY |
| 3 | 2D | 125 | ILE |
| 34 | 2c | 138 | VAL |
| 25 | 23 | 59 | VAL |
| 41 | 2j | 75 | ILE |
| 35 | 1d | 37 | PRO |
| 6 | 2G | 109 | VAL |
| 6 | 2G | 177 | GLY |
| 13 | 2R | 117 | VAL |

### 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%) | 200 (93%) | 15 (7%) | 14 40 |
| 3 | 2D | 215/218 (99%) | 206 (96%) | 9 (4%) | 26 61 |
| 4 | 1E | 164/166 (99%) | 152 (93%) | 12 (7%) | 13 38 |
| 4 | 2E | 164/166 (99%) | 148 (90%) | 16 (10%) | 7 25 |
| 5 | 1F | 160/166 (96%) | 142 (89%) | 18 (11%) | 5 19 |
| 5 | 2F | 159/166 (96%) | 137 (86%) | 22 (14%) | 3 12 |
| 6 | 1G | 143/156 (92%) | 126 (88%) | 17 (12%) | 5 17 |
| 6 | 2G | 143/156 (92%) | 120 (84%) | 23 (16%) | 2 8 |
| 7 | 1H | 144/148 (97%) | 131 (91%) | 13 (9%) | 9 28 |
| 7 | 2H | 144/148 (97%) | 128 (89%) | 16 (11%) | 6 20 |
| 8 | 1I | 113/124 (91%) | 98 (87%) | 15 (13%) | 4 14 |
| 8 | 2I | 105/124 (85%) | 73 (70%) | 32 (30%) | 0 1 |
| 9 | 1N | 118/119 (99%) | 103 (87%) | 15 (13%) | 4 15 |
| 9 | 2N | 118/119 (99%) | 103 (87%) | 15 (13%) | 4 15 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 10 | 1O | 100/100 (100%) | 95 (95%) | 5 (5%) | 22 54 |
| 10 | 2O | 100/100 (100%) | 94 (94%) | 6 (6%) | 17 47 |
| 11 | 1P | 115/116 (99%) | 99 (86%) | 16 (14%) | 3 12 |
| 11 | 2P | 115/116 (99%) | 103 (90%) | 12 (10%) | 7 22 |
| 12 | 1Q | 111/111 (100%) | 101 (91%) | 10 (9%) | 9 28 |
| 12 | 2Q | 111/111 (100%) | 99 (89%) | 12 (11%) | 6 21 |
| 13 | 1R | 101/101 (100%) | 90 (89%) | 11 (11%) | 6 21 |
| 13 | 2R | 101/101 (100%) | 93 (92%) | 8 (8%) | 11 35 |
| 14 | 1S | 86/88 (98%) | 82 (95%) | 4 (5%) | 23 57 |
| 14 | 2S | 85/88 (97%) | 72 (85%) | 13 (15%) | 3 10 |
| 15 | 1T | 115/127 (91%) | 108 (94%) | 7 (6%) | 17 46 |
| 15 | 2T | 113/127 (89%) | 104 (92%) | 9 (8%) | 11 34 |
| 16 | 1U | 93/94 (99%) | 88 (95%) | 5 (5%) | 20 51 |
| 16 | 2U | 93/94 (99%) | 86 (92%) | 7 (8%) | 12 37 |
| 17 | 1V | 80/82 (98%) | 75 (94%) | 5 (6%) | 16 45 |
| 17 | 2V | 80/82 (98%) | 72 (90%) | 8 (10%) | 7 24 |
| 18 | 1W | 90/92 (98%) | 83 (92%) | 7 (8%) | 11 35 |
| 18 | 2W | 90/92 (98%) | 82 (91%) | 8 (9%) | 9 29 |
| 19 | 1X | 77/78 (99%) | 74 (96%) | 3 (4%) | 28 64 |
| 19 | 2X | 77/78 (99%) | 69 (90%) | 8 (10%) | 7 22 |
| 20 | 1Y | 85/91 (93%) | 75 (88%) | 10 (12%) | 5 17 |
| 20 | 2Y | 85/91 (93%) | 75 (88%) | 10 (12%) | 5 17 |
| 21 | 1Z | 135/179 (75%) | 119 (88%) | 16 (12%) | 5 17 |
| 21 | 2Z | 137/179 (76%) | 119 (87%) | 18 (13%) | 4 14 |
| 22 | 10 | 65/67 (97%) | 61 (94%) | 4 (6%) | 16 45 |
| 22 | 20 | 65/67 (97%) | 61 (94%) | 4 (6%) | 16 45 |
| 23 | 11 | 80/83 (96%) | 76 (95%) | 4 (5%) | 22 54 |
| 23 | 21 | 80/83 (96%) | 73 (91%) | 7 (9%) | 9 29 |
| 24 | 12 | 65/67 (97%) | 57 (88%) | 8 (12%) | 4 16 |
| 24 | 22 | 65/67 (97%) | 58 (89%) | 7 (11%) | 6 21 |
| 25 | 13 | 51/52 (98%) | 43 (84%) | 8 (16%) | 2 9 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 25 | 23 | 50/52 (96%) | 46 (92%) | 4 (8%) | 11 34 |
| 26 | 14 | 59/63 (94%) | 46 (78%) | 13 (22%) | 1 3 |
| 26 | 24 | 53/63 (84%) | 45 (85%) | 8 (15%) | 3 10 |
| 27 | 15 | 50/52 (96%) | 44 (88%) | 6 (12%) | 5 17 |
| 27 | 25 | 50/52 (96%) | 46 (92%) | 4 (8%) | 11 34 |
| 28 | 16 | 51/52 (98%) | 44 (86%) | 7 (14%) | 3 13 |
| 28 | 26 | 50/52 (96%) | 46 (92%) | 4 (8%) | 11 34 |
| 29 | 17 | 41/42 (98%) | 38 (93%) | 3 (7%) | 13 38 |
| 29 | 27 | 41/42 (98%) | 38 (93%) | 3 (7%) | 13 38 |
| 30 | 18 | 54/55 (98%) | 52 (96%) | 2 (4%) | 30 65 |
| 30 | 28 | 54/55 (98%) | 50 (93%) | 4 (7%) | 13 37 |
| 31 | 19 | 34/34 (100%) | 33 (97%) | 1 (3%) | 37 73 |
| 31 | 29 | 34/34 (100%) | 32 (94%) | 2 (6%) | 18 48 |
| 33 | 1b | 192/220 (87%) | 170 (88%) | 22 (12%) | 5 18 |
| 33 | 2b | 187/220 (85%) | 151 (81%) | 36 (19%) | 1 5 |
| 34 | 1c | 142/188 (76%) | 127 (89%) | 15 (11%) | 6 22 |
| 34 | 2c | 140/188 (74%) | 115 (82%) | 25 (18%) | 2 6 |
| 35 | 1d | 169/181 (93%) | 153 (90%) | 16 (10%) | 8 26 |
| 35 | 2d | 173/181 (96%) | 153 (88%) | 20 (12%) | 5 18 |
| 36 | 1e | 113/123 (92%) | 106 (94%) | 7 (6%) | 16 45 |
| 36 | 2e | 114/123 (93%) | 102 (90%) | 12 (10%) | 6 22 |
| 37 | 1f | 84/90 (93%) | 79 (94%) | 5 (6%) | 17 47 |
| 37 | 2f | 85/90 (94%) | 77 (91%) | 8 (9%) | 8 27 |
| 38 | 1g | 119/127 (94%) | 115 (97%) | 4 (3%) | 32 68 |
| 38 | 2g | 120/127 (94%) | 105 (88%) | 15 (12%) | 4 15 |
| 39 | 1h | 114/119 (96%) | 99 (87%) | 15 (13%) | 4 14 |
| 39 | 2h | 114/119 (96%) | 100 (88%) | 14 (12%) | 4 16 |
| 40 | 1i | 90/99 (91%) | 81 (90%) | 9 (10%) | 7 24 |
| 40 | 2i | 89/99 (90%) | 79 (89%) | 10 (11%) | 6 19 |
| 41 | 1j | 66/92 (72%) | 56 (85%) | 10 (15%) | 3 10 |
| 41 | 2j | 69/92 (75%) | 63 (91%) | 6 (9%) | 9 30 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 42 | 1k | 82/99 (83%) | 73 (89%) | 9 (11%) | 6 20 |
| 42 | 2k | 83/99 (84%) | 76 (92%) | 7 (8%) | 10 32 |
| 43 | 1l | 96/108 (89%) | 86 (90%) | 10 (10%) | 7 22 |
| 43 | 2l | 96/108 (89%) | 87 (91%) | 9 (9%) | 8 27 |
| 44 | 1m | 92/101 (91%) | 78 (85%) | 14 (15%) | 3 10 |
| 44 | 2m | 91/101 (90%) | 76 (84%) | 15 (16%) | 2 8 |
| 45 | 1n | 49/50 (98%) | 42 (86%) | 7 (14%) | 3 11 |
| 45 | 2n | 49/50 (98%) | 43 (88%) | 6 (12%) | 5 16 |
| 46 | 1o | 78/80 (98%) | 73 (94%) | 5 (6%) | 16 44 |
| 46 | 2o | 78/80 (98%) | 70 (90%) | 8 (10%) | 7 23 |
| 47 | 1p | 69/74 (93%) | 62 (90%) | 7 (10%) | 7 23 |
| 47 | 2p | 68/74 (92%) | 60 (88%) | 8 (12%) | 5 17 |
| 48 | 1q | 94/97 (97%) | 85 (90%) | 9 (10%) | 8 26 |
| 48 | 2q | 94/97 (97%) | 87 (93%) | 7 (7%) | 13 37 |
| 49 | 1r | 59/77 (77%) | 54 (92%) | 5 (8%) | 10 31 |
| 49 | 2r | 59/77 (77%) | 50 (85%) | 9 (15%) | 3 10 |
| 50 | 1s | 69/80 (86%) | 64 (93%) | 5 (7%) | 13 39 |
| 50 | 2s | 67/80 (84%) | 59 (88%) | 8 (12%) | 5 17 |
| 51 | 1t | 70/82 (85%) | 63 (90%) | 7 (10%) | 7 24 |
| 51 | 2t | 70/82 (85%) | 65 (93%) | 5 (7%) | 13 39 |
| 52 | 1u | 18/22 (82%) | 18 (100%) | 0 | 100 100 |
| 52 | 2u | 18/22 (82%) | 17 (94%) | 1 (6%) | 19 50 |
| All | All | 9301/10064 (92%) | 8332 (90%) | 969 (10%) | 7 22 |

All (969) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | 1D | 3 | VAL |
| 3 | 1D | 27 | THR |
| 3 | 1D | 32 | SER |
| 3 | 1D | 34 | VAL |
| 3 | 1D | 35 | LYS |
| 3 | 1D | 61 | LEU |
| 3 | 1D | 113 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | 1D | 122 | ASP |
| 3 | 1D | 142 | VAL |
| 3 | 1D | 193 | VAL |
| 3 | 1D | 206 | LEU |
| 3 | 1D | 211 | ARG |
| 3 | 1D | 229 | VAL |
| 3 | 1D | 242 | ARG |
| 3 | 1D | 275 | LYS |
| 4 | 1E | 9 | VAL |
| 4 | 1E | 12 | THR |
| 4 | 1E | 33 | VAL |
| 4 | 1E | 49 | LEU |
| 4 | 1E | 82 | ARG |
| 4 | 1E | 89 | ASP |
| 4 | 1E | 116 | VAL |
| 4 | 1E | 170 | LEU |
| 4 | 1E | 181 | LEU |
| 4 | 1E | 183 | LEU |
| 4 | 1E | 184 | VAL |
| 4 | 1E | 195 | LEU |
| 5 | 1F | 17 | ARG |
| 5 | 1F | 18 | ARG |
| 5 | 1F | 33 | LEU |
| 5 | 1F | 53 | THR |
| 5 | 1F | 57 | VAL |
| 5 | 1F | 70 | THR |
| 5 | 1F | 74 | ARG |
| 5 | 1F | 106 | ARG |
| 5 | 1F | 132 | VAL |
| 5 | 1F | 140 | LEU |
| 5 | 1F | 158 | THR |
| 5 | 1F | 168 | ARG |
| 5 | 1F | 175 | THR |
| 5 | 1F | 176 | LEU |
| 5 | 1F | 183 | VAL |
| 5 | 1F | 190 | GLU |
| 5 | 1F | 192 | LEU |
| 5 | 1F | 195 | ASP |
| 6 | 1G | 3 | LEU |
| 6 | 1G | 5 | VAL |
| 6 | 1G | 28 | VAL |
| 6 | 1G | 31 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 6 | 1G | 35 | GLU |
| 6 | 1G | 60 | LEU |
| 6 | 1G | 67 | LYS |
| 6 | 1G | 82 | LEU |
| 6 | 1G | 135 | LEU |
| 6 | 1G | 140 | ILE |
| 6 | 1G | 148 | MET |
| 6 | 1G | 149 | VAL |
| 6 | 1G | 150 | ASP |
| 6 | 1G | 152 | LEU |
| 6 | 1G | 159 | VAL |
| 6 | 1G | 162 | THR |
| 6 | 1G | 175 | LEU |
| 7 | 1H | 18 | GLU |
| 7 | 1H | 44 | VAL |
| 7 | 1H | 56 | SER |
| 7 | 1H | 62 | LYS |
| 7 | 1H | 67 | LEU |
| 7 | 1H | 84 | SER |
| 7 | 1H | 95 | ARG |
| 7 | 1H | 98 | LEU |
| 7 | 1H | 114 | VAL |
| 7 | 1H | 122 | THR |
| 7 | 1H | 127 | GLU |
| 7 | 1H | 129 | THR |
| 7 | 1H | 141 | VAL |
| 8 | 1I | 12 | LEU |
| 8 | 1I | 20 | ASP |
| 8 | 1I | 40 | THR |
| 8 | 1I | 74 | ASN |
| 8 | 1I | 75 | LEU |
| 8 | 1I | 78 | THR |
| 8 | 1I | 86 | THR |
| 8 | 1I | 92 | VAL |
| 8 | 1I | 95 | LYS |
| 8 | 1I | 108 | THR |
| 8 | 1I | 109 | ILE |
| 8 | 1I | 116 | LEU |
| 8 | 1I | 129 | THR |
| 8 | 1I | 140 | LEU |
| 8 | 1I | 142 | VAL |
| 9 | 1N | 8 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 9 | 1N | 28 | THR |
| 9 | 1N | 32 | THR |
| 9 | 1N | 33 | LEU |
| 9 | 1N | 46 | VAL |
| 9 | 1N | 48 | MET |
| 9 | 1N | 61 | ARG |
| 9 | 1N | 62 | VAL |
| 9 | 1N | 67 | LEU |
| 9 | 1N | 68 | GLU |
| 9 | 1N | 71 | ILE |
| 9 | 1N | 87 | LEU |
| 9 | 1N | 99 | LEU |
| 9 | 1N | 131 | GLN |
| 9 | 1N | 138 | LEU |
| 10 | 1O | 10 | VAL |
| 10 | 1O | 58 | VAL |
| 10 | 1O | 96 | THR |
| 10 | 1O | 109 | LYS |
| 10 | 1O | 120 | GLU |
| 11 | 1P | 3 | LEU |
| 11 | 1P | 6 | LEU |
| 11 | 1P | 29 | LYS |
| 11 | 1P | 42 | SER |
| 11 | 1P | 59 | LEU |
| 11 | 1P | 65 | ARG |
| 11 | 1P | 75 | ILE |
| 11 | 1P | 76 | LYS |
| 11 | 1P | 92 | GLU |
| 11 | 1P | 101 | VAL |
| 11 | 1P | 107 | LYS |
| 11 | 1P | 119 | GLU |
| 11 | 1P | 125 | VAL |
| 11 | 1P | 133 | SER |
| 11 | 1P | 147 | LEU |
| 11 | 1P | 148 | LEU |
| 12 | 1Q | 8 | LYS |
| 12 | 1Q | 56 | ARG |
| 12 | 1Q | 63 | LYS |
| 12 | 1Q | 75 | THR |
| 12 | 1Q | 79 | LEU |
| 12 | 1Q | 81 | VAL |
| 12 | 1Q | 109 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 12 | 1Q | 110 | THR |
| 12 | 1Q | 129 | THR |
| 12 | 1Q | 133 | ARG |
| 13 | 1R | 1 | MET |
| 13 | 1R | 6 | SER |
| 13 | 1R | 8 | ARG |
| 13 | 1R | 33 | ARG |
| 13 | 1R | 36 | THR |
| 13 | 1R | 38 | VAL |
| 13 | 1R | 65 | LEU |
| 13 | 1R | 76 | VAL |
| 13 | 1R | 96 | ARG |
| 13 | 1R | 102 | GLU |
| 13 | 1R | 114 | VAL |
| 14 | 1S | 36 | TYR |
| 14 | 1S | 50 | SER |
| 14 | 1S | 69 | VAL |
| 14 | 1S | 110 | LEU |
| 15 | 1T | 28 | VAL |
| 15 | 1T | 35 | LYS |
| 15 | 1T | 40 | THR |
| 15 | 1T | 43 | GLN |
| 15 | 1T | 50 | ILE |
| 15 | 1T | 118 | ARG |
| 15 | 1T | 128 | GLU |
| 16 | 1U | 31 | SER |
| 16 | 1U | 74 | LEU |
| 16 | 1U | 77 | SER |
| 16 | 1U | 85 | LYS |
| 16 | 1U | 100 | VAL |
| 17 | 1V | 32 | THR |
| 17 | 1V | 52 | VAL |
| 17 | 1V | 61 | VAL |
| 17 | 1V | 82 | ARG |
| 17 | 1V | 85 | LYS |
| 18 | 1W | 4 | LYS |
| 18 | 1W | 11 | ARG |
| 18 | 1W | 15 | ARG |
| 18 | 1W | 17 | VAL |
| 18 | 1W | 60 | ASN |
| 18 | 1W | 97 | LYS |
| 18 | 1W | 107 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 19 | 1X | 23 | GLU |
| 19 | 1X | 57 | LEU |
| 19 | 1X | 93 | GLU |
| 20 | 1Y | 1 | MET |
| 20 | 1Y | 43 | ASN |
| 20 | 1Y | 64 | GLU |
| 20 | 1Y | 67 | LEU |
| 20 | 1Y | 70 | SER |
| 20 | 1Y | 72 | VAL |
| 20 | 1Y | 90 | LEU |
| 20 | 1Y | 91 | GLU |
| 20 | 1Y | 99 | CYS |
| 20 | 1Y | 106 | LEU |
| 21 | 1Z | 18 | LEU |
| 21 | 1Z | 24 | LEU |
| 21 | 1Z | 33 | LEU |
| 21 | 1Z | 50 | GLN |
| 21 | 1Z | 61 | LEU |
| 21 | 1Z | 71 | VAL |
| 21 | 1Z | 74 | VAL |
| 21 | 1Z | 86 | VAL |
| 21 | 1Z | 93 | ASP |
| 21 | 1Z | 119 | GLU |
| 21 | 1Z | 121 | HIS |
| 21 | 1Z | 146 | ILE |
| 21 | 1Z | 154 | ASP |
| 21 | 1Z | 155 | LEU |
| 21 | 1Z | 163 | LEU |
| 21 | 1Z | 165 | VAL |
| 22 | 10 | 3 | HIS |
| 22 | 10 | 4 | LYS |
| 22 | 10 | 14 | ARG |
| 22 | 10 | 82 | ARG |
| 23 | 11 | 3 | LYS |
| 23 | 11 | 37 | ILE |
| 23 | 11 | 74 | VAL |
| 23 | 11 | 83 | GLU |
| 24 | 12 | 3 | LEU |
| 24 | 12 | 4 | SER |
| 24 | 12 | 5 | GLU |
| 24 | 12 | 19 | VAL |
| 24 | 12 | 53 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 24 | 12 | 65 | ASN |
| 24 | 12 | 67 | LYS |
| 24 | 12 | 70 | GLN |
| 25 | 13 | 6 | VAL |
| 25 | 13 | 18 | ASP |
| 25 | 13 | 23 | LEU |
| 25 | 13 | 36 | VAL |
| 25 | 13 | 54 | VAL |
| 25 | 13 | 56 | VAL |
| 25 | 13 | 58 | VAL |
| 25 | 13 | 60 | GLU |
| 26 | 14 | 3 | GLU |
| 26 | 14 | 5 | ILE |
| 26 | 14 | 8 | LYS |
| 26 | 14 | 21 | VAL |
| 26 | 14 | 27 | THR |
| 26 | 14 | 28 | LYS |
| 26 | 14 | 49 | PHE |
| 26 | 14 | 50 | VAL |
| 26 | 14 | 52 | THR |
| 26 | 14 | 59 | PHE |
| 26 | 14 | 63 | TYR |
| 26 | 14 | 66 | SER |
| 26 | 14 | 67 | TYR |
| 27 | 15 | 6 | VAL |
| 27 | 15 | 29 | THR |
| 27 | 15 | 40 | LYS |
| 27 | 15 | 48 | GLU |
| 27 | 15 | 58 | LEU |
| 27 | 15 | 60 | VAL |
| 28 | 16 | 6 | ARG |
| 28 | 16 | 9 | LEU |
| 28 | 16 | 14 | THR |
| 28 | 16 | 19 | ARG |
| 28 | 16 | 38 | LYS |
| 28 | 16 | 48 | VAL |
| 28 | 16 | 53 | LYS |
| 29 | 17 | 1 | MET |
| 29 | 17 | 4 | THR |
| 29 | 17 | 43 | THR |
| 30 | 18 | 14 | VAL |
| 30 | 18 | 29 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 31 | 19 | 13 | LYS |
| 33 | 1b | 7 | VAL |
| 33 | 1b | 21 | ARG |
| 33 | 1b | 27 | LYS |
| 33 | 1b | 32 | ILE |
| 33 | 1b | 54 | THR |
| 33 | 1b | 56 | ARG |
| 33 | 1b | 67 | THR |
| 33 | 1b | 78 | GLN |
| 33 | 1b | 87 | ARG |
| 33 | 1b | 108 | ILE |
| 33 | 1b | 111 | ARG |
| 33 | 1b | 121 | LEU |
| 33 | 1b | 128 | GLU |
| 33 | 1b | 142 | LEU |
| 33 | 1b | 160 | ASP |
| 33 | 1b | 162 | ILE |
| 33 | 1b | 170 | GLU |
| 33 | 1b | 206 | ASP |
| 33 | 1b | 211 | ILE |
| 33 | 1b | 213 | LEU |
| 33 | 1b | 229 | VAL |
| 33 | 1b | 230 | VAL |
| 34 | 1c | 3 | ASN |
| 34 | 1c | 15 | THR |
| 34 | 1c | 17 | ASP |
| 34 | 1c | 36 | ASP |
| 34 | 1c | 38 | ARG |
| 34 | 1c | 46 | GLU |
| 34 | 1c | 49 | SER |
| 34 | 1c | 58 | GLU |
| 34 | 1c | 64 | VAL |
| 34 | 1c | 82 | GLU |
| 34 | 1c | 97 | LYS |
| 34 | 1c | 103 | VAL |
| 34 | 1c | 115 | LEU |
| 34 | 1c | 191 | THR |
| 34 | 1c | 195 | VAL |
| 35 | 1d | 8 | VAL |
| 35 | 1d | 19 | LEU |
| 35 | 1d | 31 | CYS |
| 35 | 1d | 59 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 35 | 1d | 112 | VAL |
| 35 | 1d | 141 | ARG |
| 35 | 1d | 146 | ILE |
| 35 | 1d | 158 | ILE |
| 35 | 1d | 160 | GLN |
| 35 | 1d | 166 | LYS |
| 35 | 1d | 175 | SER |
| 35 | 1d | 178 | VAL |
| 35 | 1d | 190 | ASP |
| 35 | 1d | 194 | LEU |
| 35 | 1d | 201 | GLN |
| 35 | 1d | 204 | ILE |
| 36 | 1e | 31 | LEU |
| 36 | 1e | 34 | VAL |
| 36 | 1e | 41 | VAL |
| 36 | 1e | 79 | GLU |
| 36 | 1e | 81 | GLU |
| 36 | 1e | 120 | THR |
| 36 | 1e | 151 | LEU |
| 37 | 1f | 46 | ARG |
| 37 | 1f | 55 | ASP |
| 37 | 1f | 70 | ASP |
| 37 | 1f | 72 | VAL |
| 37 | 1f | 81 | ILE |
| 38 | 1g | 24 | THR |
| 38 | 1g | 53 | LYS |
| 38 | 1g | 57 | GLU |
| 38 | 1g | 113 | GLU |
| 39 | 1h | 2 | LEU |
| 39 | 1h | 9 | MET |
| 39 | 1h | 26 | VAL |
| 39 | 1h | 35 | ILE |
| 39 | 1h | 49 | GLU |
| 39 | 1h | 51 | VAL |
| 39 | 1h | 52 | ASP |
| 39 | 1h | 77 | GLU |
| 39 | 1h | 82 | HIS |
| 39 | 1h | 91 | ARG |
| 39 | 1h | 99 | GLU |
| 39 | 1h | 109 | ILE |
| 39 | 1h | 120 | THR |
| 39 | 1h | 123 | GLU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 39 | 1h | 127 | LEU |
| 40 | 1i | 16 | ARG |
| 40 | 1i | 26 | VAL |
| 40 | 1i | 27 | THR |
| 40 | 1i | 53 | VAL |
| 40 | 1i | 64 | THR |
| 40 | 1i | 103 | THR |
| 40 | 1i | 104 | ARG |
| 40 | 1i | 108 | VAL |
| 40 | 1i | 113 | LYS |
| 41 | 1j | 17 | ASP |
| 41 | 1j | 19 | SER |
| 41 | 1j | 21 | GLN |
| 41 | 1j | 30 | SER |
| 41 | 1j | 38 | ILE |
| 41 | 1j | 44 | VAL |
| 41 | 1j | 48 | THR |
| 41 | 1j | 65 | LEU |
| 41 | 1j | 81 | THR |
| 41 | 1j | 98 | ILE |
| 42 | 1k | 29 | ILE |
| 42 | 1k | 33 | THR |
| 42 | 1k | 48 | ILE |
| 42 | 1k | 82 | VAL |
| 42 | 1k | 87 | THR |
| 42 | 1k | 109 | VAL |
| 42 | 1k | 110 | ASP |
| 42 | 1k | 114 | VAL |
| 42 | 1k | 117 | ASN |
| 43 | 1l | 18 | VAL |
| 43 | 1l | 38 | THR |
| 43 | 1l | 43 | VAL |
| 43 | 1l | 47 | LYS |
| 43 | 1l | 57 | LYS |
| 43 | 1l | 67 | THR |
| 43 | 1l | 83 | VAL |
| 43 | 1l | 86 | ARG |
| 43 | 1l | 96 | VAL |
| 43 | 1l | 124 | LYS |
| 44 | 1m | 3 | ARG |
| 44 | 1m | 4 | ILE |
| 44 | 1m | 17 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 44 | 1m | 19 | LEU |
| 44 | 1m | 49 | THR |
| 44 | 1m | 53 | VAL |
| 44 | 1m | 67 | GLU |
| 44 | 1m | 73 | GLU |
| 44 | 1m | 78 | ILE |
| 44 | 1m | 103 | THR |
| 44 | 1m | 106 | ASN |
| 44 | 1m | 109 | THR |
| 44 | 1m | 114 | ARG |
| 44 | 1m | 117 | VAL |
| 45 | 1n | 7 | ILE |
| 45 | 1n | 11 | LYS |
| 45 | 1n | 13 | THR |
| 45 | 1n | 18 | VAL |
| 45 | 1n | 22 | THR |
| 45 | 1n | 33 | VAL |
| 45 | 1n | 41 | ARG |
| 46 | 1o | 3 | ILE |
| 46 | 1o | 4 | THR |
| 46 | 1o | 34 | LEU |
| 46 | 1o | 39 | LEU |
| 46 | 1o | 87 | ILE |
| 47 | 1p | 2 | VAL |
| 47 | 1p | 11 | SER |
| 47 | 1p | 19 | ILE |
| 47 | 1p | 20 | VAL |
| 47 | 1p | 60 | LEU |
| 47 | 1p | 62 | VAL |
| 47 | 1p | 67 | THR |
| 48 | 1q | 9 | VAL |
| 48 | 1q | 19 | VAL |
| 48 | 1q | 24 | GLU |
| 48 | 1q | 49 | GLU |
| 48 | 1q | 70 | ARG |
| 48 | 1q | 72 | ARG |
| 48 | 1q | 82 | MET |
| 48 | 1q | 87 | LYS |
| 48 | 1q | 93 | GLN |
| 49 | 1r | 22 | VAL |
| 49 | 1r | 25 | THR |
| 49 | 1r | 37 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 49 | 1r | 68 | LYS |
| 49 | 1r | 82 | THR |
| 50 | 1s | 12 | ASP |
| 50 | 1s | 16 | LEU |
| 50 | 1s | 28 | LYS |
| 50 | 1s | 65 | ASN |
| 50 | 1s | 77 | THR |
| 51 | 1t | 10 | LEU |
| 51 | 1t | 37 | SER |
| 51 | 1t | 45 | GLN |
| 51 | 1t | 62 | LEU |
| 51 | 1t | 71 | THR |
| 51 | 1t | 88 | VAL |
| 51 | 1t | 100 | ILE |
| 3 | 2D | 3 | VAL |
| 3 | 2D | 87 | ASN |
| 3 | 2D | 113 | VAL |
| 3 | 2D | 141 | VAL |
| 3 | 2D | 173 | VAL |
| 3 | 2D | 193 | VAL |
| 3 | 2D | 211 | ARG |
| 3 | 2D | 242 | ARG |
| 3 | 2D | 260 | ARG |
| 4 | 2E | 1 | MET |
| 4 | 2E | 9 | VAL |
| 4 | 2E | 12 | THR |
| 4 | 2E | 27 | LEU |
| 4 | 2E | 38 | THR |
| 4 | 2E | 73 | GLU |
| 4 | 2E | 77 | ILE |
| 4 | 2E | 82 | ARG |
| 4 | 2E | 89 | ASP |
| 4 | 2E | 90 | THR |
| 4 | 2E | 101 | ARG |
| 4 | 2E | 107 | THR |
| 4 | 2E | 116 | VAL |
| 4 | 2E | 170 | LEU |
| 4 | 2E | 178 | GLU |
| 4 | 2E | 181 | LEU |
| 5 | 2F | 18 | ARG |
| 5 | 2F | 20 | LEU |
| 5 | 2F | 24 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 5 | 2F | 33 | LEU |
| 5 | 2F | 57 | VAL |
| 5 | 2F | 74 | ARG |
| 5 | 2F | 77 | ASP |
| 5 | 2F | 88 | VAL |
| 5 | 2F | 108 | LYS |
| 5 | 2F | 110 | LEU |
| 5 | 2F | 126 | VAL |
| 5 | 2F | 137 | LYS |
| 5 | 2F | 145 | GLU |
| 5 | 2F | 153 | SER |
| 5 | 2F | 158 | THR |
| 5 | 2F | 165 | ARG |
| 5 | 2F | 170 | LEU |
| 5 | 2F | 176 | LEU |
| 5 | 2F | 183 | VAL |
| 5 | 2F | 188 | ARG |
| 5 | 2F | 195 | ASP |
| 5 | 2F | 201 | VAL |
| 6 | 2G | 3 | LEU |
| 6 | 2G | 5 | VAL |
| 6 | 2G | 15 | VAL |
| 6 | 2G | 22 | ARG |
| 6 | 2G | 28 | VAL |
| 6 | 2G | 35 | GLU |
| 6 | 2G | 51 | ARG |
| 6 | 2G | 53 | LEU |
| 6 | 2G | 79 | ASN |
| 6 | 2G | 88 | ILE |
| 6 | 2G | 91 | ARG |
| 6 | 2G | 92 | VAL |
| 6 | 2G | 98 | ARG |
| 6 | 2G | 106 | LEU |
| 6 | 2G | 109 | VAL |
| 6 | 2G | 128 | ARG |
| 6 | 2G | 135 | LEU |
| 6 | 2G | 139 | LEU |
| 6 | 2G | 140 | ILE |
| 6 | 2G | 145 | THR |
| 6 | 2G | 152 | LEU |
| 6 | 2G | 159 | VAL |
| 6 | 2G | 165 | THR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 7 | 2H | 24 | VAL |
| 7 | 2H | 33 | LEU |
| 7 | 2H | 42 | ARG |
| 7 | 2H | 43 | VAL |
| 7 | 2H | 45 | VAL |
| 7 | 2H | 47 | GLU |
| 7 | 2H | 49 | VAL |
| 7 | 2H | 58 | GLU |
| 7 | 2H | 70 | THR |
| 7 | 2H | 71 | LEU |
| 7 | 2H | 88 | LEU |
| 7 | 2H | 98 | LEU |
| 7 | 2H | 114 | VAL |
| 7 | 2H | 129 | THR |
| 7 | 2H | 130 | ARG |
| 7 | 2H | 136 | ILE |
| 8 | 2I | 7 | GLU |
| 8 | 2I | 15 | VAL |
| 8 | 2I | 19 | VAL |
| 8 | 2I | 38 | LEU |
| 8 | 2I | 40 | THR |
| 8 | 2I | 43 | ASN |
| 8 | 2I | 47 | LEU |
| 8 | 2I | 52 | ARG |
| 8 | 2I | 61 | ARG |
| 8 | 2I | 73 | GLU |
| 8 | 2I | 75 | LEU |
| 8 | 2I | 76 | THR |
| 8 | 2I | 78 | THR |
| 8 | 2I | 79 | ILE |
| 8 | 2I | 81 | VAL |
| 8 | 2I | 86 | THR |
| 8 | 2I | 88 | ILE |
| 8 | 2I | 91 | SER |
| 8 | 2I | 93 | THR |
| 8 | 2I | 101 | LEU |
| 8 | 2I | 102 | SER |
| 8 | 2I | 108 | THR |
| 8 | 2I | 114 | LEU |
| 8 | 2I | 122 | GLU |
| 8 | 2I | 125 | GLU |
| 8 | 2I | 126 | TYR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 8 | 2I | 129 | THR |
| 8 | 2I | 136 | VAL |
| 8 | 2I | 138 | ILE |
| 8 | 2I | 139 | GLN |
| 8 | 2I | 140 | LEU |
| 8 | 2I | 143 | SER |
| 9 | 2N | 1 | MET |
| 9 | 2N | 5 | VAL |
| 9 | 2N | 33 | LEU |
| 9 | 2N | 38 | HIS |
| 9 | 2N | 43 | THR |
| 9 | 2N | 48 | MET |
| 9 | 2N | 55 | VAL |
| 9 | 2N | 59 | LYS |
| 9 | 2N | 61 | ARG |
| 9 | 2N | 62 | VAL |
| 9 | 2N | 63 | THR |
| 9 | 2N | 67 | LEU |
| 9 | 2N | 71 | ILE |
| 9 | 2N | 87 | LEU |
| 9 | 2N | 99 | LEU |
| 10 | 2O | 10 | VAL |
| 10 | 2O | 19 | ILE |
| 10 | 2O | 26 | LYS |
| 10 | 2O | 58 | VAL |
| 10 | 2O | 69 | ILE |
| 10 | 2O | 96 | THR |
| 11 | 2P | 1 | MET |
| 11 | 2P | 3 | LEU |
| 11 | 2P | 30 | THR |
| 11 | 2P | 56 | SER |
| 11 | 2P | 77 | ARG |
| 11 | 2P | 83 | VAL |
| 11 | 2P | 91 | PHE |
| 11 | 2P | 96 | THR |
| 11 | 2P | 101 | VAL |
| 11 | 2P | 119 | GLU |
| 11 | 2P | 125 | VAL |
| 11 | 2P | 148 | LEU |
| 12 | 2Q | 1 | MET |
| 12 | 2Q | 7 | MET |
| 12 | 2Q | 38 | GLU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 12 | 2Q | 52 | VAL |
| 12 | 2Q | 54 | MET |
| 12 | 2Q | 56 | ARG |
| 12 | 2Q | 85 | LYS |
| 12 | 2Q | 98 | LYS |
| 12 | 2Q | 106 | VAL |
| 12 | 2Q | 109 | VAL |
| 12 | 2Q | 112 | GLU |
| 12 | 2Q | 133 | ARG |
| 13 | 2R | 15 | SER |
| 13 | 2R | 35 | THR |
| 13 | 2R | 65 | LEU |
| 13 | 2R | 73 | VAL |
| 13 | 2R | 95 | THR |
| 13 | 2R | 96 | ARG |
| 13 | 2R | 114 | VAL |
| 13 | 2R | 117 | VAL |
| 14 | 2S | 8 | GLU |
| 14 | 2S | 12 | PHE |
| 14 | 2S | 13 | ARG |
| 14 | 2S | 19 | LYS |
| 14 | 2S | 36 | TYR |
| 14 | 2S | 40 | ILE |
| 14 | 2S | 43 | GLU |
| 14 | 2S | 46 | VAL |
| 14 | 2S | 49 | VAL |
| 14 | 2S | 63 | THR |
| 14 | 2S | 69 | VAL |
| 14 | 2S | 75 | GLU |
| 14 | 2S | 76 | LYS |
| 15 | 2T | 6 | LEU |
| 15 | 2T | 15 | VAL |
| 15 | 2T | 31 | SER |
| 15 | 2T | 55 | ASN |
| 15 | 2T | 63 | VAL |
| 15 | 2T | 89 | VAL |
| 15 | 2T | 95 | ARG |
| 15 | 2T | 96 | ARG |
| 15 | 2T | 107 | ASP |
| 16 | 2U | 55 | ARG |
| 16 | 2U | 74 | LEU |
| 16 | 2U | 77 | SER |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 16 | 2U | 85 | LYS |
| 16 | 2U | 100 | VAL |
| 16 | 2U | 108 | GLU |
| 16 | 2U | 117 | GLN |
| 17 | 2V | 14 | VAL |
| 17 | 2V | 15 | GLU |
| 17 | 2V | 52 | VAL |
| 17 | 2V | 56 | SER |
| 17 | 2V | 61 | VAL |
| 17 | 2V | 82 | ARG |
| 17 | 2V | 85 | LYS |
| 17 | 2V | 95 | LEU |
| 18 | 2W | 11 | ARG |
| 18 | 2W | 17 | VAL |
| 18 | 2W | 20 | VAL |
| 18 | 2W | 23 | LEU |
| 18 | 2W | 59 | VAL |
| 18 | 2W | 67 | ASP |
| 18 | 2W | 107 | LEU |
| 18 | 2W | 111 | HIS |
| 19 | 2X | 23 | GLU |
| 19 | 2X | 30 | VAL |
| 19 | 2X | 35 | THR |
| 19 | 2X | 52 | VAL |
| 19 | 2X | 65 | ARG |
| 19 | 2X | 66 | LEU |
| 19 | 2X | 72 | LYS |
| 19 | 2X | 81 | VAL |
| 20 | 2Y | 24 | VAL |
| 20 | 2Y | 42 | VAL |
| 20 | 2Y | 72 | VAL |
| 20 | 2Y | 81 | LYS |
| 20 | 2Y | 85 | VAL |
| 20 | 2Y | 90 | LEU |
| 20 | 2Y | 91 | GLU |
| 20 | 2Y | 94 | LYS |
| 20 | 2Y | 98 | VAL |
| 20 | 2Y | 99 | CYS |
| 21 | 2Z | 5 | LEU |
| 21 | 2Z | 38 | TYR |
| 21 | 2Z | 41 | LEU |
| 21 | 2Z | 53 | ILE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 21 | 2Z | 60 | GLU |
| 21 | 2Z | 71 | VAL |
| 21 | 2Z | 72 | ARG |
| 21 | 2Z | 100 | VAL |
| 21 | 2Z | 121 | HIS |
| 21 | 2Z | 123 | ASP |
| 21 | 2Z | 124 | ILE |
| 21 | 2Z | 126 | VAL |
| 21 | 2Z | 131 | ARG |
| 21 | 2Z | 154 | ASP |
| 21 | 2Z | 155 | LEU |
| 21 | 2Z | 161 | VAL |
| 21 | 2Z | 171 | ILE |
| 21 | 2Z | 174 | VAL |
| 22 | 20 | 3 | HIS |
| 22 | 20 | 10 | THR |
| 22 | 20 | 11 | ARG |
| 22 | 20 | 37 | LEU |
| 23 | 21 | 51 | VAL |
| 23 | 21 | 52 | ARG |
| 23 | 21 | 56 | GLN |
| 23 | 21 | 65 | SER |
| 23 | 21 | 74 | VAL |
| 23 | 21 | 83 | GLU |
| 23 | 21 | 92 | LYS |
| 24 | 22 | 30 | ARG |
| 24 | 22 | 32 | LEU |
| 24 | 22 | 34 | GLU |
| 24 | 22 | 35 | LEU |
| 24 | 22 | 53 | LEU |
| 24 | 22 | 65 | ASN |
| 24 | 22 | 70 | GLN |
| 25 | 23 | 6 | VAL |
| 25 | 23 | 31 | LEU |
| 25 | 23 | 54 | VAL |
| 25 | 23 | 56 | VAL |
| 26 | 24 | 13 | ARG |
| 26 | 24 | 33 | VAL |
| 26 | 24 | 34 | GLU |
| 26 | 24 | 48 | ARG |
| 26 | 24 | 49 | PHE |
| 26 | 24 | 53 | GLU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 26 | 24 | 56 | VAL |
| 26 | 24 | 63 | TYR |
| 27 | 25 | 6 | VAL |
| 27 | 25 | 8 | LYS |
| 27 | 25 | 29 | THR |
| 27 | 25 | 48 | GLU |
| 28 | 26 | 9 | LEU |
| 28 | 26 | 13 | CYS |
| 28 | 26 | 20 | ASN |
| 28 | 26 | 50 | ARG |
| 29 | 27 | 4 | THR |
| 29 | 27 | 41 | ARG |
| 29 | 27 | 46 | VAL |
| 30 | 28 | 14 | VAL |
| 30 | 28 | 37 | SER |
| 30 | 28 | 46 | ARG |
| 30 | 28 | 50 | LEU |
| 31 | 29 | 7 | VAL |
| 31 | 29 | 26 | ILE |
| 33 | 2b | 8 | LYS |
| 33 | 2b | 11 | LEU |
| 33 | 2b | 15 | VAL |
| 33 | 2b | 16 | HIS |
| 33 | 2b | 35 | GLU |
| 33 | 2b | 44 | LEU |
| 33 | 2b | 47 | THR |
| 33 | 2b | 67 | THR |
| 33 | 2b | 68 | ILE |
| 33 | 2b | 71 | VAL |
| 33 | 2b | 83 | MET |
| 33 | 2b | 93 | VAL |
| 33 | 2b | 94 | ASN |
| 33 | 2b | 103 | THR |
| 33 | 2b | 107 | THR |
| 33 | 2b | 115 | LEU |
| 33 | 2b | 117 | GLU |
| 33 | 2b | 127 | ILE |
| 33 | 2b | 137 | ARG |
| 33 | 2b | 150 | SER |
| 33 | 2b | 153 | ARG |
| 33 | 2b | 154 | LEU |
| 33 | 2b | 164 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 33 | 2b | 165 | VAL |
| 33 | 2b | 176 | GLU |
| 33 | 2b | 178 | ARG |
| 33 | 2b | 180 | LEU |
| 33 | 2b | 184 | VAL |
| 33 | 2b | 189 | ASP |
| 33 | 2b | 197 | VAL |
| 33 | 2b | 200 | ILE |
| 33 | 2b | 208 | ILE |
| 33 | 2b | 209 | ARG |
| 33 | 2b | 224 | GLN |
| 33 | 2b | 229 | VAL |
| 33 | 2b | 230 | VAL |
| 34 | 2c | 36 | ASP |
| 34 | 2c | 45 | LYS |
| 34 | 2c | 47 | LEU |
| 34 | 2c | 57 | ILE |
| 34 | 2c | 70 | VAL |
| 34 | 2c | 98 | ASN |
| 34 | 2c | 101 | LEU |
| 34 | 2c | 103 | VAL |
| 34 | 2c | 105 | GLU |
| 34 | 2c | 115 | LEU |
| 34 | 2c | 118 | GLN |
| 34 | 2c | 152 | ILE |
| 34 | 2c | 153 | VAL |
| 34 | 2c | 154 | SER |
| 34 | 2c | 156 | ARG |
| 34 | 2c | 162 | GLN |
| 34 | 2c | 164 | ARG |
| 34 | 2c | 166 | GLU |
| 34 | 2c | 172 | ARG |
| 34 | 2c | 173 | VAL |
| 34 | 2c | 190 | ARG |
| 34 | 2c | 191 | THR |
| 34 | 2c | 195 | VAL |
| 34 | 2c | 198 | VAL |
| 34 | 2c | 206 | GLU |
| 35 | 2d | 5 | ILE |
| 35 | 2d | 21 | LEU |
| 35 | 2d | 27 | TYR |
| 35 | 2d | 28 | SER |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 35 | 2d | 31 | CYS |
| 35 | 2d | 38 | TYR |
| 35 | 2d | 60 | GLU |
| 35 | 2d | 76 | ARG |
| 35 | 2d | 102 | ASP |
| 35 | 2d | 108 | LEU |
| 35 | 2d | 112 | VAL |
| 35 | 2d | 127 | THR |
| 35 | 2d | 135 | LEU |
| 35 | 2d | 150 | GLU |
| 35 | 2d | 155 | LEU |
| 35 | 2d | 156 | GLU |
| 35 | 2d | 157 | LEU |
| 35 | 2d | 175 | SER |
| 35 | 2d | 178 | VAL |
| 35 | 2d | 181 | MET |
| 36 | 2e | 6 | PHE |
| 36 | 2e | 10 | MET |
| 36 | 2e | 13 | ILE |
| 36 | 2e | 24 | ARG |
| 36 | 2e | 32 | VAL |
| 36 | 2e | 41 | VAL |
| 36 | 2e | 55 | VAL |
| 36 | 2e | 81 | GLU |
| 36 | 2e | 135 | THR |
| 36 | 2e | 140 | ARG |
| 36 | 2e | 144 | THR |
| 36 | 2e | 152 | ARG |
| 37 | 2f | 31 | GLU |
| 37 | 2f | 37 | VAL |
| 37 | 2f | 61 | LEU |
| 37 | 2f | 72 | VAL |
| 37 | 2f | 81 | ILE |
| 37 | 2f | 89 | MET |
| 37 | 2f | 94 | GLN |
| 37 | 2f | 95 | GLU |
| 38 | 2g | 8 | GLU |
| 38 | 2g | 21 | VAL |
| 38 | 2g | 28 | ASN |
| 38 | 2g | 42 | ILE |
| 38 | 2g | 49 | ILE |
| 38 | 2g | 51 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 38 | 2g | 52 | GLU |
| 38 | 2g | 57 | GLU |
| 38 | 2g | 85 | TYR |
| 38 | 2g | 87 | VAL |
| 38 | 2g | 114 | ARG |
| 38 | 2g | 115 | ARG |
| 38 | 2g | 119 | ARG |
| 38 | 2g | 135 | VAL |
| 38 | 2g | 154 | TYR |
| 39 | 2h | 2 | LEU |
| 39 | 2h | 9 | MET |
| 39 | 2h | 25 | ASP |
| 39 | 2h | 63 | LEU |
| 39 | 2h | 81 | HIS |
| 39 | 2h | 85 | ARG |
| 39 | 2h | 98 | LYS |
| 39 | 2h | 99 | GLU |
| 39 | 2h | 112 | LEU |
| 39 | 2h | 115 | SER |
| 39 | 2h | 118 | VAL |
| 39 | 2h | 123 | GLU |
| 39 | 2h | 127 | LEU |
| 39 | 2h | 137 | VAL |
| 40 | 2i | 14 | VAL |
| 40 | 2i | 41 | VAL |
| 40 | 2i | 53 | VAL |
| 40 | 2i | 64 | THR |
| 40 | 2i | 65 | VAL |
| 40 | 2i | 75 | ASP |
| 40 | 2i | 111 | ARG |
| 40 | 2i | 114 | TYR |
| 40 | 2i | 124 | GLN |
| 40 | 2i | 125 | TYR |
| 41 | 2j | 44 | VAL |
| 41 | 2j | 49 | VAL |
| 41 | 2j | 65 | LEU |
| 41 | 2j | 72 | VAL |
| 41 | 2j | 92 | THR |
| 41 | 2j | 96 | ILE |
| 42 | 2k | 14 | VAL |
| 42 | 2k | 29 | ILE |
| 42 | 2k | 48 | ILE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 42 | 2k | 50 | TYR |
| 42 | 2k | 63 | LEU |
| 42 | 2k | 80 | VAL |
| 42 | 2k | 104 | GLN |
| 43 | 2l | 6 | THR |
| 43 | 2l | 18 | VAL |
| 43 | 2l | 33 | ARG |
| 43 | 2l | 36 | VAL |
| 43 | 2l | 38 | THR |
| 43 | 2l | 40 | VAL |
| 43 | 2l | 83 | VAL |
| 43 | 2l | 104 | VAL |
| 43 | 2l | 113 | ARG |
| 44 | 2m | 15 | VAL |
| 44 | 2m | 19 | LEU |
| 44 | 2m | 34 | LEU |
| 44 | 2m | 39 | ILE |
| 44 | 2m | 47 | ASP |
| 44 | 2m | 50 | GLU |
| 44 | 2m | 55 | ARG |
| 44 | 2m | 60 | VAL |
| 44 | 2m | 69 | GLU |
| 44 | 2m | 71 | ARG |
| 44 | 2m | 81 | LEU |
| 44 | 2m | 98 | VAL |
| 44 | 2m | 103 | THR |
| 44 | 2m | 105 | THR |
| 44 | 2m | 117 | VAL |
| 45 | 2n | 3 | ARG |
| 45 | 2n | 7 | ILE |
| 45 | 2n | 11 | LYS |
| 45 | 2n | 13 | THR |
| 45 | 2n | 15 | LYS |
| 45 | 2n | 58 | LYS |
| 46 | 2o | 5 | LYS |
| 46 | 2o | 7 | GLU |
| 46 | 2o | 25 | THR |
| 46 | 2o | 35 | ARG |
| 46 | 2o | 39 | LEU |
| 46 | 2o | 62 | GLN |
| 46 | 2o | 64 | ARG |
| 46 | 2o | 83 | GLU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 47 | 2p | 2 | VAL |
| 47 | 2p | 16 | HIS |
| 47 | 2p | 20 | VAL |
| 47 | 2p | 21 | VAL |
| 47 | 2p | 42 | ARG |
| 47 | 2p | 45 | THR |
| 47 | 2p | 62 | VAL |
| 47 | 2p | 69 | THR |
| 48 | 2q | 37 | LYS |
| 48 | 2q | 43 | LEU |
| 48 | 2q | 63 | ARG |
| 48 | 2q | 66 | SER |
| 48 | 2q | 68 | ARG |
| 48 | 2q | 82 | MET |
| 48 | 2q | 99 | SER |
| 49 | 2r | 25 | THR |
| 49 | 2r | 26 | LEU |
| 49 | 2r | 31 | LEU |
| 49 | 2r | 37 | VAL |
| 49 | 2r | 54 | ARG |
| 49 | 2r | 65 | ILE |
| 49 | 2r | 68 | LYS |
| 49 | 2r | 74 | ARG |
| 49 | 2r | 85 | LEU |
| 50 | 2s | 22 | LEU |
| 50 | 2s | 28 | LYS |
| 50 | 2s | 30 | LEU |
| 50 | 2s | 48 | THR |
| 50 | 2s | 49 | ILE |
| 50 | 2s | 65 | ASN |
| 50 | 2s | 79 | THR |
| 50 | 2s | 81 | ARG |
| 51 | 2t | 30 | LYS |
| 51 | 2t | 41 | ILE |
| 51 | 2t | 54 | LYS |
| 51 | 2t | 71 | THR |
| 51 | 2t | 100 | ILE |
| 52 | 2u | 13 | ILE |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (125) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 4 | 1E | 121 | ASN |
| 5 | 1F | 8 | GLN |
| 5 | 1F | 133 | ASN |
| 6 | 1G | 26 | GLN |
| 8 | 1I | 54 | GLN |
| 8 | 1I | 139 | GLN |
| 9 | 1N | 131 | GLN |
| 10 | 1O | 5 | GLN |
| 11 | 1P | 35 | HIS |
| 12 | 1Q | 57 | HIS |
| 12 | 1Q | 123 | HIS |
| 13 | 1R | 13 | HIS |
| 13 | 1R | 31 | HIS |
| 13 | 1R | 61 | HIS |
| 13 | 1R | 71 | GLN |
| 13 | 1R | 91 | GLN |
| 14 | 1S | 61 | ASN |
| 15 | 1T | 58 | ASN |
| 16 | 1U | 94 | ASN |
| 19 | 1X | 82 | GLN |
| 20 | 1Y | 6 | HIS |
| 21 | 1Z | 73 | GLN |
| 21 | 1Z | 75 | ASN |
| 21 | 1Z | 151 | HIS |
| 22 | 10 | 3 | HIS |
| 23 | 11 | 56 | GLN |
| 24 | 12 | 38 | GLN |
| 33 | 1b | 16 | HIS |
| 33 | 1b | 78 | GLN |
| 33 | 1b | 94 | ASN |
| 34 | 1c | 6 | HIS |
| 34 | 1c | 31 | HIS |
| 34 | 1c | 98 | ASN |
| 34 | 1c | 110 | ASN |
| 34 | 1c | 162 | GLN |
| 35 | 1d | 42 | GLN |
| 35 | 1d | 45 | GLN |
| 35 | 1d | 116 | GLN |
| 35 | 1d | 119 | GLN |
| 35 | 1d | 123 | HIS |
| 36 | 1e | 78 | HIS |
| 37 | 1f | 13 | ASN |
| 37 | 1f | 18 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 37 | 1f | 100 | ASN |
| 38 | 1g | 28 | ASN |
| 38 | 1g | 64 | GLN |
| 38 | 1g | 110 | GLN |
| 39 | 1h | 15 | ASN |
| 40 | 1i | 3 | GLN |
| 40 | 1i | 34 | ASN |
| 40 | 1i | 58 | HIS |
| 40 | 1i | 73 | GLN |
| 40 | 1i | 124 | GLN |
| 41 | 1j | 56 | HIS |
| 41 | 1j | 84 | GLN |
| 42 | 1k | 99 | GLN |
| 42 | 1k | 116 | HIS |
| 44 | 1m | 12 | ASN |
| 46 | 1o | 28 | GLN |
| 46 | 1o | 46 | HIS |
| 47 | 1p | 16 | HIS |
| 47 | 1p | 65 | GLN |
| 48 | 1q | 26 | GLN |
| 49 | 1r | 63 | GLN |
| 50 | 1s | 14 | HIS |
| 50 | 1s | 57 | HIS |
| 50 | 1s | 69 | HIS |
| 50 | 1s | 83 | HIS |
| 4 | 2E | 48 | GLN |
| 5 | 2F | 75 | HIS |
| 6 | 2G | 58 | GLN |
| 8 | 2I | 133 | HIS |
| 9 | 2N | 8 | GLN |
| 12 | 2Q | 123 | HIS |
| 13 | 2R | 61 | HIS |
| 14 | 2S | 38 | GLN |
| 15 | 2T | 43 | GLN |
| 15 | 2T | 58 | ASN |
| 15 | 2T | 84 | GLN |
| 16 | 2U | 94 | ASN |
| 18 | 2W | 60 | ASN |
| 20 | 2Y | 6 | HIS |
| 20 | 2Y | 92 | ASN |
| 21 | 2Z | 73 | GLN |
| 22 | 20 | 17 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 22 | 20 | 35 | ASN |
| 23 | 21 | 56 | GLN |
| 24 | 22 | 46 | GLN |
| 24 | 22 | 56 | GLN |
| 28 | 26 | 20 | ASN |
| 30 | 28 | 43 | GLN |
| 33 | 2b | 19 | HIS |
| 33 | 2b | 40 | HIS |
| 33 | 2b | 212 | GLN |
| 33 | 2b | 224 | GLN |
| 34 | 2c | 6 | HIS |
| 34 | 2c | 108 | ASN |
| 35 | 2d | 74 | GLN |
| 35 | 2d | 77 | ASN |
| 35 | 2d | 116 | GLN |
| 35 | 2d | 119 | GLN |
| 35 | 2d | 123 | HIS |
| 35 | 2d | 125 | HIS |
| 36 | 2e | 38 | GLN |
| 36 | 2e | 78 | HIS |
| 38 | 2g | 28 | ASN |
| 38 | 2g | 86 | GLN |
| 38 | 2g | 109 | ASN |
| 38 | 2g | 122 | HIS |
| 38 | 2g | 153 | HIS |
| 40 | 2i | 3 | GLN |
| 40 | 2i | 23 | ASN |
| 40 | 2i | 124 | GLN |
| 41 | 2j | 33 | GLN |
| 42 | 2k | 99 | GLN |
| 43 | 2l | 99 | HIS |
| 44 | 2m | 77 | ASN |
| 46 | 2o | 28 | GLN |
| 46 | 2o | 62 | GLN |
| 47 | 2p | 13 | HIS |
| 47 | 2p | 16 | HIS |
| 48 | 2q | 16 | GLN |
| 48 | 2q | 26 | GLN |
| 49 | 2r | 63 | GLN |
| 50 | 2s | 23 | ASN |

### 5.3.3 RNA (i)

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|---|---|---|---|---|
| 1 | 1A | 2864/2915 (98%) | 481 (16%) | 37 (1%) |
| 1 | 2A | 2791/2915 (95%) | 530 (18%) | 25 (0%) |
| 2 | 1B | 120/121 (99%) | 12 (10%) | 1 (0%) |
| 2 | 2B | 118/121 (97%) | 31 (26%) | 0 |
| 32 | 1a | 1497/1521 (98%) | 286 (19%) | 0 |
| 32 | 2a | 1501/1521 (98%) | 262 (17%) | 0 |
| 53 | 1v | 9/24 (37%) | 4 (44%) | 0 |
| 53 | 2v | 4/24 (16%) | 0 | 0 |
| 54 | 1x | 75/77 (97%) | 8 (10%) | 0 |
| 54 | 2x | 75/77 (97%) | 11 (14%) | 0 |
| All | All | 9054/9316 (97%) | 1625 (17%) | 63 (0%) |

All (1625) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 1A | 10 | G |
| 1 | 1A | 12 | U |
| 1 | 1A | 13 | A |
| 1 | 1A | 14 | A |
| 1 | 1A | 15 | 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 | 64 | A |
| 1 | 1A | 71 | A |
| 1 | 1A | 74 | A |
| 1 | 1A | 75 | G |
| 1 | 1A | 84 | A |
| 1 | 1A | 95 | G |
| 1 | 1A | 118 | A |
| 1 | 1A | 119 | A |
| 1 | 1A | 120 | U |
| 1 | 1A | 125 | G |
| 1 | 1A | 131 | G |
| 1 | 1A | 139 | G |
| 1 | 1A | 139(A) | G |
| 1 | 1A | 154 | G |
| 1 | 1A | 181 | A |
| 1 | 1A | 182 | A |
| 1 | 1A | 188 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 1A | 196 | A |
| 1 | 1A | 199 | A |
| 1 | 1A | 205 | G |
| 1 | 1A | 214 | G |
| 1 | 1A | 216 | A |
| 1 | 1A | 222 | A |
| 1 | 1A | 225 | A |
| 1 | 1A | 228 | A |
| 1 | 1A | 229 | A |
| 1 | 1A | 233 | A |
| 1 | 1A | 248 | G |
| 1 | 1A | 250 | G |
| 1 | 1A | 271(L) | U |
| 1 | 1A | 271(M) | G |
| 1 | 1A | 271(N) | U |
| 1 | 1A | 271(R) | G |
| 1 | 1A | 272(B) | G |
| 1 | 1A | 275 | 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 | 363(B) | G |
| 1 | 1A | 363(E) | U |
| 1 | 1A | 363(F) | A |
| 1 | 1A | 370 | G |
| 1 | 1A | 380 | U |
| 1 | 1A | 386 | G |
| 1 | 1A | 389 | G |
| 1 | 1A | 396 | G |
| 1 | 1A | 405 | U |
| 1 | 1A | 411 | G |
| 1 | 1A | 428 | A |
| 1 | 1A | 442 | G |
| 1 | 1A | 444 | C |
| 1 | 1A | 446 | G |
| 1 | 1A | 448 | U |
| 1 | 1A | 457 | A |
| 1 | 1A | 481 | G |
| 1 | 1A | 504 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 1A | 505 | A |
| 1 | 1A | 509 | C |
| 1 | 1A | 512 | G |
| 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 | 555 | U |
| 1 | 1A | 563 | G |
| 1 | 1A | 573 | G |
| 1 | 1A | 574 | C |
| 1 | 1A | 575 | A |
| 1 | 1A | 594 | U |
| 1 | 1A | 603 | A |
| 1 | 1A | 604 | G |
| 1 | 1A | 607 | U |
| 1 | 1A | 614(A) | U |
| 1 | 1A | 614(B) | G |
| 1 | 1A | 615 | G |
| 1 | 1A | 619 | G |
| 1 | 1A | 627 | A |
| 1 | 1A | 637 | A |
| 1 | 1A | 645 | C |
| 1 | 1A | 646 | A |
| 1 | 1A | 652(A) | A |
| 1 | 1A | 652(E) | G |
| 1 | 1A | 652(T) | C |
| 1 | 1A | 669 | G |
| 1 | 1A | 686 | G |
| 1 | 1A | 717 | G |
| 1 | 1A | 726 | G |
| 1 | 1A | 730 | C |
| 1 | 1A | 764 | A |
| 1 | 1A | 775 | G |
| 1 | 1A | 776 | G |
| 1 | 1A | 782 | A |
| 1 | 1A | 784 | A |
| 1 | 1A | 785 | G |
| 1 | 1A | 792 | G |
| 1 | 1A | 802 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 1A | 805 | G |
| 1 | 1A | 812 | C |
| 1 | 1A | 819 | A |
| 1 | 1A | 827 | U |
| 1 | 1A | 828 | U |
| 1 | 1A | 859 | G |
| 1 | 1A | 867 | C |
| 1 | 1A | 880 | G |
| 1 | 1A | 881 | G |
| 1 | 1A | 884 | C |
| 1 | 1A | 885 | C |
| 1 | 1A | 886 | C |
| 1 | 1A | 887 | A |
| 1 | 1A | 888 | C |
| 1 | 1A | 889 | C |
| 1 | 1A | 890 | A |
| 1 | 1A | 896 | A |
| 1 | 1A | 897 | C |
| 1 | 1A | 898 | C |
| 1 | 1A | 907 | U |
| 1 | 1A | 910 | A |
| 1 | 1A | 932 | G |
| 1 | 1A | 938 | 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 | 990 | A |
| 1 | 1A | 996 | A |
| 1 | 1A | 1005 | C |
| 1 | 1A | 1006 | C |
| 1 | 1A | 1008 | C |
| 1 | 1A | 1009 | A |
| 1 | 1A | 1012 | U |
| 1 | 1A | 1013 | C |
| 1 | 1A | 1022 | G |
| 1 | 1A | 1026 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 1A | 1033 | U |
| 1 | 1A | 1038 | C |
| 1 | 1A | 1041 | C |
| 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 | 1066 | U |
| 1 | 1A | 1068 | G |
| 1 | 1A | 1070 | A |
| 1 | 1A | 1071 | G |
| 1 | 1A | 1073 | A |
| 1 | 1A | 1075 | C |
| 1 | 1A | 1076 | C |
| 1 | 1A | 1078 | U |
| 1 | 1A | 1079 | C |
| 1 | 1A | 1082 | U |
| 1 | 1A | 1083 | U |
| 1 | 1A | 1084 | A |
| 1 | 1A | 1086 | A |
| 1 | 1A | 1088 | A |
| 1 | 1A | 1089 | G |
| 1 | 1A | 1090 | U |
| 1 | 1A | 1091 | G |
| 1 | 1A | 1094 | U |
| 1 | 1A | 1096 | A |
| 1 | 1A | 1101 | U |
| 1 | 1A | 1103 | A |
| 1 | 1A | 1106 | G |
| 1 | 1A | 1108 | U |
| 1 | 1A | 1111 | A |
| 1 | 1A | 1112 | G |
| 1 | 1A | 1115 | G |
| 1 | 1A | 1116 | C |
| 1 | 1A | 1128 | A |
| 1 | 1A | 1129 | A |
| 1 | 1A | 1130 | U |
| 1 | 1A | 1132 | A |
| 1 | 1A | 1135 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 1A | 1136 | G |
| 1 | 1A | 1149 | G |
| 1 | 1A | 1155 | A |
| 1 | 1A | 1170 | 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 | 1189 | A |
| 1 | 1A | 1211 | U |
| 1 | 1A | 1218 | C |
| 1 | 1A | 1220 | A |
| 1 | 1A | 1237 | A |
| 1 | 1A | 1244 | G |
| 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 | 1274 | A |
| 1 | 1A | 1289 | C |
| 1 | 1A | 1290 | C |
| 1 | 1A | 1298 | C |
| 1 | 1A | 1300 | U |
| 1 | 1A | 1301 | A |
| 1 | 1A | 1316 | U |
| 1 | 1A | 1352 | U |
| 1 | 1A | 1354 | A |
| 1 | 1A | 1359 | A |
| 1 | 1A | 1360 | A |
| 1 | 1A | 1365 | A |
| 1 | 1A | 1370 | C |
| 1 | 1A | 1372 | U |
| 1 | 1A | 1384 | A |
| 1 | 1A | 1385 | G |
| 1 | 1A | 1396 | U |
| 1 | 1A | 1416 | G |
| 1 | 1A | 1417 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 1A | 1420 | U |
| 1 | 1A | 1421 | G |
| 1 | 1A | 1428 | C |
| 1 | 1A | 1445 | A |
| 1 | 1A | 1450 | G |
| 1 | 1A | 1455 | G |
| 1 | 1A | 1467 | C |
| 1 | 1A | 1482 | G |
| 1 | 1A | 1493 | C |
| 1 | 1A | 1497 | U |
| 1 | 1A | 1504 | C |
| 1 | 1A | 1508 | A |
| 1 | 1A | 1509 | C |
| 1 | 1A | 1509(A) | A |
| 1 | 1A | 1525 | G |
| 1 | 1A | 1541 | G |
| 1 | 1A | 1542 | A |
| 1 | 1A | 1558 | A |
| 1 | 1A | 1566 | A |
| 1 | 1A | 1569 | A |
| 1 | 1A | 1578 | U |
| 1 | 1A | 1580 | A |
| 1 | 1A | 1581 | G |
| 1 | 1A | 1584 | C |
| 1 | 1A | 1586 | A |
| 1 | 1A | 1608 | A |
| 1 | 1A | 1609 | A |
| 1 | 1A | 1616 | A |
| 1 | 1A | 1627 | G |
| 1 | 1A | 1647 | G |
| 1 | 1A | 1648 | C |
| 1 | 1A | 1653 | G |
| 1 | 1A | 1654 | A |
| 1 | 1A | 1656 | C |
| 1 | 1A | 1667 | G |
| 1 | 1A | 1674 | G |
| 1 | 1A | 1675 | C |
| 1 | 1A | 1696 | G |
| 1 | 1A | 1700 | A |
| 1 | 1A | 1701 | A |
| 1 | 1A | 1722 | A |
| 1 | 1A | 1739 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 1A | 1746 | G |
| 1 | 1A | 1756 | G |
| 1 | 1A | 1762 | A |
| 1 | 1A | 1763 | G |
| 1 | 1A | 1764 | G |
| 1 | 1A | 1773 | A |
| 1 | 1A | 1780 | A |
| 1 | 1A | 1782 | C |
| 1 | 1A | 1791 | A |
| 1 | 1A | 1800 | C |
| 1 | 1A | 1801 | G |
| 1 | 1A | 1812 | A |
| 1 | 1A | 1816 | G |
| 1 | 1A | 1817 | G |
| 1 | 1A | 1819 | A |
| 1 | 1A | 1829 | A |
| 1 | 1A | 1847 | A |
| 1 | 1A | 1853 | A |
| 1 | 1A | 1858 | G |
| 1 | 1A | 1861 | G |
| 1 | 1A | 1878 | G |
| 1 | 1A | 1889 | A |
| 1 | 1A | 1900 | A |
| 1 | 1A | 1906 | G |
| 1 | 1A | 1913 | A |
| 1 | 1A | 1915 | 5MU |
| 1 | 1A | 1919 | A |
| 1 | 1A | 1927 | A |
| 1 | 1A | 1929 | G |
| 1 | 1A | 1930 | G |
| 1 | 1A | 1938 | A |
| 1 | 1A | 1955 | U |
| 1 | 1A | 1962 | 5MC |
| 1 | 1A | 1963 | U |
| 1 | 1A | 1964 | G |
| 1 | 1A | 1967 | C |
| 1 | 1A | 1970 | A |
| 1 | 1A | 1971 | A |
| 1 | 1A | 1972 | A |
| 1 | 1A | 1983 | C |
| 1 | 1A | 1993 | U |
| 1 | 1A | 1997 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 1A | 2020 | A |
| 1 | 1A | 2023 | G |
| 1 | 1A | 2031 | A |
| 1 | 1A | 2032 | G |
| 1 | 1A | 2033 | A |
| 1 | 1A | 2043 | C |
| 1 | 1A | 2055 | C |
| 1 | 1A | 2056 | G |
| 1 | 1A | 2060 | A |
| 1 | 1A | 2061 | G |
| 1 | 1A | 2062 | A |
| 1 | 1A | 2069 | G |
| 1 | 1A | 2092 | U |
| 1 | 1A | 2097 | C |
| 1 | 1A | 2101 | G |
| 1 | 1A | 2104 | G |
| 1 | 1A | 2111 | C |
| 1 | 1A | 2113 | U |
| 1 | 1A | 2116 | G |
| 1 | 1A | 2123 | 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 | 2141 | G |
| 1 | 1A | 2142 | C |
| 1 | 1A | 2144 | U |
| 1 | 1A | 2146 | C |
| 1 | 1A | 2147 | G |
| 1 | 1A | 2150 | U |
| 1 | 1A | 2151 | G |
| 1 | 1A | 2156 | G |
| 1 | 1A | 2157 | G |
| 1 | 1A | 2158 | A |
| 1 | 1A | 2159 | G |
| 1 | 1A | 2162 | G |
| 1 | 1A | 2165 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 1A | 2166 | G |
| 1 | 1A | 2171 | A |
| 1 | 1A | 2172 | U |
| 1 | 1A | 2173 | A |
| 1 | 1A | 2175 | C |
| 1 | 1A | 2181 | G |
| 1 | 1A | 2182 | G |
| 1 | 1A | 2183 | C |
| 1 | 1A | 2184 | G |
| 1 | 1A | 2189 | U |
| 1 | 1A | 2192 | G |
| 1 | 1A | 2198 | A |
| 1 | 1A | 2206 | G |
| 1 | 1A | 2207 | G |
| 1 | 1A | 2208 | A |
| 1 | 1A | 2218 | U |
| 1 | 1A | 2219 | G |
| 1 | 1A | 2225 | A |
| 1 | 1A | 2238 | G |
| 1 | 1A | 2239 | G |
| 1 | 1A | 2242 | G |
| 1 | 1A | 2249 | U |
| 1 | 1A | 2268 | A |
| 1 | 1A | 2269 | A |
| 1 | 1A | 2273 | A |
| 1 | 1A | 2282 | G |
| 1 | 1A | 2283 | C |
| 1 | 1A | 2286 | A |
| 1 | 1A | 2287 | A |
| 1 | 1A | 2289 | G |
| 1 | 1A | 2305 | A |
| 1 | 1A | 2307 | G |
| 1 | 1A | 2308 | G |
| 1 | 1A | 2320 | A |
| 1 | 1A | 2325 | G |
| 1 | 1A | 2334 | G |
| 1 | 1A | 2336 | A |
| 1 | 1A | 2347 | C |
| 1 | 1A | 2350 | C |
| 1 | 1A | 2354 | G |
| 1 | 1A | 2361 | A |
| 1 | 1A | 2372 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 1A | 2379 | G |
| 1 | 1A | 2383 | G |
| 1 | 1A | 2385 | C |
| 1 | 1A | 2396 | G |
| 1 | 1A | 2405 | G |
| 1 | 1A | 2406 | U |
| 1 | 1A | 2407 | G |
| 1 | 1A | 2410 | G |
| 1 | 1A | 2422 | A |
| 1 | 1A | 2425 | A |
| 1 | 1A | 2429 | G |
| 1 | 1A | 2430 | A |
| 1 | 1A | 2431 | U |
| 1 | 1A | 2435 | A |
| 1 | 1A | 2438 | U |
| 1 | 1A | 2439 | A |
| 1 | 1A | 2441 | C |
| 1 | 1A | 2448 | A |
| 1 | 1A | 2468 | G |
| 1 | 1A | 2476 | A |
| 1 | 1A | 2477 | C |
| 1 | 1A | 2481 | G |
| 1 | 1A | 2487 | G |
| 1 | 1A | 2490 | G |
| 1 | 1A | 2502 | G |
| 1 | 1A | 2505 | G |
| 1 | 1A | 2506 | U |
| 1 | 1A | 2507 | C |
| 1 | 1A | 2518 | A |
| 1 | 1A | 2525 | G |
| 1 | 1A | 2529 | G |
| 1 | 1A | 2554 | U |
| 1 | 1A | 2566 | A |
| 1 | 1A | 2567 | G |
| 1 | 1A | 2573 | C |
| 1 | 1A | 2579 | C |
| 1 | 1A | 2582 | G |
| 1 | 1A | 2585 | U |
| 1 | 1A | 2602 | A |
| 1 | 1A | 2609 | U |
| 1 | 1A | 2611 | U |
| 1 | 1A | 2612 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 1A | 2629 | A |
| 1 | 1A | 2630 | G |
| 1 | 1A | 2638 | G |
| 1 | 1A | 2654 | A |
| 1 | 1A | 2689 | U |
| 1 | 1A | 2690 | 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 | 2758 | A |
| 1 | 1A | 2764 | A |
| 1 | 1A | 2765 | A |
| 1 | 1A | 2778 | A |
| 1 | 1A | 2780 | G |
| 1 | 1A | 2790 | A |
| 1 | 1A | 2791 | C |
| 1 | 1A | 2802 | G |
| 1 | 1A | 2805 | G |
| 1 | 1A | 2818 | G |
| 1 | 1A | 2820 | A |
| 1 | 1A | 2821 | A |
| 1 | 1A | 2835 | A |
| 1 | 1A | 2839 | G |
| 1 | 1A | 2855 | C |
| 1 | 1A | 2861 | G |
| 1 | 1A | 2872 | G |
| 1 | 1A | 2880 | C |
| 1 | 1A | 2892 | A |
| 1 | 1A | 2894 | G |
| 2 | 1B | 2 | C |
| 2 | 1B | 13 | A |
| 2 | 1B | 15 | A |
| 2 | 1B | 35 | U |
| 2 | 1B | 50 | G |
| 2 | 1B | 52 | A |
| 2 | 1B | 56 | G |
| 2 | 1B | 73 | A |
| 2 | 1B | 85 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | 1B | 91 | C |
| 2 | 1B | 106 | G |
| 2 | 1B | 110 | G |
| 32 | 1a | 9 | G |
| 32 | 1a | 26 | A |
| 32 | 1a | 31 | G |
| 32 | 1a | 32 | A |
| 32 | 1a | 39 | G |
| 32 | 1a | 44 | G |
| 32 | 1a | 48 | C |
| 32 | 1a | 50 | A |
| 32 | 1a | 51 | A |
| 32 | 1a | 61 | G |
| 32 | 1a | 78 | G |
| 32 | 1a | 79 | G |
| 32 | 1a | 91 | C |
| 32 | 1a | 98 | G |
| 32 | 1a | 101 | A |
| 32 | 1a | 105 | G |
| 32 | 1a | 116 | A |
| 32 | 1a | 121 | C |
| 32 | 1a | 129(A) | G |
| 32 | 1a | 131 | C |
| 32 | 1a | 151 | A |
| 32 | 1a | 162 | A |
| 32 | 1a | 163 | C |
| 32 | 1a | 164 | U |
| 32 | 1a | 174 | C |
| 32 | 1a | 176 | C |
| 32 | 1a | 182 | U |
| 32 | 1a | 189(F) | U |
| 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 | 247 | G |
| 32 | 1a | 251 | G |
| 32 | 1a | 258 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 32 | 1a | 266 | G |
| 32 | 1a | 267 | C |
| 32 | 1a | 279 | A |
| 32 | 1a | 289 | G |
| 32 | 1a | 316 | G |
| 32 | 1a | 321 | A |
| 32 | 1a | 327 | A |
| 32 | 1a | 328 | C |
| 32 | 1a | 330 | C |
| 32 | 1a | 332 | G |
| 32 | 1a | 345 | C |
| 32 | 1a | 348 | G |
| 32 | 1a | 352 | C |
| 32 | 1a | 353 | A |
| 32 | 1a | 354 | G |
| 32 | 1a | 358 | U |
| 32 | 1a | 359 | U |
| 32 | 1a | 363 | A |
| 32 | 1a | 367 | U |
| 32 | 1a | 372 | C |
| 32 | 1a | 373 | A |
| 32 | 1a | 378 | G |
| 32 | 1a | 382 | A |
| 32 | 1a | 384 | G |
| 32 | 1a | 397 | A |
| 32 | 1a | 398 | C |
| 32 | 1a | 406 | G |
| 32 | 1a | 412 | A |
| 32 | 1a | 414 | A |
| 32 | 1a | 415 | A |
| 32 | 1a | 421 | U |
| 32 | 1a | 423 | G |
| 32 | 1a | 424 | G |
| 32 | 1a | 429 | U |
| 32 | 1a | 430 | A |
| 32 | 1a | 433 | C |
| 32 | 1a | 437 | U |
| 32 | 1a | 438 | G |
| 32 | 1a | 439 | A |
| 32 | 1a | 442 | C |
| 32 | 1a | 451 | A |
| 32 | 1a | 452 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 32 | 1a | 457 | C |
| 32 | 1a | 461 | A |
| 32 | 1a | 470 | C |
| 32 | 1a | 471 | G |
| 32 | 1a | 474 | G |
| 32 | 1a | 480 | U |
| 32 | 1a | 485 | G |
| 32 | 1a | 496 | A |
| 32 | 1a | 498 | U |
| 32 | 1a | 505 | G |
| 32 | 1a | 506 | G |
| 32 | 1a | 509 | A |
| 32 | 1a | 510 | A |
| 32 | 1a | 511 | C |
| 32 | 1a | 518 | C |
| 32 | 1a | 519 | C |
| 32 | 1a | 531 | U |
| 32 | 1a | 532 | A |
| 32 | 1a | 533 | A |
| 32 | 1a | 534 | U |
| 32 | 1a | 536 | C |
| 32 | 1a | 547 | A |
| 32 | 1a | 559 | A |
| 32 | 1a | 560 | U |
| 32 | 1a | 561 | U |
| 32 | 1a | 562 | C |
| 32 | 1a | 568 | G |
| 32 | 1a | 572 | A |
| 32 | 1a | 573 | A |
| 32 | 1a | 574 | A |
| 32 | 1a | 576 | G |
| 32 | 1a | 577 | G |
| 32 | 1a | 596 | C |
| 32 | 1a | 607 | A |
| 32 | 1a | 618 | C |
| 32 | 1a | 630 | G |
| 32 | 1a | 633 | G |
| 32 | 1a | 653 | A |
| 32 | 1a | 657 | G |
| 32 | 1a | 659 | U |
| 32 | 1a | 665 | A |
| 32 | 1a | 671 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 32 | 1a | 684 | A |
| 32 | 1a | 686 | U |
| 32 | 1a | 687 | A |
| 32 | 1a | 688 | G |
| 32 | 1a | 693 | G |
| 32 | 1a | 695 | A |
| 32 | 1a | 723 | U |
| 32 | 1a | 724 | G |
| 32 | 1a | 731 | G |
| 32 | 1a | 749 | C |
| 32 | 1a | 755 | G |
| 32 | 1a | 759 | A |
| 32 | 1a | 766 | A |
| 32 | 1a | 773 | G |
| 32 | 1a | 774 | G |
| 32 | 1a | 777 | A |
| 32 | 1a | 792 | A |
| 32 | 1a | 793 | U |
| 32 | 1a | 794 | A |
| 32 | 1a | 810 | C |
| 32 | 1a | 815 | A |
| 32 | 1a | 817 | C |
| 32 | 1a | 821 | G |
| 32 | 1a | 828 | A |
| 32 | 1a | 832 | C |
| 32 | 1a | 836 | G |
| 32 | 1a | 840 | C |
| 32 | 1a | 841 | U |
| 32 | 1a | 851 | G |
| 32 | 1a | 855 | G |
| 32 | 1a | 859 | A |
| 32 | 1a | 870 | U |
| 32 | 1a | 873 | A |
| 32 | 1a | 902 | G |
| 32 | 1a | 914 | A |
| 32 | 1a | 926 | G |
| 32 | 1a | 927 | G |
| 32 | 1a | 934 | C |
| 32 | 1a | 935 | A |
| 32 | 1a | 936 | C |
| 32 | 1a | 960 | U |
| 32 | 1a | 961 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 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 | 994 | A |
| 32 | 1a | 997 | U |
| 32 | 1a | 998 | G |
| 32 | 1a | 999 | C |
| 32 | 1a | 1000 | U |
| 32 | 1a | 1003 | G |
| 32 | 1a | 1005 | A |
| 32 | 1a | 1006 | C |
| 32 | 1a | 1009 | G |
| 32 | 1a | 1011 | G |
| 32 | 1a | 1020 | U |
| 32 | 1a | 1022 | G |
| 32 | 1a | 1023 | G |
| 32 | 1a | 1025 | U |
| 32 | 1a | 1026 | G |
| 32 | 1a | 1027 | C |
| 32 | 1a | 1028 | C |
| 32 | 1a | 1030 | C |
| 32 | 1a | 1030(A) | G |
| 32 | 1a | 1030(C) | G |
| 32 | 1a | 1031 | G |
| 32 | 1a | 1035 | A |
| 32 | 1a | 1039 | C |
| 32 | 1a | 1043 | C |
| 32 | 1a | 1044 | A |
| 32 | 1a | 1045 | C |
| 32 | 1a | 1050 | G |
| 32 | 1a | 1054 | C |
| 32 | 1a | 1056 | U |
| 32 | 1a | 1065 | U |
| 32 | 1a | 1066 | C |
| 32 | 1a | 1068 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 32 | 1a | 1081 | G |
| 32 | 1a | 1086 | U |
| 32 | 1a | 1094 | G |
| 32 | 1a | 1095 | U |
| 32 | 1a | 1096 | C |
| 32 | 1a | 1101 | A |
| 32 | 1a | 1121 | U |
| 32 | 1a | 1122 | U |
| 32 | 1a | 1124 | G |
| 32 | 1a | 1125 | U |
| 32 | 1a | 1134 | G |
| 32 | 1a | 1137 | C |
| 32 | 1a | 1138 | G |
| 32 | 1a | 1139 | G |
| 32 | 1a | 1141 | C |
| 32 | 1a | 1146 | A |
| 32 | 1a | 1152 | A |
| 32 | 1a | 1154 | G |
| 32 | 1a | 1157 | A |
| 32 | 1a | 1159 | U |
| 32 | 1a | 1183 | A |
| 32 | 1a | 1184 | G |
| 32 | 1a | 1196 | U |
| 32 | 1a | 1197 | G |
| 32 | 1a | 1202 | G |
| 32 | 1a | 1212 | U |
| 32 | 1a | 1213 | A |
| 32 | 1a | 1214 | C |
| 32 | 1a | 1222 | G |
| 32 | 1a | 1227 | A |
| 32 | 1a | 1233 | G |
| 32 | 1a | 1236 | A |
| 32 | 1a | 1238 | A |
| 32 | 1a | 1256 | A |
| 32 | 1a | 1257 | U |
| 32 | 1a | 1258 | G |
| 32 | 1a | 1260 | C |
| 32 | 1a | 1270 | C |
| 32 | 1a | 1275 | A |
| 32 | 1a | 1278 | U |
| 32 | 1a | 1279 | A |
| 32 | 1a | 1280 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 32 | 1a | 1286 | A |
| 32 | 1a | 1287 | A |
| 32 | 1a | 1299 | A |
| 32 | 1a | 1300 | G |
| 32 | 1a | 1302 | U |
| 32 | 1a | 1312 | G |
| 32 | 1a | 1320 | C |
| 32 | 1a | 1323 | G |
| 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 | 1379 | G |
| 32 | 1a | 1394 | A |
| 32 | 1a | 1396 | A |
| 32 | 1a | 1397 | C |
| 32 | 1a | 1403 | C |
| 32 | 1a | 1419 | G |
| 32 | 1a | 1442 | G |
| 32 | 1a | 1442(A) | G |
| 32 | 1a | 1446 | U |
| 32 | 1a | 1447 | A |
| 32 | 1a | 1487 | G |
| 32 | 1a | 1492 | A |
| 32 | 1a | 1494 | G |
| 32 | 1a | 1503 | A |
| 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 | 14 | A |
| 53 | 1v | 15 | A |
| 53 | 1v | 19 | U |
| 53 | 1v | 21 | C |
| 54 | 1x | 9 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 54 | 1x | 14 | A |
| 54 | 1x | 18 | G |
| 54 | 1x | 19 | G |
| 54 | 1x | 21 | A |
| 54 | 1x | 32 | 5MC |
| 54 | 1x | 47 | U |
| 54 | 1x | 76 | A |
| 1 | 2A | 8 | A |
| 1 | 2A | 10 | G |
| 1 | 2A | 14 | A |
| 1 | 2A | 15 | G |
| 1 | 2A | 34 | C |
| 1 | 2A | 35 | G |
| 1 | 2A | 45 | C |
| 1 | 2A | 61 | G |
| 1 | 2A | 64 | A |
| 1 | 2A | 71 | A |
| 1 | 2A | 72 | U |
| 1 | 2A | 74 | A |
| 1 | 2A | 75 | G |
| 1 | 2A | 84 | A |
| 1 | 2A | 90 | U |
| 1 | 2A | 94 | C |
| 1 | 2A | 100 | G |
| 1 | 2A | 102 | G |
| 1 | 2A | 118 | A |
| 1 | 2A | 119 | A |
| 1 | 2A | 120 | U |
| 1 | 2A | 121 | G |
| 1 | 2A | 125 | G |
| 1 | 2A | 126 | A |
| 1 | 2A | 131 | G |
| 1 | 2A | 141 | A |
| 1 | 2A | 154(A) | C |
| 1 | 2A | 157 | U |
| 1 | 2A | 181 | A |
| 1 | 2A | 196 | A |
| 1 | 2A | 199 | A |
| 1 | 2A | 205 | G |
| 1 | 2A | 214 | G |
| 1 | 2A | 216 | A |
| 1 | 2A | 221 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 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 | 250 | 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 | 274 | G |
| 1 | 2A | 277 | C |
| 1 | 2A | 278 | A |
| 1 | 2A | 279 | C |
| 1 | 2A | 280 | C |
| 1 | 2A | 294 | A |
| 1 | 2A | 303 | U |
| 1 | 2A | 311 | A |
| 1 | 2A | 317 | G |
| 1 | 2A | 324 | A |
| 1 | 2A | 327 | G |
| 1 | 2A | 329 | G |
| 1 | 2A | 330 | A |
| 1 | 2A | 333 | 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 | 372 | G |
| 1 | 2A | 386 | G |
| 1 | 2A | 396 | G |
| 1 | 2A | 399 | G |
| 1 | 2A | 405 | U |
| 1 | 2A | 407 | G |
| 1 | 2A | 411 | G |
| 1 | 2A | 421 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 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 | 474 | G |
| 1 | 2A | 479 | A |
| 1 | 2A | 481 | G |
| 1 | 2A | 496 | G |
| 1 | 2A | 499 | U |
| 1 | 2A | 504 | U |
| 1 | 2A | 505 | A |
| 1 | 2A | 509 | C |
| 1 | 2A | 519 | U |
| 1 | 2A | 529 | A |
| 1 | 2A | 530 | G |
| 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 | 575 | A |
| 1 | 2A | 588 | U |
| 1 | 2A | 595 | C |
| 1 | 2A | 599 | G |
| 1 | 2A | 603 | A |
| 1 | 2A | 604 | G |
| 1 | 2A | 607 | U |
| 1 | 2A | 609 | A |
| 1 | 2A | 614(A) | U |
| 1 | 2A | 614(B) | G |
| 1 | 2A | 614(C) | A |
| 1 | 2A | 615 | G |
| 1 | 2A | 620 | G |
| 1 | 2A | 627 | A |
| 1 | 2A | 637 | A |
| 1 | 2A | 645 | C |
| 1 | 2A | 652(B) | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 2A | 669 | G |
| 1 | 2A | 686 | G |
| 1 | 2A | 709 | U |
| 1 | 2A | 717 | G |
| 1 | 2A | 718 | A |
| 1 | 2A | 726 | G |
| 1 | 2A | 730 | C |
| 1 | 2A | 752 | A |
| 1 | 2A | 753 | C |
| 1 | 2A | 771 | G |
| 1 | 2A | 775 | G |
| 1 | 2A | 776 | G |
| 1 | 2A | 779 | U |
| 1 | 2A | 782 | A |
| 1 | 2A | 783 | A |
| 1 | 2A | 784 | A |
| 1 | 2A | 785 | G |
| 1 | 2A | 790 | C |
| 1 | 2A | 791 | C |
| 1 | 2A | 792 | G |
| 1 | 2A | 805 | G |
| 1 | 2A | 812 | C |
| 1 | 2A | 819 | A |
| 1 | 2A | 825 | C |
| 1 | 2A | 827 | U |
| 1 | 2A | 828 | U |
| 1 | 2A | 832 | G |
| 1 | 2A | 847 | U |
| 1 | 2A | 857 | C |
| 1 | 2A | 859 | G |
| 1 | 2A | 869 | G |
| 1 | 2A | 870 | A |
| 1 | 2A | 874 | 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 |
| 1 | 2A | 892 | G |
| 1 | 2A | 893 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 2A | 894 | C |
| 1 | 2A | 895 | U |
| 1 | 2A | 896 | A |
| 1 | 2A | 900 | A |
| 1 | 2A | 901 | A |
| 1 | 2A | 904 | C |
| 1 | 2A | 910 | A |
| 1 | 2A | 914 | C |
| 1 | 2A | 917 | A |
| 1 | 2A | 932 | G |
| 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 | 983 | A |
| 1 | 2A | 996 | A |
| 1 | 2A | 997 | G |
| 1 | 2A | 998 | C |
| 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 | 1033 | U |
| 1 | 2A | 1038 | C |
| 1 | 2A | 1039 | G |
| 1 | 2A | 1043 | C |
| 1 | 2A | 1116 | C |
| 1 | 2A | 1117 | G |
| 1 | 2A | 1126 | A |
| 1 | 2A | 1130 | U |
| 1 | 2A | 1135 | C |
| 1 | 2A | 1136 | G |
| 1 | 2A | 1139 | G |
| 1 | 2A | 1143 | A |
| 1 | 2A | 1155 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 2A | 1159 | U |
| 1 | 2A | 1171 | G |
| 1 | 2A | 1188 | U |
| 1 | 2A | 1195 | G |
| 1 | 2A | 1204 | A |
| 1 | 2A | 1211 | U |
| 1 | 2A | 1220 | A |
| 1 | 2A | 1229 | G |
| 1 | 2A | 1236 | G |
| 1 | 2A | 1237 | A |
| 1 | 2A | 1247 | A |
| 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 | 1300 | U |
| 1 | 2A | 1301 | A |
| 1 | 2A | 1303 | G |
| 1 | 2A | 1314 | C |
| 1 | 2A | 1318 | C |
| 1 | 2A | 1352 | U |
| 1 | 2A | 1359 | A |
| 1 | 2A | 1360 | A |
| 1 | 2A | 1365 | A |
| 1 | 2A | 1368 | G |
| 1 | 2A | 1370 | C |
| 1 | 2A | 1380 | G |
| 1 | 2A | 1384 | A |
| 1 | 2A | 1385 | G |
| 1 | 2A | 1386 | C |
| 1 | 2A | 1395 | A |
| 1 | 2A | 1400 | G |
| 1 | 2A | 1416 | G |
| 1 | 2A | 1417 | C |
| 1 | 2A | 1420 | U |
| 1 | 2A | 1421 | G |
| 1 | 2A | 1427 | A |
| 1 | 2A | 1428 | C |
| 1 | 2A | 1437 | C |
| 1 | 2A | 1445 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 2A | 1445(A) | C |
| 1 | 2A | 1449 | A |
| 1 | 2A | 1450 | G |
| 1 | 2A | 1455 | G |
| 1 | 2A | 1460 | A |
| 1 | 2A | 1461 | G |
| 1 | 2A | 1467 | C |
| 1 | 2A | 1471 | A |
| 1 | 2A | 1482 | G |
| 1 | 2A | 1493 | C |
| 1 | 2A | 1495 | A |
| 1 | 2A | 1497 | U |
| 1 | 2A | 1508 | A |
| 1 | 2A | 1509 | C |
| 1 | 2A | 1509(A) | A |
| 1 | 2A | 1531 | C |
| 1 | 2A | 1532 | C |
| 1 | 2A | 1533 | G |
| 1 | 2A | 1541 | G |
| 1 | 2A | 1543 | C |
| 1 | 2A | 1558 | A |
| 1 | 2A | 1559 | G |
| 1 | 2A | 1566 | A |
| 1 | 2A | 1569 | A |
| 1 | 2A | 1578 | U |
| 1 | 2A | 1580 | A |
| 1 | 2A | 1584 | C |
| 1 | 2A | 1586 | A |
| 1 | 2A | 1589 | C |
| 1 | 2A | 1595 | G |
| 1 | 2A | 1603 | A |
| 1 | 2A | 1608 | A |
| 1 | 2A | 1609 | A |
| 1 | 2A | 1610 | A |
| 1 | 2A | 1613 | G |
| 1 | 2A | 1616 | A |
| 1 | 2A | 1640 | C |
| 1 | 2A | 1647 | G |
| 1 | 2A | 1648 | C |
| 1 | 2A | 1654 | A |
| 1 | 2A | 1664 | A |
| 1 | 2A | 1672 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 2A | 1674 | G |
| 1 | 2A | 1675 | C |
| 1 | 2A | 1696 | G |
| 1 | 2A | 1700 | A |
| 1 | 2A | 1701 | A |
| 1 | 2A | 1708 | C |
| 1 | 2A | 1722 | A |
| 1 | 2A | 1739 | U |
| 1 | 2A | 1740 | G |
| 1 | 2A | 1745(A) | C |
| 1 | 2A | 1746 | G |
| 1 | 2A | 1748 | G |
| 1 | 2A | 1756 | 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 | 1828 | G |
| 1 | 2A | 1829 | A |
| 1 | 2A | 1835 | G |
| 1 | 2A | 1836 | C |
| 1 | 2A | 1847 | A |
| 1 | 2A | 1857 | G |
| 1 | 2A | 1877 | A |
| 1 | 2A | 1878 | G |
| 1 | 2A | 1885 | A |
| 1 | 2A | 1900 | A |
| 1 | 2A | 1906 | G |
| 1 | 2A | 1910 | G |
| 1 | 2A | 1913 | A |
| 1 | 2A | 1914 | C |
| 1 | 2A | 1915 | 5MU |
| 1 | 2A | 1929 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 2A | 1930 | G |
| 1 | 2A | 1931 | U |
| 1 | 2A | 1936 | A |
| 1 | 2A | 1937 | A |
| 1 | 2A | 1938 | A |
| 1 | 2A | 1955 | U |
| 1 | 2A | 1963 | U |
| 1 | 2A | 1964 | G |
| 1 | 2A | 1967 | C |
| 1 | 2A | 1970 | A |
| 1 | 2A | 1971 | A |
| 1 | 2A | 1972 | A |
| 1 | 2A | 1993 | U |
| 1 | 2A | 1997 | G |
| 1 | 2A | 2020 | A |
| 1 | 2A | 2023 | G |
| 1 | 2A | 2031 | A |
| 1 | 2A | 2032 | G |
| 1 | 2A | 2033 | A |
| 1 | 2A | 2036 | C |
| 1 | 2A | 2043 | C |
| 1 | 2A | 2055 | C |
| 1 | 2A | 2056 | G |
| 1 | 2A | 2060 | A |
| 1 | 2A | 2061 | G |
| 1 | 2A | 2062 | A |
| 1 | 2A | 2069 | G |
| 1 | 2A | 2093 | G |
| 1 | 2A | 2098 | U |
| 1 | 2A | 2104 | G |
| 1 | 2A | 2108 | C |
| 1 | 2A | 2110 | G |
| 1 | 2A | 2111 | C |
| 1 | 2A | 2112 | G |
| 1 | 2A | 2116 | G |
| 1 | 2A | 2117 | A |
| 1 | 2A | 2119 | A |
| 1 | 2A | 2120 | G |
| 1 | 2A | 2122 | U |
| 1 | 2A | 2126 | A |
| 1 | 2A | 2127 | G |
| 1 | 2A | 2129 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 2A | 2131 | G |
| 1 | 2A | 2132 | U |
| 1 | 2A | 2133 | G |
| 1 | 2A | 2134 | A |
| 1 | 2A | 2135 | A |
| 1 | 2A | 2136 | C |
| 1 | 2A | 2137 | C |
| 1 | 2A | 2138 | C |
| 1 | 2A | 2140 | C |
| 1 | 2A | 2142 | C |
| 1 | 2A | 2143 | C |
| 1 | 2A | 2146 | C |
| 1 | 2A | 2150 | U |
| 1 | 2A | 2151 | G |
| 1 | 2A | 2153 | G |
| 1 | 2A | 2154 | G |
| 1 | 2A | 2155 | G |
| 1 | 2A | 2156 | G |
| 1 | 2A | 2157 | G |
| 1 | 2A | 2158 | A |
| 1 | 2A | 2160 | G |
| 1 | 2A | 2161 | C |
| 1 | 2A | 2162 | G |
| 1 | 2A | 2164 | C |
| 1 | 2A | 2166 | G |
| 1 | 2A | 2167 | U |
| 1 | 2A | 2168 | G |
| 1 | 2A | 2171 | A |
| 1 | 2A | 2172 | U |
| 1 | 2A | 2177 | C |
| 1 | 2A | 2178 | C |
| 1 | 2A | 2181 | G |
| 1 | 2A | 2182 | G |
| 1 | 2A | 2185 | C |
| 1 | 2A | 2186 | G |
| 1 | 2A | 2189 | U |
| 1 | 2A | 2190 | G |
| 1 | 2A | 2192 | G |
| 1 | 2A | 2197 | U |
| 1 | 2A | 2198 | A |
| 1 | 2A | 2200 | C |
| 1 | 2A | 2206 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 2A | 2207 | G |
| 1 | 2A | 2208 | A |
| 1 | 2A | 2218 | U |
| 1 | 2A | 2225 | A |
| 1 | 2A | 2235 | G |
| 1 | 2A | 2238 | G |
| 1 | 2A | 2239 | G |
| 1 | 2A | 2275 | C |
| 1 | 2A | 2278 | A |
| 1 | 2A | 2279 | G |
| 1 | 2A | 2283 | C |
| 1 | 2A | 2287 | A |
| 1 | 2A | 2288 | A |
| 1 | 2A | 2294 | C |
| 1 | 2A | 2305 | A |
| 1 | 2A | 2308 | G |
| 1 | 2A | 2312 | U |
| 1 | 2A | 2319 | G |
| 1 | 2A | 2320 | A |
| 1 | 2A | 2325 | G |
| 1 | 2A | 2334 | G |
| 1 | 2A | 2336 | A |
| 1 | 2A | 2347 | C |
| 1 | 2A | 2350 | C |
| 1 | 2A | 2372 | G |
| 1 | 2A | 2376 | A |
| 1 | 2A | 2377 | A |
| 1 | 2A | 2383 | G |
| 1 | 2A | 2385 | C |
| 1 | 2A | 2391 | G |
| 1 | 2A | 2403 | C |
| 1 | 2A | 2406 | U |
| 1 | 2A | 2410 | G |
| 1 | 2A | 2414 | G |
| 1 | 2A | 2422 | A |
| 1 | 2A | 2425 | A |
| 1 | 2A | 2428 | G |
| 1 | 2A | 2429 | G |
| 1 | 2A | 2430 | A |
| 1 | 2A | 2435 | A |
| 1 | 2A | 2439 | A |
| 1 | 2A | 2441 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 2A | 2448 | A |
| 1 | 2A | 2458 | G |
| 1 | 2A | 2465 | C |
| 1 | 2A | 2468 | G |
| 1 | 2A | 2469 | A |
| 1 | 2A | 2474 | C |
| 1 | 2A | 2476 | A |
| 1 | 2A | 2477 | C |
| 1 | 2A | 2480 | C |
| 1 | 2A | 2486 | G |
| 1 | 2A | 2487 | G |
| 1 | 2A | 2490 | G |
| 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 | 2525 | G |
| 1 | 2A | 2529 | G |
| 1 | 2A | 2543 | G |
| 1 | 2A | 2554 | U |
| 1 | 2A | 2555 | U |
| 1 | 2A | 2566 | A |
| 1 | 2A | 2567 | G |
| 1 | 2A | 2569 | G |
| 1 | 2A | 2574 | G |
| 1 | 2A | 2585 | U |
| 1 | 2A | 2592 | G |
| 1 | 2A | 2601 | C |
| 1 | 2A | 2602 | A |
| 1 | 2A | 2608 | G |
| 1 | 2A | 2609 | U |
| 1 | 2A | 2611 | U |
| 1 | 2A | 2612 | C |
| 1 | 2A | 2620 | C |
| 1 | 2A | 2630 | G |
| 1 | 2A | 2634 | G |
| 1 | 2A | 2654 | A |
| 1 | 2A | 2679 | A |
| 1 | 2A | 2689 | U |
| 1 | 2A | 2690 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 2A | 2702 | U |
| 1 | 2A | 2703 | 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 | 2757 | A |
| 1 | 2A | 2758 | A |
| 1 | 2A | 2759 | G |
| 1 | 2A | 2761 | G |
| 1 | 2A | 2764 | A |
| 1 | 2A | 2765 | A |
| 1 | 2A | 2766 | G |
| 1 | 2A | 2778 | A |
| 1 | 2A | 2789 | C |
| 1 | 2A | 2793 | G |
| 1 | 2A | 2802 | G |
| 1 | 2A | 2803 | C |
| 1 | 2A | 2808 | U |
| 1 | 2A | 2818 | G |
| 1 | 2A | 2820 | A |
| 1 | 2A | 2821 | A |
| 1 | 2A | 2833 | G |
| 1 | 2A | 2835 | A |
| 1 | 2A | 2872 | G |
| 1 | 2A | 2873 | A |
| 1 | 2A | 2880 | C |
| 1 | 2A | 2894 | G |
| 1 | 2A | 2895 | U |
| 1 | 2A | 2897 | U |
| 2 | 2B | 2 | C |
| 2 | 2B | 5 | C |
| 2 | 2B | 8 | U |
| 2 | 2B | 19 | G |
| 2 | 2B | 20 | C |
| 2 | 2B | 25 | A |
| 2 | 2B | 30 | C |
| 2 | 2B | 41 | U |
| 2 | 2B | 42 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | 2B | 52 | A |
| 2 | 2B | 53 | A |
| 2 | 2B | 56 | G |
| 2 | 2B | 63 | G |
| 2 | 2B | 67 | G |
| 2 | 2B | 73 | A |
| 2 | 2B | 74 | U |
| 2 | 2B | 75 | G |
| 2 | 2B | 85 | G |
| 2 | 2B | 88 | C |
| 2 | 2B | 89 | G |
| 2 | 2B | 91 | C |
| 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 | 117 | G |
| 2 | 2B | 119 | G |
| 2 | 2B | 120 | A |
| 32 | 2a | 9 | G |
| 32 | 2a | 16 | A |
| 32 | 2a | 22 | G |
| 32 | 2a | 32 | A |
| 32 | 2a | 39 | G |
| 32 | 2a | 41 | G |
| 32 | 2a | 47 | C |
| 32 | 2a | 48 | C |
| 32 | 2a | 50 | A |
| 32 | 2a | 51 | A |
| 32 | 2a | 59 | A |
| 32 | 2a | 65 | U |
| 32 | 2a | 66 | G |
| 32 | 2a | 73 | G |
| 32 | 2a | 88 | A |
| 32 | 2a | 89 | C |
| 32 | 2a | 90 | U |
| 32 | 2a | 92 | C |
| 32 | 2a | 98 | G |
| 32 | 2a | 101 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 32 | 2a | 115 | G |
| 32 | 2a | 116 | A |
| 32 | 2a | 121 | C |
| 32 | 2a | 129(A) | G |
| 32 | 2a | 131 | C |
| 32 | 2a | 159 | G |
| 32 | 2a | 163 | C |
| 32 | 2a | 174 | C |
| 32 | 2a | 182 | U |
| 32 | 2a | 189 | G |
| 32 | 2a | 189(A) | C |
| 32 | 2a | 189(E) | 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 | 266 | G |
| 32 | 2a | 267 | C |
| 32 | 2a | 289 | G |
| 32 | 2a | 306 | G |
| 32 | 2a | 321 | A |
| 32 | 2a | 328 | C |
| 32 | 2a | 332 | G |
| 32 | 2a | 351 | G |
| 32 | 2a | 352 | C |
| 32 | 2a | 353 | A |
| 32 | 2a | 354 | G |
| 32 | 2a | 367 | U |
| 32 | 2a | 372 | C |
| 32 | 2a | 397 | A |
| 32 | 2a | 398 | C |
| 32 | 2a | 406 | G |
| 32 | 2a | 412 | A |
| 32 | 2a | 413 | G |
| 32 | 2a | 424 | G |
| 32 | 2a | 429 | U |
| 32 | 2a | 430 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 32 | 2a | 439 | A |
| 32 | 2a | 442 | C |
| 32 | 2a | 452 | A |
| 32 | 2a | 461 | A |
| 32 | 2a | 470 | C |
| 32 | 2a | 482 | A |
| 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 | 518 | C |
| 32 | 2a | 521 | G |
| 32 | 2a | 531 | U |
| 32 | 2a | 532 | A |
| 32 | 2a | 533 | A |
| 32 | 2a | 547 | A |
| 32 | 2a | 559 | A |
| 32 | 2a | 561 | U |
| 32 | 2a | 562 | C |
| 32 | 2a | 564 | C |
| 32 | 2a | 572 | A |
| 32 | 2a | 573 | A |
| 32 | 2a | 576 | G |
| 32 | 2a | 596 | C |
| 32 | 2a | 603 | U |
| 32 | 2a | 618 | C |
| 32 | 2a | 630 | G |
| 32 | 2a | 647 | C |
| 32 | 2a | 651 | C |
| 32 | 2a | 653 | A |
| 32 | 2a | 665 | A |
| 32 | 2a | 666 | G |
| 32 | 2a | 687 | A |
| 32 | 2a | 688 | G |
| 32 | 2a | 695 | A |
| 32 | 2a | 723 | U |
| 32 | 2a | 731 | G |
| 32 | 2a | 742 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 32 | 2a | 749 | C |
| 32 | 2a | 753 | A |
| 32 | 2a | 755 | G |
| 32 | 2a | 763 | G |
| 32 | 2a | 777 | A |
| 32 | 2a | 782 | A |
| 32 | 2a | 792 | A |
| 32 | 2a | 793 | U |
| 32 | 2a | 794 | A |
| 32 | 2a | 796 | C |
| 32 | 2a | 810 | C |
| 32 | 2a | 816 | A |
| 32 | 2a | 817 | C |
| 32 | 2a | 819 | A |
| 32 | 2a | 821 | G |
| 32 | 2a | 828 | A |
| 32 | 2a | 840 | C |
| 32 | 2a | 841 | U |
| 32 | 2a | 851 | G |
| 32 | 2a | 853 | G |
| 32 | 2a | 854 | G |
| 32 | 2a | 859 | A |
| 32 | 2a | 872 | A |
| 32 | 2a | 902 | G |
| 32 | 2a | 914 | A |
| 32 | 2a | 926 | G |
| 32 | 2a | 927 | G |
| 32 | 2a | 934 | C |
| 32 | 2a | 942 | G |
| 32 | 2a | 961 | U |
| 32 | 2a | 968 | A |
| 32 | 2a | 969 | A |
| 32 | 2a | 971 | G |
| 32 | 2a | 972 | C |
| 32 | 2a | 974 | A |
| 32 | 2a | 975 | A |
| 32 | 2a | 976 | G |
| 32 | 2a | 977 | A |
| 32 | 2a | 982 | U |
| 32 | 2a | 989 | C |
| 32 | 2a | 992 | U |
| 32 | 2a | 993 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 32 | 2a | 997 | U |
| 32 | 2a | 998 | G |
| 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 | 1020 | U |
| 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 | 1030 | C |
| 32 | 2a | 1030(A) | G |
| 32 | 2a | 1031 | G |
| 32 | 2a | 1037 | C |
| 32 | 2a | 1039 | C |
| 32 | 2a | 1040 | U |
| 32 | 2a | 1043 | C |
| 32 | 2a | 1045 | C |
| 32 | 2a | 1046 | A |
| 32 | 2a | 1065 | U |
| 32 | 2a | 1066 | C |
| 32 | 2a | 1068 | G |
| 32 | 2a | 1077 | G |
| 32 | 2a | 1081 | G |
| 32 | 2a | 1086 | U |
| 32 | 2a | 1094 | G |
| 32 | 2a | 1095 | U |
| 32 | 2a | 1101 | A |
| 32 | 2a | 1108 | G |
| 32 | 2a | 1113 | C |
| 32 | 2a | 1117 | G |
| 32 | 2a | 1122 | U |
| 32 | 2a | 1129 | C |
| 32 | 2a | 1130 | A |
| 32 | 2a | 1133 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 32 | 2a | 1136 | U |
| 32 | 2a | 1137 | C |
| 32 | 2a | 1138 | G |
| 32 | 2a | 1139 | G |
| 32 | 2a | 1146 | A |
| 32 | 2a | 1152 | A |
| 32 | 2a | 1157 | A |
| 32 | 2a | 1159 | U |
| 32 | 2a | 1160 | G |
| 32 | 2a | 1182 | G |
| 32 | 2a | 1183 | A |
| 32 | 2a | 1184 | G |
| 32 | 2a | 1196 | U |
| 32 | 2a | 1197 | G |
| 32 | 2a | 1202 | G |
| 32 | 2a | 1211 | U |
| 32 | 2a | 1212 | U |
| 32 | 2a | 1213 | A |
| 32 | 2a | 1227 | A |
| 32 | 2a | 1228 | C |
| 32 | 2a | 1238 | A |
| 32 | 2a | 1240 | U |
| 32 | 2a | 1241 | G |
| 32 | 2a | 1256 | A |
| 32 | 2a | 1257 | U |
| 32 | 2a | 1260 | C |
| 32 | 2a | 1262 | C |
| 32 | 2a | 1270 | C |
| 32 | 2a | 1272 | G |
| 32 | 2a | 1273 | G |
| 32 | 2a | 1275 | A |
| 32 | 2a | 1277 | C |
| 32 | 2a | 1278 | U |
| 32 | 2a | 1279 | A |
| 32 | 2a | 1280 | A |
| 32 | 2a | 1287 | A |
| 32 | 2a | 1297 | C |
| 32 | 2a | 1299 | A |
| 32 | 2a | 1302 | U |
| 32 | 2a | 1303 | C |
| 32 | 2a | 1305 | G |
| 32 | 2a | 1312 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 32 | 2a | 1319 | A |
| 32 | 2a | 1322 | C |
| 32 | 2a | 1323 | G |
| 32 | 2a | 1346 | A |
| 32 | 2a | 1347 | G |
| 32 | 2a | 1358 | U |
| 32 | 2a | 1363 | C |
| 32 | 2a | 1368 | G |
| 32 | 2a | 1370 | G |
| 32 | 2a | 1398 | A |
| 32 | 2a | 1399 | C |
| 32 | 2a | 1401 | G |
| 32 | 2a | 1402 | 4OC |
| 32 | 2a | 1410 | G |
| 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 | 1475 | G |
| 32 | 2a | 1492 | A |
| 32 | 2a | 1494 | G |
| 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 |
| 54 | 2x | 8 | 4SU |
| 54 | 2x | 9 | G |
| 54 | 2x | 19 | G |
| 54 | 2x | 21 | A |
| 54 | 2x | 22 | G |
| 54 | 2x | 47 | U |
| 54 | 2x | 52 | G |
| 54 | 2x | 56 | C |
| 54 | 2x | 59 | A |
| 54 | 2x | 68 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 54 | 2x | 76 | A |

All (63) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 1A | 90 | U |
| 1 | 1A | 195 | A |
| 1 | 1A | 266 | G |
| 1 | 1A | 271(K) | U |
| 1 | 1A | 278 | A |
| 1 | 1A | 351 | G |
| 1 | 1A | 548 | A |
| 1 | 1A | 574 | C |
| 1 | 1A | 746 | A |
| 1 | 1A | 774 | A |
| 1 | 1A | 895 | U |
| 1 | 1A | 974 | G |
| 1 | 1A | 1047 | G |
| 1 | 1A | 1065 | U |
| 1 | 1A | 1067 | A |
| 1 | 1A | 1078 | U |
| 1 | 1A | 1107 | G |
| 1 | 1A | 1174 | A |
| 1 | 1A | 1175 | U |
| 1 | 1A | 1176 | G |
| 1 | 1A | 1210 | A |
| 1 | 1A | 1384 | A |
| 1 | 1A | 1442 | G |
| 1 | 1A | 1508 | A |
| 1 | 1A | 1608 | A |
| 1 | 1A | 1653 | G |
| 1 | 1A | 1992 | G |
| 1 | 1A | 2134 | A |
| 1 | 1A | 2156 | G |
| 1 | 1A | 2158 | A |
| 1 | 1A | 2181 | G |
| 1 | 1A | 2183 | C |
| 1 | 1A | 2406 | U |
| 1 | 1A | 2422 | A |
| 1 | 1A | 2430 | A |
| 1 | 1A | 2601 | C |
| 1 | 1A | 2689 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | 1B | 1 | U |
| 1 | 2A | 34 | C |
| 1 | 2A | 196 | A |
| 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 | 774 | A |
| 1 | 2A | 805 | G |
| 1 | 2A | 856 | C |
| 1 | 2A | 900 | A |
| 1 | 2A | 1210 | A |
| 1 | 2A | 1379 | A |
| 1 | 2A | 1420 | U |
| 1 | 2A | 1442 | G |
| 1 | 2A | 1530 | C |
| 1 | 2A | 1608 | A |
| 1 | 2A | 1653 | G |
| 1 | 2A | 1913 | A |
| 1 | 2A | 1992 | G |
| 1 | 2A | 2119 | A |
| 1 | 2A | 2126 | A |
| 1 | 2A | 2689 | U |

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

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

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 1 | 5MU | 1A | 1939 | 1,55 | 19,22,23 | 1.40 | 5 (26%) | 27,32,35 | 2.29 | 6 (22%) |
| 1 | 5MC | 2A | 1962 | 1,55 | 19,22,23 | 1.55 | 3 (15%) | 26,32,35 | 1.15 | 2 (7%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 32 | 5MC | 1a | 1407 | 32 | 19,22,23 | 1.66 | 3 (15%) | 26,32,35 | 1.08 | 2 (7%) |
| 32 | PSU | 2a | 516 | 32,55 | 18,21,22 | 1.35 | 2 (11%) | 21,30,33 | 1.94 | 4 (19%) |
| 32 | 5MC | 2a | 1400 | 54,32 | 19,22,23 | 1.71 | 3 (15%) | 26,32,35 | 1.30 | 3 (11%) |
| 1 | 2MA | 2A | 2503 | 1,55 | 22,25,26 | 1.47 | 5 (22%) | 32,37,40 | 2.22 | 9 (28%) |
| 32 | UR3 | 1a | 1498 | 32 | 19,22,23 | 1.02 | 1 (5%) | 26,32,35 | 1.78 | 3 (11%) |
| 1 | OMG | 1A | 2251 | 54,1,55 | 23,26,27 | 1.24 | 3 (13%) | 32,38,41 | 1.98 | 6 (18%) |
| 1 | 5MU | 2A | 1915 | 1 | 19,22,23 | 1.56 | 5 (26%) | 27,32,35 | 2.03 | 7 (25%) |
| 54 | 5MC | 2x | 32 | 54 | 19,22,23 | 1.75 | 3 (15%) | 26,32,35 | 1.21 | 3 (11%) |
| 1 | 2MU | 1A | 2552 | 1,55 | 19,22,24 | 1.18 | 1 (5%) | 25,31,36 | 2.05 | 6 (24%) |
| 32 | PSU | 1a | 516 | 32,55 | 18,21,22 | 1.40 | 2 (11%) | 21,30,33 | 1.94 | 4 (19%) |
| 32 | 4OC | 1a | 1402 | 32 | 20,23,24 | 0.79 | 0 | 25,32,35 | 0.97 | 2 (8%) |
| 1 | 5MC | 2A | 1942 | 1 | 19,22,23 | 1.65 | 3 (15%) | 26,32,35 | 1.13 | 2 (7%) |
| 54 | 4SU | 2x | 8 | 54 | 18,21,22 | 2.03 | 6 (33%) | 25,30,33 | 1.50 | 4 (16%) |
| 1 | PSU | 2A | 2605 | 1 | 18,21,22 | 1.39 | 3 (16%) | 21,30,33 | 2.00 | 4 (19%) |
| 32 | 5MC | 2a | 1407 | 32 | 19,22,23 | 1.51 | 3 (15%) | 26,32,35 | 1.14 | 2 (7%) |
| 32 | MA6 | 1a | 1519 | 32 | 23,26,27 | 1.58 | 5 (21%) | 33,38,41 | 2.21 | 13 (39%) |
| 32 | UR3 | 2a | 1498 | 32 | 19,22,23 | 1.02 | 2 (10%) | 26,32,35 | 1.76 | 3 (11%) |
| 1 | 4OC | 1A | 1920 | 1 | 19,22,24 | 0.79 | 0 | 25,31,35 | 1.00 | 1 (4%) |
| 1 | 2MA | 1A | 2503 | 1,55 | 22,25,26 | 1.47 | 5 (22%) | 32,37,40 | 2.17 | 9 (28%) |
| 32 | M2G | 2a | 966 | 32,55 | 24,27,28 | 1.35 | 4 (16%) | 33,40,43 | 1.95 | 5 (15%) |
| 43 | 0TD | 2l | 92 | 43 | 8,9,10 | 4.58 | 1 (12%) | 6,11,13 | 6.85 | 3 (50%) |
| 54 | 5MU | 1x | 54 | 54,55 | 19,22,23 | 1.39 | 5 (26%) | 27,32,35 | 1.84 | 7 (25%) |
| 32 | MA6 | 1a | 1518 | 32 | 23,26,27 | 1.48 | 6 (26%) | 33,38,41 | 2.37 | 13 (39%) |
| 1 | 4OC | 2A | 1920 | 1 | 19,22,24 | 0.77 | 0 | 25,31,35 | 1.05 | 2 (8%) |
| 54 | 4SU | 1x | 8 | 54 | 18,21,22 | 2.12 | 4 (22%) | 25,30,33 | 1.59 | 5 (20%) |
| 32 | 5MC | 1a | 1404 | 32 | 19,22,23 | 1.86 | 3 (15%) | 26,32,35 | 1.17 | 3 (11%) |
| 32 | MA6 | 2a | 1518 | 32 | 23,26,27 | 1.55 | 5 (21%) | 33,38,41 | 2.27 | 13 (39%) |
| 32 | 5MC | 2a | 967 | 32 | 19,22,23 | 1.67 | 3 (15%) | 26,32,35 | 1.16 | 3 (11%) |
| 54 | PSU | 1x | 55 | 54 | 18,21,22 | 1.32 | 2 (11%) | 21,30,33 | 1.98 | 4 (19%) |
| 1 | 5MC | 1A | 1962 | 1,55 | 19,22,23 | 1.57 | 3 (15%) | 26,32,35 | 1.06 | 2 (7%) |
| 1 | PSU | 2A | 1911 | 1 | 18,21,22 | 1.39 | 2 (11%) | 21,30,33 | 2.03 | 3 (14%) |
| 1 | PSU | 1A | 1911 | 1 | 18,21,22 | 1.33 | 2 (11%) | 21,30,33 | 1.99 | 3 (14%) |
| 1 | 2MU | 2A | 2552 | 1,55 | 19,22,24 | 1.27 | 3 (15%) | 25,31,36 | 1.86 | 5 (20%) |
| 1 | PSU | 1A | 1917 | 1 | 18,21,22 | 1.35 | 3 (16%) | 21,30,33 | 2.08 | 4 (19%) |
| 32 | 7MG | 1a | 527 | 32,55 | 23,26,27 | 1.35 | 3 (13%) | 27,39,42 | 2.64 | 7 (25%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 32 | 2MG | 1a | 1207 | 32,55 | 23,26,27 | 1.23 | 2 (8%) | 33,38,41 | 2.18 | 8 (24%) |
| 54 | 5MC | 1x | 32 | 54 | 19,22,23 | 1.64 | 3 (15%) | 26,32,35 | 1.26 | 2 (7%) |
| 1 | 5MU | 2A | 1939 | 1 | 19,22,23 | 1.44 | 5 (26%) | 27,32,35 | 2.40 | 6 (22%) |
| 32 | 4OC | 2a | 1402 | 32,55 | 20,23,24 | 0.80 | 0 | 25,32,35 | 0.98 | 1 (4%) |
| 32 | MA6 | 2a | 1519 | 32 | 23,26,27 | 1.57 | 4 (17%) | 33,38,41 | 2.29 | 11 (33%) |
| 1 | PSU | 2A | 1917 | 1,55 | 18,21,22 | 1.41 | 2 (11%) | 21,30,33 | 1.91 | 3 (14%) |
| 32 | 5MC | 1a | 967 | 32 | 19,22,23 | 1.53 | 3 (15%) | 26,32,35 | 1.23 | 4 (15%) |
| 1 | 5MU | 1A | 1915 | 1 | 19,22,23 | 1.42 | 5 (26%) | 27,32,35 | 2.08 | 7 (25%) |
| 1 | 5MC | 1A | 1942 | 1,55 | 19,22,23 | 1.46 | 3 (15%) | 26,32,35 | 1.16 | 2 (7%) |
| 1 | OMG | 2A | 2251 | 54,1,55 | 23,26,27 | 1.22 | 3 (13%) | 32,38,41 | 1.93 | 6 (18%) |
| 43 | 0TD | 1l | 92 | 43 | 8,9,10 | 4.46 | 1 (12%) | 6,11,13 | 4.35 | 3 (50%) |
| 1 | PSU | 1A | 2605 | 1 | 18,21,22 | 1.41 | 4 (22%) | 21,30,33 | 2.00 | 4 (19%) |
| 54 | 5MU | 2x | 54 | 54 | 19,22,23 | 1.39 | 5 (26%) | 27,32,35 | 2.05 | 7 (25%) |
| 32 | 5MC | 1a | 1400 | 32 | 19,22,23 | 1.71 | 3 (15%) | 26,32,35 | 1.16 | 2 (7%) |
| 32 | 5MC | 2a | 1404 | 32 | 19,22,23 | 1.55 | 3 (15%) | 26,32,35 | 1.11 | 2 (7%) |
| 32 | M2G | 1a | 966 | 32,55 | 24,27,28 | 1.33 | 4 (16%) | 33,40,43 | 1.85 | 5 (15%) |
| 32 | 7MG | 2a | 527 | 32,55 | 23,26,27 | 1.38 | 4 (17%) | 27,39,42 | 2.54 | 5 (18%) |
| 54 | PSU | 2x | 55 | 54 | 18,21,22 | 1.39 | 2 (11%) | 21,30,33 | 2.00 | 4 (19%) |
| 32 | 2MG | 2a | 1207 | 32 | 23,26,27 | 1.26 | 4 (17%) | 33,38,41 | 2.13 | 8 (24%) |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 1 | 5MU | 1A | 1939 | 1,55 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | 5MC | 2A | 1962 | 1,55 | - | 0/7/25/26 | 0/2/2/2 |
| 32 | 5MC | 1a | 1407 | 32 | - | 0/7/25/26 | 0/2/2/2 |
| 32 | PSU | 2a | 516 | 32,55 | - | 0/7/25/26 | 0/2/2/2 |
| 32 | 5MC | 2a | 1400 | 54,32 | - | 2/7/25/26 | 0/2/2/2 |
| 1 | 2MA | 2A | 2503 | 1,55 | - | 0/7/25/26 | 0/3/3/3 |
| 32 | UR3 | 1a | 1498 | 32 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | OMG | 1A | 2251 | 54,1,55 | - | 0/9/27/28 | 0/3/3/3 |
| 1 | 5MU | 2A | 1915 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 54 | 5MC | 2x | 32 | 54 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | 2MU | 1A | 2552 | 1,55 | - | 0/9/27/28 | 0/2/2/2 |
| 32 | PSU | 1a | 516 | 32,55 | - | 0/7/25/26 | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 32 | 4OC | 1a | 1402 | 32 | - | 1/9/29/30 | 0/2/2/2 |
| 1 | 5MC | 2A | 1942 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 54 | 4SU | 2x | 8 | 54 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | PSU | 2A | 2605 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 32 | 5MC | 2a | 1407 | 32 | - | 0/7/25/26 | 0/2/2/2 |
| 32 | MA6 | 1a | 1519 | 32 | - | 4/11/29/30 | 0/3/3/3 |
| 32 | UR3 | 2a | 1498 | 32 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | 4OC | 1A | 1920 | 1 | - | 0/9/27/30 | 0/2/2/2 |
| 1 | 2MA | 1A | 2503 | 1,55 | - | 1/7/25/26 | 0/3/3/3 |
| 32 | M2G | 2a | 966 | 32,55 | - | 0/11/29/30 | 0/3/3/3 |
| 43 | 0TD | 2l | 92 | 43 | - | 3/7/12/14 | - |
| 54 | 5MU | 1x | 54 | 54,55 | - | 0/7/25/26 | 0/2/2/2 |
| 32 | MA6 | 1a | 1518 | 32 | - | 3/11/29/30 | 0/3/3/3 |
| 1 | 4OC | 2A | 1920 | 1 | - | 2/9/27/30 | 0/2/2/2 |
| 54 | 4SU | 1x | 8 | 54 | - | 0/7/25/26 | 0/2/2/2 |
| 32 | 5MC | 1a | 1404 | 32 | - | 0/7/25/26 | 0/2/2/2 |
| 32 | MA6 | 2a | 1518 | 32 | - | 2/11/29/30 | 0/3/3/3 |
| 32 | 5MC | 2a | 967 | 32 | - | 0/7/25/26 | 0/2/2/2 |
| 54 | PSU | 1x | 55 | 54 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | 5MC | 1A | 1962 | 1,55 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | PSU | 2A | 1911 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | PSU | 1A | 1911 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | 2MU | 2A | 2552 | 1,55 | - | 0/9/27/28 | 0/2/2/2 |
| 1 | PSU | 1A | 1917 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 32 | 7MG | 1a | 527 | 32,55 | - | 1/7/37/38 | 0/3/3/3 |
| 32 | 2MG | 1a | 1207 | 32,55 | - | 0/9/27/28 | 0/3/3/3 |
| 54 | 5MC | 1x | 32 | 54 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | 5MU | 2A | 1939 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 32 | 4OC | 2a | 1402 | 32,55 | - | 2/9/29/30 | 0/2/2/2 |
| 32 | MA6 | 2a | 1519 | 32 | - | 4/11/29/30 | 0/3/3/3 |
| 1 | PSU | 2A | 1917 | 1,55 | - | 0/7/25/26 | 0/2/2/2 |
| 32 | 5MC | 1a | 967 | 32 | - | 2/7/25/26 | 0/2/2/2 |
| 1 | 5MU | 1A | 1915 | 1 | - | 2/7/25/26 | 0/2/2/2 |
| 1 | 5MC | 1A | 1942 | 1,55 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | OMG | 2A | 2251 | 54,1,55 | - | 0/9/27/28 | 0/3/3/3 |
| 43 | 0TD | 1l | 92 | 43 | - | 1/7/12/14 | - |
| 1 | PSU | 1A | 2605 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 54 | 5MU | 2x | 54 | 54 | - | 0/7/25/26 | 0/2/2/2 |
| 32 | 5MC | 1a | 1400 | 32 | - | 0/7/25/26 | 0/2/2/2 |
| 32 | 5MC | 2a | 1404 | 32 | - | 0/7/25/26 | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 32 | M2G | 1a | 966 | 32,55 | - | 0/11/29/30 | 0/3/3/3 |
| 32 | 7MG | 2a | 527 | 32,55 | - | 2/7/37/38 | 0/3/3/3 |
| 54 | PSU | 2x | 55 | 54 | - | 2/7/25/26 | 0/2/2/2 |
| 32 | 2MG | 2a | 1207 | 32 | - | 0/9/27/28 | 0/3/3/3 |

All (172) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 43 | 2l | 92 | 0TD | CB-SB | -12.61 | 1.69 | 1.82 |
| 43 | 1l | 92 | 0TD | CB-SB | -12.16 | 1.70 | 1.82 |
| 32 | 1a | 1404 | 5MC | C5-C4 | 6.96 | 1.49 | 1.44 |
| 54 | 2x | 32 | 5MC | C5-C4 | 6.25 | 1.48 | 1.44 |
| 32 | 1a | 1400 | 5MC | C5-C4 | 6.20 | 1.48 | 1.44 |
| 32 | 2a | 967 | 5MC | C5-C4 | 6.13 | 1.48 | 1.44 |
| 32 | 2a | 1400 | 5MC | C5-C4 | 6.03 | 1.48 | 1.44 |
| 32 | 1a | 1407 | 5MC | C5-C4 | 6.03 | 1.48 | 1.44 |
| 1 | 2A | 1942 | 5MC | C5-C4 | 6.00 | 1.48 | 1.44 |
| 54 | 1x | 32 | 5MC | C5-C4 | 5.67 | 1.48 | 1.44 |
| 1 | 1A | 1962 | 5MC | C5-C4 | 5.61 | 1.48 | 1.44 |
| 32 | 2a | 1404 | 5MC | C5-C4 | 5.51 | 1.48 | 1.44 |
| 1 | 2A | 1962 | 5MC | C5-C4 | 5.40 | 1.48 | 1.44 |
| 32 | 1a | 967 | 5MC | C5-C4 | 5.27 | 1.48 | 1.44 |
| 32 | 2a | 1407 | 5MC | C5-C4 | 5.20 | 1.48 | 1.44 |
| 54 | 1x | 8 | 4SU | C4-S4 | -4.92 | 1.60 | 1.68 |
| 1 | 1A | 1942 | 5MC | C5-C4 | 4.88 | 1.47 | 1.44 |
| 32 | 1a | 1519 | MA6 | C5-C4 | 4.86 | 1.47 | 1.39 |
| 32 | 2a | 1519 | MA6 | C5-C4 | 4.85 | 1.47 | 1.39 |
| 32 | 2a | 1518 | MA6 | C5-C4 | 4.78 | 1.47 | 1.39 |
| 54 | 2x | 8 | 4SU | C4-S4 | -4.51 | 1.60 | 1.68 |
| 54 | 1x | 8 | 4SU | C4-N3 | -4.48 | 1.33 | 1.37 |
| 32 | 1a | 1518 | MA6 | C5-C4 | 4.48 | 1.47 | 1.39 |
| 54 | 2x | 8 | 4SU | C4-N3 | -4.48 | 1.33 | 1.37 |
| 1 | 1A | 2503 | 2MA | C5-C4 | 4.40 | 1.46 | 1.39 |
| 1 | 2A | 2503 | 2MA | C5-C4 | 4.38 | 1.46 | 1.39 |
| 54 | 1x | 8 | 4SU | C2-N3 | -3.90 | 1.31 | 1.38 |
| 54 | 2x | 55 | PSU | C6-C5 | 3.88 | 1.39 | 1.35 |
| 32 | 1a | 516 | PSU | C6-C5 | 3.87 | 1.39 | 1.35 |
| 1 | 2A | 1917 | PSU | C6-C5 | 3.84 | 1.39 | 1.35 |
| 54 | 1x | 55 | PSU | C6-C5 | 3.60 | 1.39 | 1.35 |
| 1 | 2A | 1911 | PSU | C6-C5 | 3.54 | 1.39 | 1.35 |
| 54 | 1x | 8 | 4SU | C5-C4 | -3.47 | 1.38 | 1.42 |
| 1 | 1A | 1911 | PSU | C6-C5 | 3.44 | 1.39 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 32 | 2a | 1207 | 2MG | C5-C4 | 3.37 | 1.48 | 1.38 |
| 32 | 2a | 966 | M2G | C5-C4 | 3.34 | 1.47 | 1.38 |
| 32 | 2a | 527 | 7MG | C5-C4 | 3.33 | 1.47 | 1.37 |
| 1 | 2A | 2605 | PSU | C6-C5 | 3.31 | 1.39 | 1.35 |
| 32 | 1a | 966 | M2G | C5-C4 | 3.31 | 1.47 | 1.38 |
| 32 | 1a | 527 | 7MG | C5-C4 | 3.27 | 1.47 | 1.37 |
| 1 | 2A | 2251 | OMG | C5-C4 | 3.21 | 1.47 | 1.38 |
| 32 | 2a | 516 | PSU | C6-C5 | 3.19 | 1.38 | 1.35 |
| 1 | 2A | 1915 | 5MU | C6-C5 | 3.17 | 1.39 | 1.34 |
| 54 | 2x | 32 | 5MC | C6-C5 | 3.16 | 1.39 | 1.34 |
| 32 | 1a | 527 | 7MG | C4-N9 | -3.15 | 1.34 | 1.37 |
| 54 | 1x | 32 | 5MC | C6-C5 | 3.11 | 1.39 | 1.34 |
| 1 | 1A | 1917 | PSU | C6-C5 | 3.08 | 1.38 | 1.35 |
| 54 | 2x | 8 | 4SU | C5-C4 | -3.07 | 1.38 | 1.42 |
| 32 | 2a | 527 | 7MG | C4-N9 | -3.06 | 1.34 | 1.37 |
| 32 | 1a | 1207 | 2MG | C5-C4 | 3.04 | 1.47 | 1.38 |
| 1 | 1A | 1939 | 5MU | C6-C5 | 3.02 | 1.39 | 1.34 |
| 1 | 2A | 1915 | 5MU | C2-N1 | 3.01 | 1.43 | 1.38 |
| 1 | 1A | 2251 | OMG | C5-C4 | 3.00 | 1.47 | 1.38 |
| 1 | 1A | 2605 | PSU | C4-N3 | -2.99 | 1.33 | 1.38 |
| 32 | 2a | 966 | M2G | C2-N2 | 2.98 | 1.40 | 1.35 |
| 1 | 2A | 2552 | 2MU | C4-N3 | -2.94 | 1.33 | 1.38 |
| 54 | 2x | 8 | 4SU | C2-N3 | -2.93 | 1.32 | 1.38 |
| 32 | 2a | 1519 | MA6 | C5-C6 | 2.93 | 1.48 | 1.41 |
| 32 | 1a | 1404 | 5MC | C6-C5 | 2.92 | 1.39 | 1.34 |
| 1 | 2A | 1939 | 5MU | C4-N3 | -2.91 | 1.33 | 1.38 |
| 32 | 1a | 1519 | MA6 | C5-C6 | 2.90 | 1.48 | 1.41 |
| 32 | 2a | 1518 | MA6 | C5-C6 | 2.88 | 1.48 | 1.41 |
| 1 | 2A | 1915 | 5MU | C4-C5 | 2.87 | 1.49 | 1.44 |
| 32 | 1a | 1518 | MA6 | C5-C6 | 2.87 | 1.48 | 1.41 |
| 32 | 1a | 1400 | 5MC | C6-C5 | 2.82 | 1.39 | 1.34 |
| 1 | 1A | 1942 | 5MC | C6-C5 | 2.82 | 1.39 | 1.34 |
| 32 | 1a | 966 | M2G | C2-N2 | 2.82 | 1.40 | 1.35 |
| 32 | 1a | 1407 | 5MC | C6-C5 | 2.81 | 1.39 | 1.34 |
| 1 | 1A | 2251 | OMG | C6-N1 | -2.81 | 1.33 | 1.38 |
| 32 | 2a | 1400 | 5MC | C6-C5 | 2.81 | 1.39 | 1.34 |
| 1 | 2A | 1939 | 5MU | C6-C5 | 2.80 | 1.39 | 1.34 |
| 32 | 2a | 1404 | 5MC | C6-C5 | 2.78 | 1.39 | 1.34 |
| 1 | 1A | 1939 | 5MU | C4-N3 | -2.77 | 1.33 | 1.38 |
| 1 | 1A | 2552 | 2MU | C4-N3 | -2.77 | 1.33 | 1.38 |
| 1 | 1A | 1962 | 5MC | C6-C5 | 2.75 | 1.39 | 1.34 |
| 54 | 2x | 54 | 5MU | C6-C5 | 2.74 | 1.39 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 54 | 1x | 54 | 5MU | C4-N3 | -2.73 | 1.33 | 1.38 |
| 1 | 1A | 1915 | 5MU | C2-N1 | 2.73 | 1.42 | 1.38 |
| 1 | 1A | 1917 | PSU | C4-N3 | -2.72 | 1.33 | 1.38 |
| 32 | 1a | 967 | 5MC | C6-C5 | 2.71 | 1.39 | 1.34 |
| 1 | 1A | 1915 | 5MU | C6-C5 | 2.69 | 1.39 | 1.34 |
| 32 | 1a | 966 | M2G | C6-N1 | -2.66 | 1.33 | 1.38 |
| 32 | 2a | 527 | 7MG | C6-N1 | -2.66 | 1.33 | 1.38 |
| 54 | 1x | 54 | 5MU | C6-C5 | 2.66 | 1.38 | 1.34 |
| 1 | 2A | 2251 | OMG | C6-N1 | -2.65 | 1.33 | 1.38 |
| 1 | 2A | 2605 | PSU | C4-N3 | -2.64 | 1.33 | 1.38 |
| 32 | 2a | 967 | 5MC | C6-C5 | 2.61 | 1.38 | 1.34 |
| 1 | 2A | 1911 | PSU | C4-N3 | -2.61 | 1.34 | 1.38 |
| 1 | 2A | 1962 | 5MC | C6-C5 | 2.61 | 1.38 | 1.34 |
| 1 | 2A | 1942 | 5MC | C6-C5 | 2.60 | 1.38 | 1.34 |
| 1 | 2A | 1939 | 5MU | C6-N1 | -2.60 | 1.33 | 1.38 |
| 1 | 2A | 1915 | 5MU | C4-N3 | -2.58 | 1.34 | 1.38 |
| 54 | 2x | 54 | 5MU | C4-N3 | -2.58 | 1.34 | 1.38 |
| 32 | 1a | 1207 | 2MG | C6-N1 | -2.58 | 1.34 | 1.38 |
| 32 | 2a | 1407 | 5MC | C6-N1 | -2.57 | 1.33 | 1.38 |
| 1 | 2A | 2503 | 2MA | C5-N7 | -2.55 | 1.34 | 1.39 |
| 1 | 1A | 2503 | 2MA | C5-C6 | 2.54 | 1.48 | 1.41 |
| 32 | 2a | 966 | M2G | C6-N1 | -2.51 | 1.34 | 1.38 |
| 1 | 2A | 1939 | 5MU | C4-C5 | 2.51 | 1.48 | 1.44 |
| 1 | 1A | 1915 | 5MU | C4-C5 | 2.51 | 1.48 | 1.44 |
| 32 | 2a | 1518 | MA6 | C8-N7 | 2.47 | 1.36 | 1.31 |
| 32 | 2a | 1407 | 5MC | C6-C5 | 2.46 | 1.38 | 1.34 |
| 32 | 2a | 1400 | 5MC | C6-N1 | -2.46 | 1.33 | 1.38 |
| 54 | 2x | 54 | 5MU | C4-C5 | 2.46 | 1.48 | 1.44 |
| 1 | 2A | 2503 | 2MA | C5-C6 | 2.44 | 1.47 | 1.41 |
| 1 | 1A | 1939 | 5MU | C6-N1 | -2.44 | 1.33 | 1.38 |
| 54 | 2x | 55 | PSU | C4-N3 | -2.43 | 1.34 | 1.38 |
| 32 | 2a | 516 | PSU | C4-N3 | -2.43 | 1.34 | 1.38 |
| 1 | 1A | 2605 | PSU | C2-N3 | -2.43 | 1.33 | 1.37 |
| 1 | 1A | 2503 | 2MA | C4-N9 | -2.42 | 1.32 | 1.37 |
| 1 | 1A | 2503 | 2MA | C8-N7 | 2.42 | 1.36 | 1.31 |
| 1 | 1A | 1942 | 5MC | C6-N1 | -2.40 | 1.33 | 1.38 |
| 1 | 2A | 1939 | 5MU | C2-N3 | -2.39 | 1.33 | 1.38 |
| 1 | 1A | 1915 | 5MU | C4-N3 | -2.39 | 1.34 | 1.38 |
| 54 | 1x | 55 | PSU | C4-N3 | -2.38 | 1.34 | 1.38 |
| 32 | 1a | 1498 | UR3 | C2-N1 | 2.37 | 1.41 | 1.38 |
| 1 | 2A | 1917 | PSU | C4-N3 | -2.37 | 1.34 | 1.38 |
| 1 | 1A | 2605 | PSU | C2-N1 | -2.37 | 1.33 | 1.36 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | 2A | 1962 | 5MC | C6-N1 | -2.37 | 1.34 | 1.38 |
| 32 | 1a | 516 | PSU | C4-N3 | -2.36 | 1.34 | 1.38 |
| 1 | 2A | 2251 | OMG | C5-N7 | -2.36 | 1.34 | 1.39 |
| 1 | 2A | 2552 | 2MU | C5-C4 | 2.35 | 1.48 | 1.43 |
| 1 | 1A | 1911 | PSU | C4-N3 | -2.35 | 1.34 | 1.38 |
| 1 | 2A | 2503 | 2MA | C8-N7 | 2.34 | 1.36 | 1.31 |
| 1 | 1A | 1939 | 5MU | C2-N3 | -2.34 | 1.33 | 1.38 |
| 32 | 2a | 1519 | MA6 | C5-N7 | -2.32 | 1.34 | 1.39 |
| 1 | 2A | 2552 | 2MU | C2-N3 | -2.32 | 1.33 | 1.38 |
| 1 | 1A | 2503 | 2MA | C5-N7 | -2.31 | 1.34 | 1.39 |
| 1 | 2A | 1942 | 5MC | C6-N1 | -2.31 | 1.34 | 1.38 |
| 54 | 1x | 32 | 5MC | C6-N1 | -2.30 | 1.34 | 1.38 |
| 32 | 1a | 1519 | MA6 | C4-N9 | -2.30 | 1.32 | 1.37 |
| 32 | 2a | 1518 | MA6 | C4-N9 | -2.30 | 1.32 | 1.37 |
| 54 | 2x | 8 | 4SU | C2-N1 | 2.29 | 1.42 | 1.38 |
| 32 | 1a | 1519 | MA6 | C5-N7 | -2.29 | 1.34 | 1.39 |
| 1 | 1A | 2605 | PSU | C6-C5 | 2.29 | 1.37 | 1.35 |
| 32 | 2a | 1519 | MA6 | C8-N7 | 2.28 | 1.36 | 1.31 |
| 32 | 1a | 967 | 5MC | C6-N1 | -2.27 | 1.34 | 1.38 |
| 32 | 2a | 1207 | 2MG | C6-N1 | -2.26 | 1.34 | 1.38 |
| 32 | 1a | 1400 | 5MC | C6-N1 | -2.24 | 1.34 | 1.38 |
| 54 | 1x | 54 | 5MU | C4-C5 | 2.23 | 1.48 | 1.44 |
| 32 | 2a | 1498 | UR3 | C2-N1 | 2.23 | 1.41 | 1.38 |
| 32 | 1a | 527 | 7MG | C6-N1 | -2.23 | 1.34 | 1.38 |
| 54 | 2x | 54 | 5MU | C2-N1 | 2.20 | 1.41 | 1.38 |
| 32 | 2a | 966 | M2G | C5-N7 | -2.19 | 1.34 | 1.39 |
| 32 | 2a | 967 | 5MC | C6-N1 | -2.19 | 1.34 | 1.38 |
| 1 | 2A | 2503 | 2MA | C4-N9 | -2.19 | 1.33 | 1.37 |
| 32 | 1a | 1404 | 5MC | C6-N1 | -2.19 | 1.34 | 1.38 |
| 32 | 2a | 527 | 7MG | C8-N9 | 2.19 | 1.47 | 1.45 |
| 54 | 1x | 54 | 5MU | C2-N3 | -2.18 | 1.34 | 1.38 |
| 32 | 1a | 1518 | MA6 | C4-N9 | -2.17 | 1.33 | 1.37 |
| 1 | 1A | 1962 | 5MC | C6-N1 | -2.17 | 1.34 | 1.38 |
| 32 | 2a | 1518 | MA6 | C5-N7 | -2.16 | 1.35 | 1.39 |
| 54 | 1x | 54 | 5MU | C6-N1 | -2.15 | 1.34 | 1.38 |
| 32 | 1a | 1518 | MA6 | C5-N7 | -2.13 | 1.35 | 1.39 |
| 32 | 1a | 1519 | MA6 | C8-N7 | 2.12 | 1.35 | 1.31 |
| 32 | 2a | 1404 | 5MC | C6-N1 | -2.11 | 1.34 | 1.38 |
| 54 | 2x | 8 | 4SU | O2-C2 | 2.11 | 1.26 | 1.23 |
| 1 | 1A | 2251 | OMG | C5-N7 | -2.09 | 1.34 | 1.39 |
| 32 | 1a | 966 | M2G | C5-N7 | -2.08 | 1.34 | 1.39 |
| 1 | 1A | 1915 | 5MU | C6-N1 | -2.07 | 1.34 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 32 | 1a | 1518 | MA6 | C8-N7 | 2.06 | 1.35 | 1.31 |
| 1 | 1A | 1917 | PSU | C2-N3 | -2.06 | 1.34 | 1.37 |
| 32 | 2a | 1498 | UR3 | C6-C5 | 2.05 | 1.39 | 1.35 |
| 54 | 2x | 54 | 5MU | C6-N1 | -2.05 | 1.34 | 1.38 |
| 32 | 2a | 1207 | 2MG | C5-N7 | -2.04 | 1.35 | 1.39 |
| 32 | 1a | 1407 | 5MC | C6-N1 | -2.02 | 1.34 | 1.38 |
| 1 | 1A | 1939 | 5MU | C4-C5 | 2.02 | 1.48 | 1.44 |
| 54 | 2x | 32 | 5MC | C6-N1 | -2.02 | 1.34 | 1.38 |
| 32 | 2a | 1207 | 2MG | C2-N3 | 2.02 | 1.35 | 1.32 |
| 1 | 2A | 1915 | 5MU | C2-N3 | -2.02 | 1.34 | 1.38 |
| 32 | 1a | 1518 | MA6 | C8-N9 | -2.01 | 1.34 | 1.37 |
| 1 | 2A | 2605 | PSU | C2-N3 | -2.00 | 1.34 | 1.37 |

All (267) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 43 | 2l | 92 | 0TD | CSB-SB-CB | -16.09 | 73.45 | 102.36 |
| 43 | 1l | 92 | 0TD | CSB-SB-CB | -9.64 | 85.04 | 102.36 |
| 32 | 1a | 527 | 7MG | N9-C4-N3 | 8.98 | 138.62 | 125.46 |
| 32 | 2a | 527 | 7MG | N9-C4-N3 | 8.54 | 137.97 | 125.46 |
| 1 | 2A | 2503 | 2MA | C5-C4-N3 | -7.80 | 118.96 | 127.18 |
| 1 | 1A | 2503 | 2MA | C5-C4-N3 | -7.22 | 119.58 | 127.18 |
| 32 | 1a | 1498 | UR3 | C4-N3-C2 | -7.08 | 118.89 | 124.58 |
| 32 | 2a | 1498 | UR3 | C4-N3-C2 | -7.04 | 118.92 | 124.58 |
| 32 | 1a | 1207 | 2MG | C2-N3-C4 | 6.89 | 120.62 | 112.00 |
| 32 | 2a | 1207 | 2MG | C2-N3-C4 | 6.88 | 120.61 | 112.00 |
| 32 | 2a | 966 | M2G | C5-C4-N3 | -6.71 | 117.71 | 128.39 |
| 32 | 1a | 966 | M2G | C5-C4-N3 | -6.30 | 118.37 | 128.39 |
| 1 | 1A | 1917 | PSU | N1-C2-N3 | 6.28 | 121.79 | 115.17 |
| 54 | 2x | 55 | PSU | N1-C2-N3 | 6.25 | 121.76 | 115.17 |
| 1 | 2A | 1911 | PSU | N1-C2-N3 | 6.23 | 121.74 | 115.17 |
| 1 | 2A | 2605 | PSU | N1-C2-N3 | 6.15 | 121.66 | 115.17 |
| 1 | 2A | 2251 | OMG | C5-C4-N3 | -6.10 | 118.68 | 128.39 |
| 1 | 1A | 1911 | PSU | N1-C2-N3 | 6.02 | 121.52 | 115.17 |
| 1 | 2A | 1939 | 5MU | C4-N3-C2 | -6.00 | 119.47 | 127.34 |
| 1 | 2A | 1917 | PSU | N1-C2-N3 | 5.98 | 121.48 | 115.17 |
| 32 | 2a | 1207 | 2MG | C5-C4-N3 | -5.98 | 118.88 | 128.39 |
| 54 | 1x | 55 | PSU | N1-C2-N3 | 5.96 | 121.46 | 115.17 |
| 32 | 1a | 516 | PSU | N1-C2-N3 | 5.94 | 121.44 | 115.17 |
| 1 | 1A | 2605 | PSU | N1-C2-N3 | 5.86 | 121.35 | 115.17 |
| 1 | 1A | 2251 | OMG | C5-C4-N3 | -5.83 | 119.11 | 128.39 |
| 32 | 2a | 516 | PSU | N1-C2-N3 | 5.82 | 121.31 | 115.17 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | 2A | 2503 | 2MA | N3-C4-N9 | 5.78 | 134.32 | 126.99 |
| 32 | 1a | 1207 | 2MG | C5-C4-N3 | -5.77 | 119.20 | 128.39 |
| 1 | 2A | 1939 | 5MU | N3-C2-N1 | 5.71 | 122.32 | 114.89 |
| 32 | 2a | 1519 | MA6 | C5-C4-N3 | -5.54 | 119.08 | 126.72 |
| 1 | 1A | 1939 | 5MU | N3-C2-N1 | 5.50 | 122.06 | 114.89 |
| 32 | 1a | 527 | 7MG | C5-C4-N3 | -5.43 | 117.94 | 128.13 |
| 32 | 1a | 1518 | MA6 | C5-C4-N3 | -5.43 | 119.24 | 126.72 |
| 1 | 1A | 1939 | 5MU | C4-N3-C2 | -5.39 | 120.28 | 127.34 |
| 32 | 2a | 527 | 7MG | C5-C4-N3 | -5.38 | 118.03 | 128.13 |
| 32 | 1a | 527 | 7MG | N9-C8-N7 | -5.33 | 95.83 | 103.37 |
| 1 | 1A | 2503 | 2MA | N3-C4-N9 | 5.33 | 133.75 | 126.99 |
| 1 | 1A | 2552 | 2MU | N3-C2-N1 | 5.31 | 121.80 | 114.89 |
| 1 | 2A | 1915 | 5MU | N3-C2-N1 | 5.22 | 121.68 | 114.89 |
| 32 | 2a | 527 | 7MG | N9-C8-N7 | -5.13 | 96.11 | 103.37 |
| 32 | 2a | 966 | M2G | N9-C4-N3 | 5.12 | 136.18 | 125.95 |
| 32 | 1a | 1518 | MA6 | C9-N6-C6 | -5.07 | 107.61 | 120.52 |
| 54 | 2x | 54 | 5MU | N3-C2-N1 | 5.05 | 121.47 | 114.89 |
| 1 | 2A | 2251 | OMG | N9-C4-N3 | 5.02 | 136.00 | 125.95 |
| 1 | 1A | 1915 | 5MU | C4-N3-C2 | -4.98 | 120.82 | 127.34 |
| 1 | 2A | 2552 | 2MU | N3-C2-N1 | 4.95 | 121.33 | 114.89 |
| 32 | 2a | 1518 | MA6 | C5-C4-N3 | -4.94 | 119.91 | 126.72 |
| 32 | 1a | 1519 | MA6 | C5-C4-N3 | -4.94 | 119.92 | 126.72 |
| 1 | 1A | 2552 | 2MU | C4-N3-C2 | -4.88 | 120.56 | 126.61 |
| 1 | 2A | 1939 | 5MU | C5-C4-N3 | 4.87 | 119.55 | 115.32 |
| 32 | 2a | 1518 | MA6 | C9-N6-C6 | -4.86 | 108.16 | 120.52 |
| 54 | 2x | 54 | 5MU | C4-N3-C2 | -4.86 | 120.97 | 127.34 |
| 1 | 1A | 1915 | 5MU | N3-C2-N1 | 4.83 | 121.18 | 114.89 |
| 1 | 1A | 2251 | OMG | C2-N3-C4 | 4.82 | 120.60 | 112.30 |
| 1 | 2A | 1915 | 5MU | C4-N3-C2 | -4.82 | 121.02 | 127.34 |
| 1 | 2A | 2552 | 2MU | C4-N3-C2 | -4.79 | 120.67 | 126.61 |
| 1 | 2A | 1939 | 5MU | C5-C6-N1 | -4.68 | 118.23 | 123.31 |
| 32 | 2a | 966 | M2G | C2-N3-C4 | 4.66 | 121.13 | 112.51 |
| 32 | 1a | 966 | M2G | N9-C4-N3 | 4.58 | 135.10 | 125.95 |
| 1 | 2A | 2251 | OMG | C2-N3-C4 | 4.52 | 120.09 | 112.30 |
| 54 | 1x | 54 | 5MU | N3-C2-N1 | 4.51 | 120.76 | 114.89 |
| 32 | 1a | 527 | 7MG | C2-N3-C4 | 4.49 | 120.04 | 112.30 |
| 54 | 1x | 8 | 4SU | C5-C4-N3 | 4.48 | 118.92 | 114.75 |
| 1 | 1A | 1917 | PSU | C4-N3-C2 | -4.47 | 120.22 | 126.37 |
| 1 | 1A | 1939 | 5MU | O2-C2-N1 | -4.46 | 116.99 | 122.80 |
| 32 | 1a | 1519 | MA6 | C2-N1-C6 | 4.45 | 122.71 | 111.83 |
| 32 | 2a | 1518 | MA6 | C2-N1-C6 | 4.43 | 122.64 | 111.83 |
| 1 | 1A | 1915 | 5MU | C5-C4-N3 | 4.42 | 119.16 | 115.32 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | 1A | 1939 | 5MU | O4-C4-C5 | -4.40 | 119.89 | 124.92 |
| 32 | 1a | 1518 | MA6 | C4-C5-N7 | -4.38 | 105.58 | 110.58 |
| 32 | 2a | 527 | 7MG | C2-N3-C4 | 4.35 | 119.79 | 112.30 |
| 32 | 1a | 1518 | MA6 | C2-N1-C6 | 4.31 | 122.37 | 111.83 |
| 1 | 1A | 2251 | OMG | N9-C4-N3 | 4.31 | 134.57 | 125.95 |
| 32 | 2a | 1519 | MA6 | C2-N1-C6 | 4.30 | 122.32 | 111.83 |
| 1 | 1A | 1939 | 5MU | C5-C6-N1 | -4.28 | 118.66 | 123.31 |
| 32 | 1a | 966 | M2G | C2-N3-C4 | 4.28 | 120.42 | 112.51 |
| 54 | 1x | 54 | 5MU | C4-N3-C2 | -4.27 | 121.75 | 127.34 |
| 32 | 2a | 1519 | MA6 | N3-C4-N9 | 4.24 | 134.38 | 127.17 |
| 54 | 2x | 55 | PSU | C4-N3-C2 | -4.20 | 120.58 | 126.37 |
| 1 | 1A | 1939 | 5MU | C5-C4-N3 | 4.17 | 118.95 | 115.32 |
| 1 | 2A | 1915 | 5MU | C5-C4-N3 | 4.14 | 118.92 | 115.32 |
| 1 | 1A | 2605 | PSU | C4-N3-C2 | -4.14 | 120.67 | 126.37 |
| 32 | 1a | 1518 | MA6 | N3-C4-N9 | 4.12 | 134.17 | 127.17 |
| 32 | 2a | 1207 | 2MG | N9-C4-N3 | 4.12 | 134.19 | 125.95 |
| 54 | 2x | 54 | 5MU | C5-C4-N3 | 4.11 | 118.90 | 115.32 |
| 32 | 1a | 1207 | 2MG | N9-C4-N3 | 4.11 | 134.17 | 125.95 |
| 1 | 2A | 2605 | PSU | C4-N3-C2 | -4.09 | 120.73 | 126.37 |
| 32 | 1a | 1519 | MA6 | C9-N6-C6 | -4.06 | 110.20 | 120.52 |
| 1 | 1A | 1915 | 5MU | O4-C4-C5 | -4.06 | 120.28 | 124.92 |
| 1 | 1A | 1911 | PSU | C4-N3-C2 | -4.05 | 120.80 | 126.37 |
| 54 | 1x | 55 | PSU | C4-N3-C2 | -4.04 | 120.80 | 126.37 |
| 32 | 2a | 1519 | MA6 | C9-N6-C6 | -4.03 | 110.26 | 120.52 |
| 1 | 1A | 2552 | 2MU | O2-C2-N1 | -4.02 | 117.56 | 122.80 |
| 32 | 2a | 1518 | MA6 | C4-C5-N7 | -3.99 | 106.02 | 110.58 |
| 32 | 1a | 1519 | MA6 | N3-C4-N9 | 3.98 | 133.93 | 127.17 |
| 1 | 2A | 1939 | 5MU | O2-C2-N1 | -3.96 | 117.65 | 122.80 |
| 54 | 1x | 32 | 5MC | C5-C6-N1 | -3.95 | 119.02 | 123.31 |
| 1 | 2A | 1911 | PSU | C4-N3-C2 | -3.95 | 120.93 | 126.37 |
| 1 | 2A | 1939 | 5MU | O4-C4-C5 | -3.92 | 120.43 | 124.92 |
| 32 | 1a | 1404 | 5MC | C5-C6-N1 | -3.82 | 119.16 | 123.31 |
| 32 | 2a | 1519 | MA6 | C4-C5-N7 | -3.80 | 106.24 | 110.58 |
| 32 | 2a | 516 | PSU | C4-N3-C2 | -3.79 | 121.15 | 126.37 |
| 54 | 2x | 54 | 5MU | O4-C4-C5 | -3.78 | 120.60 | 124.92 |
| 1 | 2A | 1911 | PSU | O2-C2-N1 | -3.75 | 118.92 | 122.79 |
| 54 | 2x | 8 | 4SU | C5-C4-N3 | 3.75 | 118.24 | 114.75 |
| 1 | 1A | 1911 | PSU | O2-C2-N1 | -3.75 | 118.92 | 122.79 |
| 32 | 1a | 516 | PSU | C4-N3-C2 | -3.74 | 121.22 | 126.37 |
| 1 | 2A | 1917 | PSU | C4-N3-C2 | -3.74 | 121.22 | 126.37 |
| 32 | 1a | 1400 | 5MC | C5-C6-N1 | -3.72 | 119.27 | 123.31 |
| 54 | 1x | 54 | 5MU | C5-C4-N3 | 3.72 | 118.55 | 115.32 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 32 | 1a | 1519 | MA6 | C4-C5-N7 | -3.70 | 106.36 | 110.58 |
| 1 | 2A | 2503 | 2MA | C4-C5-N7 | -3.65 | 106.41 | 110.58 |
| 43 | 2l | 92 | 0TD | OD2-CG-CB | 3.64 | 121.02 | 113.15 |
| 32 | 2a | 1518 | MA6 | N3-C4-N9 | 3.63 | 133.34 | 127.17 |
| 32 | 1a | 1518 | MA6 | C2-N3-C4 | 3.62 | 120.67 | 111.83 |
| 54 | 2x | 32 | 5MC | C5-C6-N1 | -3.61 | 119.39 | 123.31 |
| 32 | 1a | 1207 | 2MG | C6-C5-N7 | 3.58 | 136.80 | 130.29 |
| 43 | 1l | 92 | 0TD | OD2-CG-CB | 3.54 | 120.79 | 113.15 |
| 32 | 2a | 516 | PSU | O2-C2-N1 | -3.53 | 119.15 | 122.79 |
| 1 | 1A | 2503 | 2MA | C4-C5-N7 | -3.52 | 106.56 | 110.58 |
| 54 | 1x | 8 | 4SU | C6-C5-C4 | -3.51 | 116.91 | 119.95 |
| 1 | 1A | 2251 | OMG | C6-C5-N7 | 3.51 | 136.68 | 130.29 |
| 1 | 1A | 1942 | 5MC | C5-C6-N1 | -3.50 | 119.51 | 123.31 |
| 32 | 2a | 1519 | MA6 | C2-N3-C4 | 3.50 | 120.38 | 111.83 |
| 54 | 2x | 8 | 4SU | C1'-N1-C2 | 3.44 | 123.78 | 117.59 |
| 1 | 2A | 1942 | 5MC | C5-C6-N1 | -3.42 | 119.60 | 123.31 |
| 1 | 1A | 2552 | 2MU | C2'-C1'-N1 | -3.42 | 107.75 | 114.24 |
| 32 | 2a | 1518 | MA6 | C2-N3-C4 | 3.40 | 120.13 | 111.83 |
| 1 | 1A | 1917 | PSU | O2-C2-N1 | -3.40 | 119.29 | 122.79 |
| 32 | 2a | 1207 | 2MG | C6-C5-N7 | 3.39 | 136.46 | 130.29 |
| 54 | 1x | 54 | 5MU | O4-C4-C5 | -3.36 | 121.08 | 124.92 |
| 1 | 2A | 1962 | 5MC | C5-C6-N1 | -3.35 | 119.67 | 123.31 |
| 1 | 2A | 2605 | PSU | O2-C2-N1 | -3.35 | 119.34 | 122.79 |
| 32 | 2a | 967 | 5MC | C5-C6-N1 | -3.34 | 119.68 | 123.31 |
| 32 | 1a | 1519 | MA6 | C2-N3-C4 | 3.34 | 119.99 | 111.83 |
| 1 | 2A | 2552 | 2MU | O2-C2-N1 | -3.33 | 118.46 | 122.80 |
| 1 | 1A | 2605 | PSU | O2-C2-N1 | -3.33 | 119.36 | 122.79 |
| 32 | 1a | 1518 | MA6 | N1-C2-N3 | -3.32 | 123.56 | 128.58 |
| 32 | 1a | 1498 | UR3 | C5-C4-N3 | 3.32 | 119.41 | 115.04 |
| 32 | 2a | 1400 | 5MC | C5-C6-N1 | -3.30 | 119.73 | 123.31 |
| 32 | 2a | 1518 | MA6 | N1-C2-N3 | -3.30 | 123.59 | 128.58 |
| 32 | 2a | 1498 | UR3 | C5-C4-N3 | 3.30 | 119.38 | 115.04 |
| 32 | 1a | 1519 | MA6 | N1-C2-N3 | -3.26 | 123.64 | 128.58 |
| 1 | 2A | 1917 | PSU | O2-C2-N1 | -3.25 | 119.44 | 122.79 |
| 32 | 2a | 1519 | MA6 | N1-C6-N6 | 3.25 | 120.81 | 116.86 |
| 32 | 1a | 1518 | MA6 | C4-N9-C8 | 3.24 | 109.14 | 105.74 |
| 54 | 1x | 55 | PSU | O2-C2-N1 | -3.24 | 119.45 | 122.79 |
| 1 | 1A | 1962 | 5MC | C5-C6-N1 | -3.19 | 119.85 | 123.31 |
| 32 | 1a | 516 | PSU | O2-C2-N1 | -3.18 | 119.51 | 122.79 |
| 1 | 2A | 2552 | 2MU | C5-C4-N3 | 3.17 | 119.24 | 114.80 |
| 1 | 1A | 2503 | 2MA | N6-C6-N1 | 3.12 | 121.24 | 117.03 |
| 32 | 1a | 1518 | MA6 | C5-N7-C8 | 3.12 | 108.35 | 103.45 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 32 | 2a | 1519 | MA6 | N1-C2-N3 | -3.12 | 123.86 | 128.58 |
| 32 | 1a | 1519 | MA6 | C4-N9-C8 | 3.10 | 109.00 | 105.74 |
| 32 | 2a | 1400 | 5MC | C5-C4-N3 | -3.08 | 118.60 | 121.75 |
| 54 | 1x | 54 | 5MU | C5-C6-N1 | -3.07 | 119.98 | 123.31 |
| 1 | 2A | 1915 | 5MU | O4-C4-C5 | -3.07 | 121.41 | 124.92 |
| 1 | 1A | 2503 | 2MA | C2-N1-C6 | 3.05 | 122.79 | 118.10 |
| 1 | 1A | 2552 | 2MU | C5-C4-N3 | 3.01 | 119.02 | 114.80 |
| 54 | 1x | 32 | 5MC | C5-C4-N3 | -3.01 | 118.67 | 121.75 |
| 32 | 2a | 1407 | 5MC | C5-C6-N1 | -3.00 | 120.05 | 123.31 |
| 1 | 2A | 1915 | 5MU | C5-C6-N1 | -3.00 | 120.06 | 123.31 |
| 1 | 1A | 1942 | 5MC | C5-C4-N3 | -2.99 | 118.69 | 121.75 |
| 32 | 1a | 966 | M2G | C6-C5-N7 | 2.99 | 135.73 | 130.29 |
| 1 | 1A | 2552 | 2MU | O4-C4-C5 | -2.98 | 120.02 | 125.16 |
| 32 | 2a | 1407 | 5MC | C5-C4-N3 | -2.97 | 118.71 | 121.75 |
| 54 | 2x | 54 | 5MU | C5-C6-N1 | -2.92 | 120.14 | 123.31 |
| 32 | 2a | 1207 | 2MG | C4-C5-N7 | -2.89 | 106.09 | 110.67 |
| 32 | 1a | 1407 | 5MC | C5-C4-N3 | -2.89 | 118.79 | 121.75 |
| 32 | 2a | 1518 | MA6 | C4-N9-C8 | 2.88 | 108.76 | 105.74 |
| 54 | 2x | 8 | 4SU | C6-C5-C4 | -2.87 | 117.46 | 119.95 |
| 54 | 2x | 32 | 5MC | C5-C4-N3 | -2.83 | 118.85 | 121.75 |
| 1 | 1A | 1915 | 5MU | C5-C6-N1 | -2.81 | 120.26 | 123.31 |
| 32 | 1a | 1407 | 5MC | C5-C6-N1 | -2.81 | 120.27 | 123.31 |
| 32 | 2a | 527 | 7MG | C5-C6-N1 | 2.81 | 115.88 | 110.94 |
| 54 | 2x | 55 | PSU | O2-C2-N1 | -2.80 | 119.90 | 122.79 |
| 1 | 1A | 2503 | 2MA | C4-N9-C8 | 2.78 | 108.65 | 105.74 |
| 32 | 2a | 1404 | 5MC | C5-C4-N3 | -2.75 | 118.93 | 121.75 |
| 32 | 2a | 1404 | 5MC | C5-C6-N1 | -2.75 | 120.33 | 123.31 |
| 32 | 2a | 1518 | MA6 | C10-N6-C6 | -2.74 | 113.55 | 120.52 |
| 32 | 1a | 527 | 7MG | C5-C6-N1 | 2.74 | 115.76 | 110.94 |
| 1 | 2A | 2503 | 2MA | C2-N1-C6 | 2.73 | 122.30 | 118.10 |
| 1 | 1A | 2251 | OMG | C4-C5-N7 | -2.72 | 106.35 | 110.67 |
| 32 | 2a | 1518 | MA6 | C10-N6-C9 | -2.72 | 107.44 | 116.18 |
| 54 | 2x | 54 | 5MU | O2-C2-N1 | -2.70 | 119.28 | 122.80 |
| 32 | 1a | 1207 | 2MG | C4-C5-N7 | -2.70 | 106.40 | 110.67 |
| 32 | 2a | 967 | 5MC | C5-C4-N3 | -2.69 | 119.00 | 121.75 |
| 1 | 2A | 2503 | 2MA | N6-C6-N1 | 2.68 | 120.64 | 117.03 |
| 54 | 2x | 32 | 5MC | O2-C2-N3 | -2.67 | 118.11 | 122.33 |
| 32 | 2a | 966 | M2G | C6-C5-N7 | 2.67 | 135.15 | 130.29 |
| 32 | 2a | 1518 | MA6 | C5-N7-C8 | 2.66 | 107.63 | 103.45 |
| 1 | 2A | 1920 | 4OC | O2-C2-N3 | -2.65 | 118.15 | 122.33 |
| 32 | 1a | 966 | M2G | C4-C5-N7 | -2.65 | 106.47 | 110.67 |
| 1 | 2A | 2503 | 2MA | C5-N7-C8 | 2.65 | 107.62 | 103.45 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 32 | 1a | 967 | 5MC | C5-C6-N1 | -2.65 | 120.44 | 123.31 |
| 32 | 1a | 1518 | MA6 | C6-C5-N7 | 2.65 | 137.66 | 133.43 |
| 32 | 1a | 1207 | 2MG | N1-C2-N2 | 2.64 | 119.26 | 116.56 |
| 32 | 2a | 1519 | MA6 | C5-N7-C8 | 2.64 | 107.59 | 103.45 |
| 1 | 2A | 1962 | 5MC | C5-C4-N3 | -2.63 | 119.06 | 121.75 |
| 32 | 2a | 1519 | MA6 | C10-N6-C6 | -2.63 | 113.84 | 120.52 |
| 43 | 2l | 92 | 0TD | OD1-CG-CB | -2.62 | 116.95 | 122.44 |
| 54 | 1x | 8 | 4SU | O2-C2-N1 | 2.59 | 126.16 | 122.80 |
| 32 | 1a | 1519 | MA6 | C5-N7-C8 | 2.58 | 107.50 | 103.45 |
| 32 | 1a | 1518 | MA6 | C10-N6-C6 | -2.57 | 113.98 | 120.52 |
| 32 | 1a | 1404 | 5MC | C5-C4-N3 | -2.57 | 119.12 | 121.75 |
| 1 | 1A | 1917 | PSU | C5-C6-N1 | -2.56 | 118.58 | 122.14 |
| 32 | 1a | 967 | 5MC | C5-C4-N3 | -2.55 | 119.14 | 121.75 |
| 1 | 2A | 2503 | 2MA | C4-N9-C8 | 2.55 | 108.42 | 105.74 |
| 32 | 1a | 967 | 5MC | C1'-N1-C6 | -2.54 | 116.96 | 121.15 |
| 1 | 1A | 1962 | 5MC | C5-C4-N3 | -2.54 | 119.16 | 121.75 |
| 32 | 1a | 1518 | MA6 | N9-C8-N7 | -2.53 | 110.34 | 113.94 |
| 32 | 1a | 1400 | 5MC | C5-C4-N3 | -2.52 | 119.17 | 121.75 |
| 1 | 2A | 1942 | 5MC | C5-C4-N3 | -2.51 | 119.18 | 121.75 |
| 32 | 1a | 1519 | MA6 | N1-C6-N6 | 2.50 | 119.90 | 116.86 |
| 32 | 2a | 966 | M2G | C4-C5-N7 | -2.48 | 106.73 | 110.67 |
| 1 | 2A | 2251 | OMG | C6-C5-N7 | 2.47 | 134.79 | 130.29 |
| 54 | 1x | 54 | 5MU | O2-C2-N1 | -2.45 | 119.60 | 122.80 |
| 32 | 2a | 1519 | MA6 | C4-N9-C8 | 2.45 | 108.31 | 105.74 |
| 1 | 1A | 2503 | 2MA | C6-C5-N7 | 2.44 | 136.80 | 132.09 |
| 1 | 1A | 1915 | 5MU | C5M-C5-C4 | 2.44 | 121.39 | 118.78 |
| 32 | 1a | 1519 | MA6 | C10-N6-C6 | -2.43 | 114.34 | 120.52 |
| 1 | 2A | 2251 | OMG | O6-C6-C5 | -2.43 | 120.12 | 126.53 |
| 1 | 1A | 2503 | 2MA | C5-N7-C8 | 2.42 | 107.26 | 103.45 |
| 32 | 2a | 1518 | MA6 | C6-C5-N7 | 2.42 | 137.29 | 133.43 |
| 32 | 2a | 1498 | UR3 | C3U-N3-C4 | 2.40 | 121.20 | 117.87 |
| 54 | 1x | 8 | 4SU | C1'-N1-C2 | 2.38 | 121.87 | 117.59 |
| 32 | 1a | 1518 | MA6 | C10-N6-C9 | -2.35 | 108.64 | 116.18 |
| 32 | 2a | 1400 | 5MC | O2-C2-N3 | -2.34 | 118.64 | 122.33 |
| 54 | 2x | 54 | 5MU | C5M-C5-C4 | 2.31 | 121.25 | 118.78 |
| 1 | 2A | 2605 | PSU | C5-C6-N1 | -2.30 | 118.95 | 122.14 |
| 32 | 2a | 1207 | 2MG | N1-C2-N2 | 2.29 | 118.90 | 116.56 |
| 1 | 2A | 1915 | 5MU | C5M-C5-C4 | 2.29 | 121.23 | 118.78 |
| 54 | 1x | 8 | 4SU | O2-C2-N3 | -2.29 | 117.27 | 121.49 |
| 54 | 1x | 55 | PSU | C5-C6-N1 | -2.28 | 118.98 | 122.14 |
| 32 | 2a | 1402 | 4OC | C6-C5-C4 | 2.28 | 119.74 | 117.00 |
| 32 | 1a | 527 | 7MG | C5-C4-N9 | -2.27 | 103.43 | 106.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 32 | 1a | 967 | 5MC | O2-C2-N3 | -2.26 | 118.76 | 122.33 |
| 54 | 2x | 8 | 4SU | O2-C2-N1 | 2.26 | 125.74 | 122.80 |
| 1 | 2A | 2503 | 2MA | C6-C5-N7 | 2.23 | 136.39 | 132.09 |
| 32 | 1a | 527 | 7MG | O6-C6-C5 | -2.23 | 122.15 | 127.62 |
| 32 | 1a | 1207 | 2MG | N2-C2-N3 | -2.21 | 117.69 | 120.51 |
| 32 | 1a | 516 | PSU | C6-C5-C4 | -2.21 | 116.68 | 118.17 |
| 1 | 2A | 1915 | 5MU | O2-C2-N3 | -2.19 | 117.44 | 121.49 |
| 32 | 2a | 1518 | MA6 | N9-C8-N7 | -2.19 | 110.83 | 113.94 |
| 1 | 2A | 2503 | 2MA | N9-C8-N7 | -2.19 | 110.83 | 113.94 |
| 1 | 1A | 2503 | 2MA | N9-C8-N7 | -2.17 | 110.86 | 113.94 |
| 43 | 1l | 92 | 0TD | OD1-CG-CB | -2.16 | 117.91 | 122.44 |
| 32 | 2a | 967 | 5MC | O2-C2-N3 | -2.16 | 118.92 | 122.33 |
| 32 | 1a | 1498 | UR3 | C3U-N3-C4 | 2.15 | 120.86 | 117.87 |
| 32 | 1a | 1402 | 4OC | CM4-N4-C4 | -2.14 | 118.27 | 122.45 |
| 32 | 2a | 516 | PSU | O4'-C1'-C2' | 2.14 | 108.11 | 105.15 |
| 32 | 1a | 1207 | 2MG | CM2-N2-C2 | -2.12 | 119.10 | 123.65 |
| 1 | 1A | 2605 | PSU | C5-C6-N1 | -2.11 | 119.21 | 122.14 |
| 1 | 1A | 1915 | 5MU | O2-C2-N1 | -2.11 | 120.05 | 122.80 |
| 32 | 2a | 1207 | 2MG | CM2-N2-C2 | -2.11 | 119.12 | 123.65 |
| 1 | 1A | 2251 | OMG | O6-C6-C5 | -2.10 | 121.00 | 126.53 |
| 32 | 1a | 1404 | 5MC | CM5-C5-C6 | -2.09 | 120.02 | 122.85 |
| 32 | 1a | 1519 | MA6 | C6-C5-N7 | 2.08 | 136.76 | 133.43 |
| 32 | 1a | 1519 | MA6 | N9-C8-N7 | -2.07 | 110.99 | 113.94 |
| 32 | 1a | 1402 | 4OC | C6-C5-C4 | 2.06 | 119.49 | 117.00 |
| 54 | 2x | 55 | PSU | C5-C6-N1 | -2.06 | 119.28 | 122.14 |
| 1 | 2A | 2552 | 2MU | O4-C4-C5 | -2.06 | 121.61 | 125.16 |
| 1 | 1A | 1920 | 4OC | O2-C2-N3 | -2.06 | 119.09 | 122.33 |
| 32 | 2a | 1207 | 2MG | N2-C2-N3 | -2.03 | 117.92 | 120.51 |
| 1 | 2A | 2251 | OMG | C4-C5-N7 | -2.03 | 107.45 | 110.67 |
| 1 | 2A | 1920 | 4OC | C1'-N1-C2 | 2.02 | 122.91 | 118.44 |
| 54 | 1x | 54 | 5MU | C5M-C5-C4 | 2.01 | 120.93 | 118.78 |

There are no chirality outliers.

All (34) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 32 | 1a | 1518 | MA6 | C5-C6-N6-C9 |
| 32 | 1a | 1519 | MA6 | O4'-C4'-C5'-O5' |
| 32 | 2a | 1402 | 4OC | O4'-C4'-C5'-O5' |
| 32 | 2a | 1519 | MA6 | O4'-C4'-C5'-O5' |
| 1 | 1A | 1915 | 5MU | O4'-C4'-C5'-O5' |
| 32 | 1a | 967 | 5MC | O4'-C4'-C5'-O5' |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 32 | 1a | 967 | 5MC | C3'-C4'-C5'-O5' |
| 32 | 1a | 1519 | MA6 | C3'-C4'-C5'-O5' |
| 32 | 1a | 1518 | MA6 | N1-C6-N6-C9 |
| 32 | 2a | 1402 | 4OC | C3'-C4'-C5'-O5' |
| 1 | 1A | 1915 | 5MU | C3'-C4'-C5'-O5' |
| 32 | 2a | 1519 | MA6 | C3'-C4'-C5'-O5' |
| 32 | 2a | 1518 | MA6 | C5-C6-N6-C10 |
| 32 | 2a | 527 | 7MG | C3'-C4'-C5'-O5' |
| 32 | 2a | 1400 | 5MC | O4'-C4'-C5'-O5' |
| 32 | 1a | 1519 | MA6 | C5-C6-N6-C10 |
| 32 | 2a | 1518 | MA6 | C5-C6-N6-C9 |
| 54 | 2x | 55 | PSU | O4'-C1'-C5-C4 |
| 32 | 1a | 527 | 7MG | C3'-C4'-C5'-O5' |
| 32 | 2a | 527 | 7MG | O4'-C4'-C5'-O5' |
| 32 | 1a | 1519 | MA6 | C5-C6-N6-C9 |
| 32 | 2a | 1519 | MA6 | C5-C6-N6-C10 |
| 1 | 2A | 1920 | 4OC | C3'-C2'-O2'-CM2 |
| 32 | 1a | 1402 | 4OC | O4'-C4'-C5'-O5' |
| 32 | 2a | 1400 | 5MC | C3'-C4'-C5'-O5' |
| 32 | 2a | 1519 | MA6 | C4'-C5'-O5'-P |
| 43 | 2l | 92 | 0TD | SB-CB-CG-OD2 |
| 54 | 2x | 55 | PSU | O4'-C1'-C5-C6 |
| 32 | 1a | 1518 | MA6 | C5-C6-N6-C10 |
| 43 | 2l | 92 | 0TD | CA-CB-CG-OD2 |
| 43 | 1l | 92 | 0TD | CG-CB-SB-CSB |
| 43 | 2l | 92 | 0TD | CG-CB-SB-CSB |
| 1 | 1A | 2503 | 2MA | C4'-C5'-O5'-P |
| 1 | 2A | 1920 | 4OC | C2'-C1'-N1-C2 |

There are no ring outliers.

32 monomers are involved in 47 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 1 | 1A | 1939 | 5MU | 1 | 0 |
| 1 | 2A | 1962 | 5MC | 1 | 0 |
| 32 | 2a | 516 | PSU | 2 | 0 |
| 32 | 2a | 1400 | 5MC | 1 | 0 |
| 1 | 2A | 2503 | 2MA | 2 | 0 |
| 1 | 1A | 2251 | OMG | 1 | 0 |
| 1 | 2A | 1915 | 5MU | 1 | 0 |
| 54 | 2x | 32 | 5MC | 1 | 0 |
| 1 | 1A | 2552 | 2MU | 2 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 32 | 1a | 1402 | 4OC | 1 | 0 |
| 1 | 2A | 1942 | 5MC | 2 | 0 |
| 54 | 2x | 8 | 4SU | 2 | 0 |
| 32 | 1a | 1519 | MA6 | 2 | 0 |
| 1 | 1A | 1920 | 4OC | 1 | 0 |
| 43 | 2l | 92 | 0TD | 2 | 0 |
| 32 | 1a | 1518 | MA6 | 2 | 0 |
| 1 | 2A | 1920 | 4OC | 2 | 0 |
| 54 | 1x | 8 | 4SU | 3 | 0 |
| 32 | 2a | 1518 | MA6 | 3 | 0 |
| 32 | 2a | 967 | 5MC | 1 | 0 |
| 1 | 2A | 1911 | PSU | 1 | 0 |
| 1 | 2A | 2552 | 2MU | 3 | 0 |
| 1 | 1A | 1917 | PSU | 1 | 0 |
| 32 | 1a | 1207 | 2MG | 1 | 0 |
| 54 | 1x | 32 | 5MC | 1 | 0 |
| 1 | 2A | 1939 | 5MU | 1 | 0 |
| 32 | 2a | 1402 | 4OC | 2 | 0 |
| 32 | 2a | 1519 | MA6 | 3 | 0 |
| 32 | 1a | 967 | 5MC | 2 | 0 |
| 1 | 2A | 2251 | OMG | 1 | 0 |
| 32 | 2a | 1404 | 5MC | 2 | 0 |
| 32 | 1a | 966 | M2G | 1 | 0 |

## 5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry (i)

Of 2715 ligands modelled in this entry, 2711 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 | V7A | 2a | 3210 | 55 | 37,38,38 | 3.93 | 11 (29%) | 43,60,60 | 1.65 | 9 (20%) |
| 58 | SF4 | 2d | 303 | 35 | 0,12,12 | - | - | - | | |
| 57 | V7A | 1a | 1835 | 55 | 37,38,38 | 4.19 | 12 (32%) | 43,60,60 | 1.77 | 9 (20%) |
| 58 | SF4 | 1d | 501 | 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 | V7A | 2a | 3210 | 55 | - | 4/13/72/72 | 0/4/4/4 |
| 58 | SF4 | 2d | 303 | 35 | - | - | 0/6/5/5 |
| 57 | V7A | 1a | 1835 | 55 | - | 4/13/72/72 | 0/4/4/4 |
| 58 | SF4 | 1d | 501 | 35 | - | - | 0/6/5/5 |

All (23) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 57 | 1a | 1835 | V7A | CAM-CAL | -14.48 | 1.39 | 1.52 |
| 57 | 2a | 3210 | V7A | CAM-CAL | -12.85 | 1.40 | 1.52 |
| 57 | 1a | 1835 | V7A | CAM-CAP | -11.58 | 1.39 | 1.55 |
| 57 | 1a | 1835 | V7A | CAJ-CAI | -11.22 | 1.40 | 1.51 |
| 57 | 2a | 3210 | V7A | CAJ-CAI | -10.67 | 1.40 | 1.51 |
| 57 | 2a | 3210 | V7A | CAM-CAP | -10.41 | 1.41 | 1.55 |
| 57 | 1a | 1835 | V7A | CAS-CAA | -7.08 | 1.39 | 1.51 |
| 57 | 2a | 3210 | V7A | CAS-CAA | -7.04 | 1.39 | 1.51 |
| 57 | 2a | 3210 | V7A | CAG-CAF | -6.80 | 1.41 | 1.51 |
| 57 | 1a | 1835 | V7A | CAG-CAF | -6.49 | 1.41 | 1.51 |
| 57 | 1a | 1835 | V7A | CAO-CAR | -5.35 | 1.41 | 1.51 |
| 57 | 2a | 3210 | V7A | CAO-CAR | -5.28 | 1.41 | 1.51 |
| 57 | 2a | 3210 | V7A | CAQ-CBC | -3.72 | 1.39 | 1.47 |
| 57 | 1a | 1835 | V7A | CAQ-CBC | -3.51 | 1.40 | 1.47 |
| 57 | 1a | 1835 | V7A | CAI-CAH | -3.32 | 1.39 | 1.46 |
| 57 | 2a | 3210 | V7A | CAI-CAL | 3.22 | 1.40 | 1.36 |
| 57 | 2a | 3210 | V7A | CAI-CAH | -3.12 | 1.39 | 1.46 |
| 57 | 1a | 1835 | V7A | CAE-CAH | -3.05 | 1.38 | 1.46 |
| 57 | 2a | 3210 | V7A | CAE-CAH | -2.90 | 1.39 | 1.46 |
| 57 | 1a | 1835 | V7A | CAQ-CAP | -2.60 | 1.39 | 1.46 |
| 57 | 2a | 3210 | V7A | CAQ-CAP | -2.51 | 1.39 | 1.46 |
| 57 | 1a | 1835 | V7A | CAM-CAN | -2.44 | 1.51 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 57 | 1a | 1835 | V7A | CAI-CAL | 2.15 | 1.38 | 1.36 |

All (18) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | 1a | 1835 | V7A | CAJ-CAK-CAN | -3.90 | 103.74 | 110.38 |
| 57 | 1a | 1835 | V7A | OAZ-CAL-CAI | -3.74 | 116.27 | 123.52 |
| 57 | 2a | 3210 | V7A | OBI-CAR-CAQ | -3.73 | 116.69 | 122.93 |
| 57 | 1a | 1835 | V7A | OBI-CAR-CAQ | -3.62 | 116.88 | 122.93 |
| 57 | 2a | 3210 | V7A | OAZ-CAL-CAI | -3.61 | 116.51 | 123.52 |
| 57 | 2a | 3210 | V7A | CAJ-CAK-CAN | -3.50 | 104.42 | 110.38 |
| 57 | 1a | 1835 | V7A | CBG-NBF-CAO | -3.31 | 106.57 | 114.10 |
| 57 | 1a | 1835 | V7A | OAZ-CAL-CAM | 3.19 | 117.99 | 113.37 |
| 57 | 2a | 3210 | V7A | CAM-CAP-CAQ | 3.11 | 120.70 | 115.75 |
| 57 | 1a | 1835 | V7A | CAM-CAP-CAQ | 2.90 | 120.35 | 115.75 |
| 57 | 2a | 3210 | V7A | OAZ-CAL-CAM | 2.87 | 117.52 | 113.37 |
| 57 | 2a | 3210 | V7A | CAM-CAL-CAI | 2.85 | 125.96 | 123.06 |
| 57 | 1a | 1835 | V7A | CAM-CAL-CAI | 2.63 | 125.73 | 123.06 |
| 57 | 2a | 3210 | V7A | OAX-CAD-CAE | -2.43 | 116.66 | 121.14 |
| 57 | 1a | 1835 | V7A | OAX-CAD-CAE | -2.36 | 116.78 | 121.14 |
| 57 | 1a | 1835 | V7A | CAK-CAN-CAO | 2.33 | 117.10 | 113.73 |
| 57 | 2a | 3210 | V7A | CBH-NBF-CAO | -2.32 | 108.81 | 114.10 |
| 57 | 2a | 3210 | V7A | OBB-CAP-CAQ | -2.13 | 118.73 | 123.23 |

There are no chirality outliers.

All (8) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 57 | 1a | 1835 | V7A | CAN-CAO-NBF-CBH |
| 57 | 1a | 1835 | V7A | CAA-CAS-NAT-CAW |
| 57 | 1a | 1835 | V7A | CAA-CAS-NAT-OAU |
| 57 | 1a | 1835 | V7A | CAW-NAT-OAU-CAV |
| 57 | 2a | 3210 | V7A | CAA-CAS-NAT-CAW |
| 57 | 2a | 3210 | V7A | CAA-CAS-NAT-OAU |
| 57 | 2a | 3210 | V7A | CAW-NAT-OAU-CAV |
| 57 | 2a | 3210 | V7A | CAF-CAA-CAS-NAT |

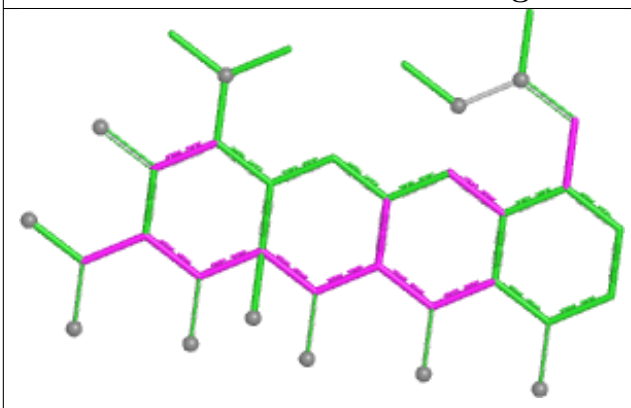
There are no ring outliers.

4 monomers are involved in 10 short contacts:

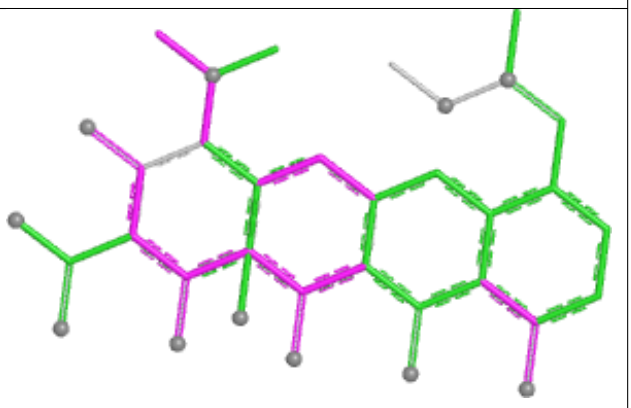
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 57 | 2a | 3210 | V7A | 4 | 0 |
| 58 | 2d | 303 | SF4 | 1 | 0 |
| 57 | 1a | 1835 | V7A | 2 | 0 |
| 58 | 1d | 501 | SF4 | 3 | 0 |

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

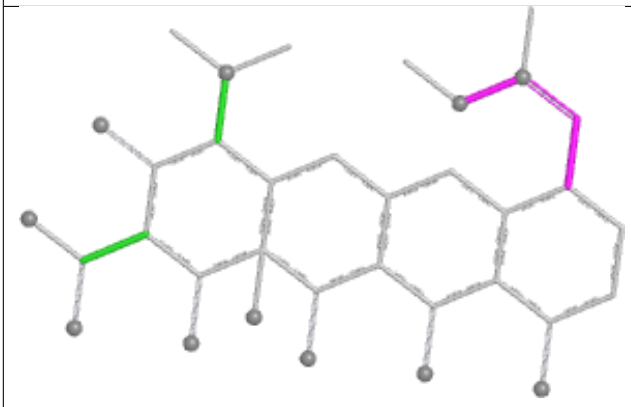
**Ligand V7A 2a 3210**



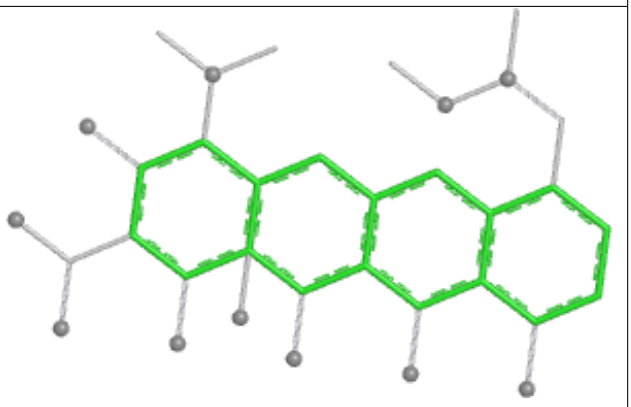
**Bond lengths**



**Bond angles**

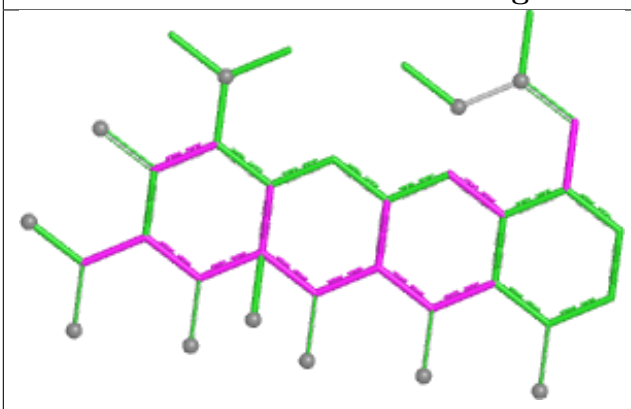


**Torsions**

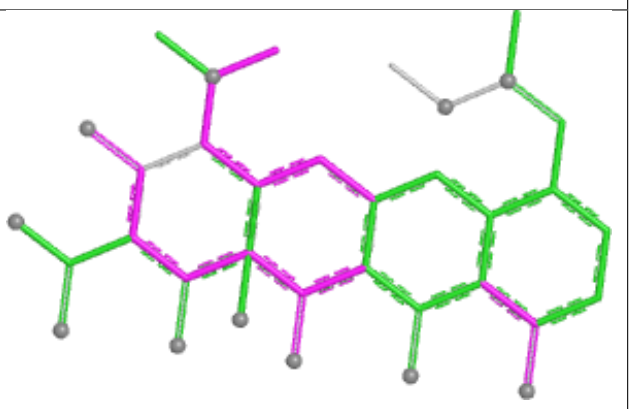


**Rings**

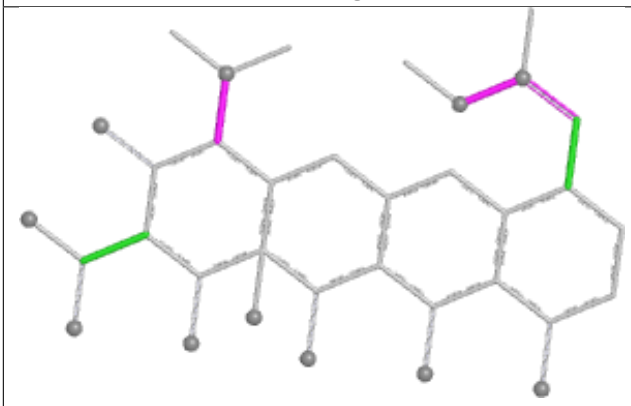
**Ligand V7A 1a 1835**



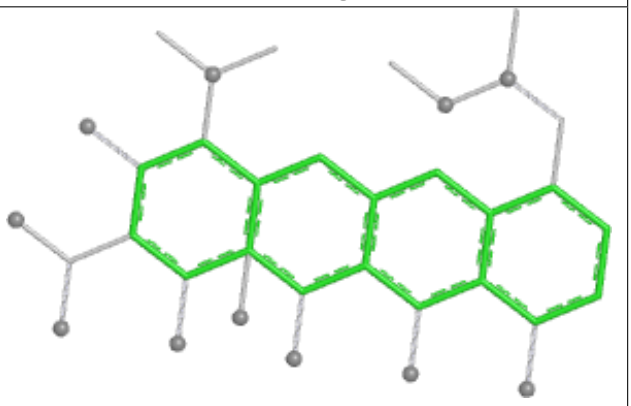
Bond lengths



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 | 71 (2%) 58 48 | 17, 35, 97, 110 | 0 |
| 1 | 2A | 2789/2915 (95%) | -0.06 | 82 (2%) 53 43 | 28, 55, 93, 117 | 0 |
| 2 | 1B | 120/121 (99%) | -0.41 | 1 (0%) 82 75 | 25, 50, 67, 89 | 0 |
| 2 | 2B | 120/121 (99%) | 0.60 | 6 (5%) 34 26 | 58, 79, 89, 99 | 0 |
| 3 | 1D | 275/276 (99%) | -0.05 | 3 (1%) 78 70 | 19, 36, 50, 75 | 0 |
| 3 | 2D | 275/276 (99%) | 0.17 | 4 (1%) 72 63 | 28, 48, 62, 79 | 0 |
| 4 | 1E | 204/206 (99%) | -0.25 | 0 100 100 | 18, 38, 58, 75 | 0 |
| 4 | 2E | 204/206 (99%) | 0.21 | 2 (0%) 79 72 | 32, 53, 69, 78 | 0 |
| 5 | 1F | 203/210 (96%) | -0.15 | 0 100 100 | 19, 40, 65, 83 | 0 |
| 5 | 2F | 203/210 (96%) | 0.43 | 3 (1%) 72 63 | 33, 64, 80, 88 | 0 |
| 6 | 1G | 181/182 (99%) | 0.51 | 11 (6%) 27 20 | 37, 58, 72, 86 | 0 |
| 6 | 2G | 181/182 (99%) | 1.06 | 14 (7%) 19 14 | 63, 79, 86, 94 | 0 |
| 7 | 1H | 174/180 (96%) | -0.05 | 1 (0%) 85 80 | 35, 51, 64, 72 | 0 |
| 7 | 2H | 174/180 (96%) | 0.95 | 16 (9%) 14 10 | 67, 80, 89, 95 | 0 |
| 8 | 1I | 146/148 (98%) | 0.43 | 1 (0%) 84 77 | 40, 70, 78, 83 | 0 |
| 8 | 2I | 146/148 (98%) | 2.22 | 74 (50%) 0 0 | 52, 87, 98, 104 | 0 |
| 9 | 1N | 140/140 (100%) | -0.18 | 0 100 100 | 22, 38, 60, 71 | 0 |
| 9 | 2N | 140/140 (100%) | 0.29 | 1 (0%) 84 77 | 44, 63, 78, 87 | 0 |
| 10 | 1O | 122/122 (100%) | -0.12 | 1 (0%) 82 75 | 28, 40, 55, 60 | 0 |
| 10 | 2O | 122/122 (100%) | 0.11 | 2 (1%) 70 61 | 40, 52, 64, 72 | 0 |
| 11 | 1P | 149/150 (99%) | 0.04 | 2 (1%) 75 66 | 18, 43, 64, 71 | 0 |
| 11 | 2P | 149/150 (99%) | 0.52 | 8 (5%) 31 24 | 37, 65, 80, 88 | 0 |
| 12 | 1Q | 141/141 (100%) | 0.04 | 2 (1%) 73 64 | 28, 39, 54, 69 | 0 |
| 12 | 2Q | 141/141 (100%) | 0.64 | 7 (4%) 34 26 | 46, 62, 74, 79 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|
| 13 | 1R | 118/118 (100%) | -0.15 | 0 100 100 | 24, 32, 47, 60 | 0 |
| 13 | 2R | 118/118 (100%) | -0.04 | 0 100 100 | 37, 49, 61, 66 | 0 |
| 14 | 1S | 110/112 (98%) | -0.03 | 0 100 100 | 35, 48, 58, 63 | 0 |
| 14 | 2S | 110/112 (98%) | 0.96 | 13 (11%) 9 7 | 59, 72, 80, 87 | 0 |
| 15 | 1T | 131/146 (89%) | -0.05 | 5 (3%) 44 35 | 30, 44, 68, 78 | 0 |
| 15 | 2T | 131/146 (89%) | 0.41 | 2 (1%) 72 63 | 47, 57, 73, 82 | 0 |
| 16 | 1U | 116/118 (98%) | -0.35 | 1 (0%) 81 74 | 20, 29, 43, 63 | 0 |
| 16 | 2U | 116/118 (98%) | 0.32 | 1 (0%) 81 74 | 40, 59, 72, 80 | 0 |
| 17 | 1V | 101/101 (100%) | -0.34 | 0 100 100 | 21, 36, 58, 67 | 0 |
| 17 | 2V | 101/101 (100%) | 0.41 | 4 (3%) 42 33 | 40, 68, 79, 84 | 0 |
| 18 | 1W | 112/113 (99%) | -0.44 | 0 100 100 | 19, 29, 46, 82 | 0 |
| 18 | 2W | 112/113 (99%) | 0.24 | 1 (0%) 81 74 | 39, 49, 66, 86 | 0 |
| 19 | 1X | 95/96 (98%) | -0.10 | 1 (1%) 78 70 | 24, 36, 56, 75 | 0 |
| 19 | 2X | 95/96 (98%) | 0.56 | 5 (5%) 32 24 | 47, 59, 75, 81 | 0 |
| 20 | 1Y | 107/110 (97%) | 0.22 | 1 (0%) 81 74 | 33, 47, 69, 79 | 0 |
| 20 | 2Y | 107/110 (97%) | 0.91 | 9 (8%) 17 12 | 56, 70, 80, 92 | 0 |
| 21 | 1Z | 154/206 (74%) | 0.33 | 4 (2%) 57 47 | 38, 56, 70, 78 | 0 |
| 21 | 2Z | 160/206 (77%) | 0.99 | 17 (10%) 11 8 | 63, 74, 86, 94 | 0 |
| 22 | 10 | 83/85 (97%) | 0.26 | 9 (10%) 11 8 | 25, 35, 69, 86 | 0 |
| 22 | 20 | 83/85 (97%) | 0.86 | 11 (13%) 7 5 | 50, 61, 79, 89 | 0 |
| 23 | 11 | 97/98 (98%) | 0.13 | 1 (1%) 79 72 | 23, 41, 68, 75 | 0 |
| 23 | 21 | 97/98 (98%) | 0.54 | 3 (3%) 51 41 | 40, 54, 73, 81 | 0 |
| 24 | 12 | 70/72 (97%) | 0.23 | 2 (2%) 53 43 | 35, 47, 57, 76 | 0 |
| 24 | 22 | 70/72 (97%) | 0.54 | 2 (2%) 53 43 | 56, 69, 80, 85 | 0 |
| 25 | 13 | 59/60 (98%) | -0.28 | 0 100 100 | 23, 35, 54, 72 | 0 |
| 25 | 23 | 59/60 (98%) | 0.43 | 0 100 100 | 47, 58, 75, 83 | 0 |
| 26 | 14 | 69/71 (97%) | 0.58 | 4 (5%) 29 22 | 56, 74, 88, 94 | 0 |
| 26 | 24 | 69/71 (97%) | 1.17 | 14 (20%) 3 2 | 75, 86, 93, 98 | 0 |
| 27 | 15 | 59/60 (98%) | -0.35 | 1 (1%) 69 60 | 18, 32, 51, 67 | 0 |
| 27 | 25 | 59/60 (98%) | 0.09 | 2 (3%) 48 39 | 35, 50, 66, 83 | 0 |
| 28 | 16 | 53/54 (98%) | -0.11 | 0 100 100 | 28, 38, 51, 59 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|
| 28 | 26 | 53/54 (98%) | 0.83 | 3 (5%) 29 22 | 49, 58, 69, 71 | 0 |
| 29 | 17 | 48/49 (97%) | 0.03 | 4 (8%) 17 12 | 22, 26, 55, 59 | 0 |
| 29 | 27 | 48/49 (97%) | 0.17 | 3 (6%) 26 19 | 31, 41, 62, 75 | 0 |
| 30 | 18 | 64/65 (98%) | -0.07 | 0 100 100 | 25, 31, 39, 53 | 0 |
| 30 | 28 | 64/65 (98%) | 0.45 | 0 100 100 | 44, 54, 61, 73 | 0 |
| 31 | 19 | 37/37 (100%) | -0.03 | 0 100 100 | 28, 38, 56, 62 | 0 |
| 31 | 29 | 37/37 (100%) | 0.86 | 2 (5%) 31 24 | 53, 64, 75, 77 | 0 |
| 32 | 1a | 1488/1521 (97%) | 0.28 | 25 (1%) 69 60 | 37, 71, 95, 109 | 0 |
| 32 | 2a | 1491/1521 (98%) | 0.32 | 32 (2%) 63 54 | 44, 75, 96, 111 | 0 |
| 33 | 1b | 231/256 (90%) | 0.92 | 24 (10%) 11 8 | 64, 78, 90, 97 | 0 |
| 33 | 2b | 231/256 (90%) | 1.09 | 34 (14%) 6 4 | 67, 83, 90, 100 | 0 |
| 34 | 1c | 206/239 (86%) | 0.86 | 15 (7%) 21 15 | 64, 76, 85, 90 | 0 |
| 34 | 2c | 206/239 (86%) | 1.16 | 26 (12%) 8 6 | 71, 82, 90, 93 | 0 |
| 35 | 1d | 208/209 (99%) | 0.97 | 28 (13%) 7 5 | 59, 74, 87, 97 | 0 |
| 35 | 2d | 208/209 (99%) | 0.75 | 12 (5%) 29 22 | 58, 70, 80, 85 | 0 |
| 36 | 1e | 148/162 (91%) | 0.41 | 1 (0%) 84 77 | 54, 66, 74, 77 | 0 |
| 36 | 2e | 148/162 (91%) | 0.68 | 8 (5%) 31 24 | 60, 71, 81, 85 | 0 |
| 37 | 1f | 100/101 (99%) | 0.56 | 3 (3%) 52 42 | 55, 69, 76, 79 | 0 |
| 37 | 2f | 100/101 (99%) | 0.54 | 5 (5%) 34 26 | 63, 71, 79, 82 | 0 |
| 38 | 1g | 155/156 (99%) | 0.61 | 9 (5%) 29 22 | 63, 73, 86, 90 | 0 |
| 38 | 2g | 155/156 (99%) | 0.68 | 8 (5%) 33 25 | 69, 80, 91, 96 | 0 |
| 39 | 1h | 137/138 (99%) | 0.49 | 3 (2%) 62 52 | 56, 68, 76, 82 | 0 |
| 39 | 2h | 137/138 (99%) | 0.64 | 6 (4%) 39 31 | 61, 74, 80, 87 | 0 |
| 40 | 1i | 127/128 (99%) | 1.37 | 25 (19%) 3 2 | 61, 78, 84, 86 | 0 |
| 40 | 2i | 127/128 (99%) | 1.55 | 33 (25%) 1 1 | 70, 85, 92, 94 | 0 |
| 41 | 1j | 97/105 (92%) | 1.32 | 15 (15%) 5 4 | 64, 80, 90, 91 | 0 |
| 41 | 2j | 96/105 (91%) | 1.70 | 33 (34%) 1 1 | 75, 85, 93, 95 | 0 |
| 42 | 1k | 114/129 (88%) | 0.41 | 6 (5%) 32 24 | 44, 67, 78, 80 | 0 |
| 42 | 2k | 114/129 (88%) | 0.58 | 4 (3%) 47 38 | 55, 73, 80, 84 | 0 |
| 43 | 1l | 121/132 (91%) | 0.45 | 4 (3%) 49 39 | 49, 61, 70, 76 | 0 |
| 43 | 2l | 121/132 (91%) | 0.55 | 4 (3%) 49 39 | 53, 63, 73, 80 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|
| 44 | 1m | 122/126 (96%) | 0.82 | 9 (7%) 20 15 | 61, 72, 82, 84 | 0 |
| 44 | 2m | 121/126 (96%) | 1.45 | 26 (21%) 2 2 | 73, 82, 87, 93 | 0 |
| 45 | 1n | 60/61 (98%) | 1.47 | 13 (21%) 2 2 | 67, 74, 80, 81 | 0 |
| 45 | 2n | 60/61 (98%) | 2.03 | 30 (50%) 0 0 | 72, 83, 87, 90 | 0 |
| 46 | 1o | 88/89 (98%) | 0.38 | 2 (2%) 61 51 | 48, 63, 76, 86 | 0 |
| 46 | 2o | 88/89 (98%) | 0.52 | 2 (2%) 61 51 | 56, 69, 76, 81 | 0 |
| 47 | 1p | 82/88 (93%) | 1.44 | 19 (23%) 2 1 | 62, 75, 84, 87 | 0 |
| 47 | 2p | 82/88 (93%) | 0.81 | 6 (7%) 21 15 | 58, 68, 77, 82 | 0 |
| 48 | 1q | 99/105 (94%) | 0.71 | 4 (4%) 42 33 | 56, 65, 74, 79 | 0 |
| 48 | 2q | 99/105 (94%) | 0.78 | 6 (6%) 27 20 | 55, 68, 78, 84 | 0 |
| 49 | 1r | 68/88 (77%) | 0.44 | 2 (2%) 53 43 | 59, 69, 77, 81 | 0 |
| 49 | 2r | 68/88 (77%) | 0.46 | 2 (2%) 53 43 | 62, 70, 79, 83 | 0 |
| 50 | 1s | 83/93 (89%) | 0.81 | 5 (6%) 27 21 | 63, 76, 85, 89 | 0 |
| 50 | 2s | 83/93 (89%) | 1.25 | 10 (12%) 9 6 | 75, 83, 91, 94 | 0 |
| 51 | 1t | 96/106 (90%) | 0.92 | 12 (12%) 8 6 | 61, 71, 80, 84 | 0 |
| 51 | 2t | 96/106 (90%) | 0.53 | 3 (3%) 51 41 | 58, 68, 76, 79 | 0 |
| 52 | 1u | 23/27 (85%) | 1.04 | 2 (8%) 16 11 | 66, 72, 77, 80 | 0 |
| 52 | 2u | 23/27 (85%) | 2.02 | 13 (56%) 0 0 | 75, 80, 82, 85 | 0 |
| 53 | 1v | 10/24 (41%) | 1.47 | 4 (40%) 1 0 | 54, 92, 98, 99 | 0 |
| 53 | 2v | 6/24 (25%) | 0.76 | 1 (16%) 4 3 | 67, 72, 86, 96 | 0 |
| 54 | 1x | 72/77 (93%) | -0.03 | 1 (1%) 73 64 | 38, 64, 78, 89 | 0 |
| 54 | 2x | 72/77 (93%) | 0.23 | 2 (2%) 55 45 | 49, 77, 89, 93 | 0 |
| All | All | 20598/21444 (96%) | 0.28 | 974 (4%) 36 29 | 17, 63, 89, 117 | 0 |

All (974) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | 2A | 2147 | G | 9.5 |
| 1 | 1A | 2145 | C | 8.9 |
| 1 | 2A | 2111 | C | 7.8 |
| 8 | 2I | 111 | PRO | 7.8 |
| 1 | 2A | 2148 | G | 7.6 |
| 8 | 2I | 119 | PRO | 7.5 |
| 8 | 2I | 145 | VAL | 7.4 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 44 | 2m | 102 | ARG | 7.2 |
| 22 | 10 | 6 | GLY | 6.9 |
| 1 | 2A | 2146 | C | 6.7 |
| 44 | 1m | 123 | ALA | 6.6 |
| 8 | 2I | 118 | LYS | 6.6 |
| 1 | 2A | 2155 | G | 6.3 |
| 1 | 2A | 2166 | G | 6.3 |
| 1 | 1A | 2121 | G | 6.2 |
| 1 | 2A | 2112 | G | 6.2 |
| 8 | 2I | 86 | THR | 5.9 |
| 23 | 21 | 2 | SER | 5.9 |
| 8 | 2I | 100 | ALA | 5.9 |
| 1 | 2A | 2120 | G | 5.8 |
| 8 | 2I | 97 | ILE | 5.8 |
| 1 | 1A | 2113 | U | 5.6 |
| 32 | 2a | 1030(B) | C | 5.6 |
| 8 | 2I | 92 | VAL | 5.6 |
| 1 | 1A | 2111 | C | 5.5 |
| 1 | 2A | 2143 | C | 5.5 |
| 44 | 2m | 6 | GLY | 5.4 |
| 1 | 1A | 2115 | G | 5.4 |
| 1 | 2A | 2145 | C | 5.4 |
| 1 | 1A | 2112 | G | 5.3 |
| 8 | 2I | 120 | ILE | 5.2 |
| 50 | 1s | 39 | THR | 5.1 |
| 8 | 2I | 124 | GLY | 5.1 |
| 8 | 2I | 93 | THR | 5.0 |
| 47 | 1p | 68 | ASP | 5.0 |
| 38 | 2g | 80 | VAL | 5.0 |
| 1 | 2A | 2167 | U | 4.9 |
| 1 | 2A | 2110 | G | 4.9 |
| 22 | 20 | 6 | GLY | 4.8 |
| 8 | 2I | 144 | VAL | 4.8 |
| 1 | 2A | 2144 | U | 4.8 |
| 44 | 2m | 7 | VAL | 4.8 |
| 1 | 2A | 2168 | G | 4.7 |
| 1 | 2A | 2138 | C | 4.7 |
| 22 | 20 | 4 | LYS | 4.7 |
| 8 | 2I | 99 | GLU | 4.7 |
| 40 | 2i | 126 | SER | 4.6 |
| 1 | 2A | 2117 | A | 4.6 |
| 8 | 2I | 109 | ILE | 4.6 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | 1A | 2117 | A | 4.6 |
| 8 | 2I | 121 | LYS | 4.6 |
| 22 | 20 | 7 | LEU | 4.5 |
| 1 | 2A | 2142 | C | 4.5 |
| 34 | 2c | 2 | GLY | 4.5 |
| 40 | 1i | 126 | SER | 4.5 |
| 40 | 2i | 102 | LEU | 4.5 |
| 17 | 2V | 73 | SER | 4.5 |
| 8 | 2I | 94 | ALA | 4.4 |
| 33 | 2b | 7 | VAL | 4.4 |
| 32 | 1a | 1030(B) | C | 4.4 |
| 1 | 2A | 2113 | U | 4.4 |
| 44 | 1m | 122 | LYS | 4.4 |
| 22 | 10 | 9 | SER | 4.4 |
| 21 | 2Z | 143 | GLY | 4.4 |
| 1 | 2A | 2122 | U | 4.4 |
| 1 | 1A | 2110 | G | 4.3 |
| 1 | 2A | 2169 | A | 4.3 |
| 22 | 20 | 2 | ALA | 4.3 |
| 1 | 2A | 2109 | U | 4.3 |
| 1 | 1A | 2147 | G | 4.3 |
| 1 | 2A | 2121 | G | 4.3 |
| 8 | 2I | 126 | TYR | 4.3 |
| 22 | 10 | 7 | LEU | 4.3 |
| 22 | 10 | 8 | GLY | 4.2 |
| 45 | 2n | 13 | THR | 4.2 |
| 45 | 2n | 25 | VAL | 4.2 |
| 34 | 2c | 206 | GLU | 4.2 |
| 31 | 29 | 12 | ASP | 4.2 |
| 41 | 2j | 5 | ARG | 4.1 |
| 40 | 1i | 106 | ALA | 4.1 |
| 1 | 1A | 2119 | A | 4.1 |
| 45 | 1n | 2 | ALA | 4.1 |
| 51 | 1t | 103 | GLY | 4.1 |
| 21 | 2Z | 142 | SER | 4.1 |
| 1 | 2A | 2165 | G | 4.1 |
| 28 | 26 | 5 | VAL | 4.0 |
| 32 | 1a | 1030 | C | 4.0 |
| 1 | 2A | 2115 | G | 4.0 |
| 8 | 2I | 140 | LEU | 4.0 |
| 33 | 2b | 165 | VAL | 4.0 |
| 1 | 1A | 2181 | G | 4.0 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 32 | 2a | 1033 | G | 4.0 |
| 6 | 2G | 28 | VAL | 4.0 |
| 38 | 2g | 83 | ALA | 3.9 |
| 1 | 1A | 2143 | C | 3.9 |
| 8 | 2I | 83 | ALA | 3.9 |
| 40 | 1i | 105 | ASP | 3.9 |
| 44 | 2m | 121 | LYS | 3.9 |
| 1 | 1A | 2146 | C | 3.9 |
| 33 | 2b | 187 | LEU | 3.9 |
| 8 | 2I | 142 | VAL | 3.9 |
| 8 | 2I | 133 | HIS | 3.9 |
| 8 | 2I | 134 | PRO | 3.9 |
| 40 | 2i | 105 | ASP | 3.9 |
| 1 | 1A | 2120 | G | 3.9 |
| 8 | 2I | 88 | ILE | 3.9 |
| 1 | 2A | 2161 | C | 3.9 |
| 35 | 1d | 166 | LYS | 3.8 |
| 1 | 2A | 2118 | U | 3.8 |
| 33 | 1b | 7 | VAL | 3.8 |
| 16 | 1U | 117 | GLN | 3.8 |
| 44 | 2m | 5 | ALA | 3.8 |
| 22 | 10 | 4 | LYS | 3.8 |
| 1 | 1A | 2122 | U | 3.8 |
| 1 | 1A | 2170 | A | 3.8 |
| 26 | 24 | 56 | VAL | 3.8 |
| 8 | 2I | 79 | ILE | 3.8 |
| 24 | 12 | 70 | GLN | 3.8 |
| 44 | 1m | 102 | ARG | 3.8 |
| 1 | 2A | 2149 | G | 3.8 |
| 40 | 2i | 43 | ALA | 3.7 |
| 32 | 1a | 1030(A) | G | 3.7 |
| 8 | 2I | 76 | THR | 3.7 |
| 8 | 2I | 117 | GLU | 3.7 |
| 1 | 1A | 2109 | U | 3.7 |
| 1 | 1A | 2174 | C | 3.7 |
| 1 | 1A | 2141 | G | 3.7 |
| 1 | 2A | 2116 | G | 3.7 |
| 8 | 2I | 116 | LEU | 3.7 |
| 19 | 2X | 92 | LEU | 3.7 |
| 20 | 2Y | 80 | GLY | 3.7 |
| 43 | 2l | 18 | VAL | 3.7 |
| 1 | 1A | 1064 | C | 3.6 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 22 | 20 | 3 | HIS | 3.6 |
| 40 | 1i | 15 | ALA | 3.6 |
| 11 | 2P | 109 | GLY | 3.6 |
| 21 | 1Z | 146 | ILE | 3.6 |
| 33 | 1b | 201 | ILE | 3.6 |
| 14 | 2S | 32 | LEU | 3.6 |
| 32 | 1a | 1447 | A | 3.6 |
| 8 | 2I | 84 | GLY | 3.6 |
| 44 | 2m | 98 | VAL | 3.6 |
| 40 | 1i | 13 | ALA | 3.6 |
| 1 | 2A | 2108 | C | 3.6 |
| 53 | 2v | 14 | A | 3.6 |
| 6 | 2G | 139 | LEU | 3.6 |
| 47 | 1p | 1 | MET | 3.6 |
| 44 | 2m | 122 | LYS | 3.6 |
| 1 | 2A | 2140 | C | 3.6 |
| 6 | 1G | 146 | TYR | 3.6 |
| 1 | 2A | 2170 | A | 3.6 |
| 51 | 1t | 18 | GLN | 3.5 |
| 1 | 2A | 2159 | G | 3.5 |
| 26 | 24 | 49 | PHE | 3.5 |
| 23 | 11 | 2 | SER | 3.5 |
| 8 | 2I | 128 | LEU | 3.5 |
| 1 | 2A | 2114 | A | 3.5 |
| 52 | 2u | 6 | ARG | 3.5 |
| 31 | 29 | 37 | GLY | 3.5 |
| 1 | 2A | 2123 | G | 3.5 |
| 38 | 1g | 84 | ASN | 3.5 |
| 1 | 2A | 2174 | C | 3.5 |
| 6 | 2G | 53 | LEU | 3.5 |
| 8 | 2I | 123 | LEU | 3.5 |
| 32 | 2a | 1034 | G | 3.5 |
| 8 | 2I | 138 | ILE | 3.5 |
| 1 | 1A | 2179 | C | 3.5 |
| 1 | 1A | 1078 | U | 3.5 |
| 8 | 2I | 141 | LYS | 3.5 |
| 35 | 1d | 150 | GLU | 3.5 |
| 1 | 1A | 2168 | G | 3.4 |
| 8 | 2I | 101 | LEU | 3.4 |
| 8 | 2I | 112 | LYS | 3.4 |
| 21 | 2Z | 150 | LEU | 3.4 |
| 44 | 2m | 90 | LEU | 3.4 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 45 | 2n | 11 | LYS | 3.4 |
| 1 | 2A | 2139 | C | 3.4 |
| 40 | 1i | 7 | THR | 3.4 |
| 34 | 2c | 158 | GLY | 3.4 |
| 8 | 2I | 77 | LEU | 3.4 |
| 40 | 1i | 47 | LEU | 3.4 |
| 41 | 2j | 40 | LEU | 3.4 |
| 32 | 2a | 1030(A) | G | 3.4 |
| 15 | 1T | 131 | ALA | 3.4 |
| 51 | 1t | 9 | ASN | 3.4 |
| 7 | 1H | 2 | SER | 3.4 |
| 1 | 2A | 2119 | A | 3.4 |
| 1 | 2A | 2141 | G | 3.4 |
| 42 | 2k | 117 | ASN | 3.4 |
| 35 | 1d | 179 | GLU | 3.4 |
| 40 | 2i | 21 | PRO | 3.4 |
| 1 | 1A | 2180 | U | 3.4 |
| 22 | 10 | 5 | LYS | 3.4 |
| 33 | 1b | 17 | PHE | 3.4 |
| 34 | 2c | 62 | ASP | 3.4 |
| 38 | 2g | 84 | ASN | 3.3 |
| 48 | 1q | 100 | LYS | 3.3 |
| 38 | 1g | 80 | VAL | 3.3 |
| 44 | 2m | 60 | VAL | 3.3 |
| 51 | 2t | 8 | ARG | 3.3 |
| 1 | 2A | 2157 | G | 3.3 |
| 1 | 2A | 2160 | G | 3.3 |
| 8 | 2I | 72 | LEU | 3.3 |
| 6 | 2G | 29 | TRP | 3.3 |
| 33 | 1b | 129 | GLU | 3.3 |
| 48 | 2q | 30 | PRO | 3.3 |
| 6 | 1G | 52 | ILE | 3.3 |
| 38 | 1g | 79 | ARG | 3.3 |
| 8 | 2I | 110 | ASP | 3.3 |
| 40 | 1i | 125 | TYR | 3.3 |
| 41 | 1j | 77 | PRO | 3.3 |
| 34 | 2c | 92 | ALA | 3.3 |
| 40 | 2i | 119 | ALA | 3.3 |
| 1 | 2A | 2162 | G | 3.3 |
| 1 | 1A | 2114 | A | 3.2 |
| 43 | 1l | 18 | VAL | 3.2 |
| 39 | 1h | 3 | THR | 3.2 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 3 | 2D | 276 | LYS | 3.2 |
| 52 | 2u | 14 | TRP | 3.2 |
| 35 | 1d | 33 | MET | 3.2 |
| 50 | 2s | 13 | ASP | 3.2 |
| 33 | 2b | 161 | ALA | 3.2 |
| 35 | 1d | 3 | ARG | 3.2 |
| 32 | 2a | 1028 | C | 3.2 |
| 32 | 2a | 1532 | U | 3.2 |
| 35 | 2d | 154 | ASN | 3.2 |
| 33 | 2b | 10 | LEU | 3.2 |
| 6 | 2G | 160 | VAL | 3.2 |
| 45 | 2n | 38 | GLY | 3.2 |
| 45 | 2n | 22 | THR | 3.2 |
| 21 | 2Z | 153 | SER | 3.2 |
| 29 | 17 | 47 | ARG | 3.2 |
| 35 | 2d | 155 | LEU | 3.2 |
| 1 | 2A | 2133 | G | 3.2 |
| 8 | 2I | 132 | PRO | 3.2 |
| 1 | 1A | 1095 | A | 3.1 |
| 8 | 2I | 98 | ALA | 3.1 |
| 45 | 2n | 20 | ALA | 3.1 |
| 41 | 2j | 47 | PHE | 3.1 |
| 42 | 2k | 124 | LYS | 3.1 |
| 32 | 2a | 1116 | C | 3.1 |
| 1 | 1A | 1063 | G | 3.1 |
| 24 | 12 | 69 | ARG | 3.1 |
| 38 | 1g | 38 | LEU | 3.1 |
| 48 | 2q | 32 | TYR | 3.1 |
| 26 | 24 | 66 | SER | 3.1 |
| 41 | 2j | 32 | ALA | 3.1 |
| 49 | 1r | 78 | LEU | 3.1 |
| 12 | 2Q | 63 | LYS | 3.1 |
| 29 | 27 | 45 | ALA | 3.1 |
| 43 | 2l | 64 | TYR | 3.1 |
| 45 | 1n | 21 | TYR | 3.1 |
| 1 | 1A | 2182 | G | 3.1 |
| 1 | 2A | 2182 | G | 3.1 |
| 38 | 2g | 33 | ASP | 3.1 |
| 40 | 1i | 14 | VAL | 3.1 |
| 40 | 1i | 33 | PHE | 3.1 |
| 1 | 1A | 2169 | A | 3.1 |
| 6 | 2G | 20 | ILE | 3.1 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 39 | 2h | 112 | LEU | 3.1 |
| 7 | 2H | 115 | VAL | 3.1 |
| 26 | 24 | 59 | PHE | 3.1 |
| 1 | 2A | 2156 | G | 3.1 |
| 11 | 2P | 15 | ARG | 3.1 |
| 41 | 2j | 8 | LEU | 3.1 |
| 40 | 2i | 5 | TYR | 3.0 |
| 47 | 1p | 28 | ARG | 3.0 |
| 52 | 2u | 15 | ARG | 3.0 |
| 28 | 26 | 4 | GLU | 3.0 |
| 15 | 1T | 130 | ALA | 3.0 |
| 11 | 2P | 44 | GLY | 3.0 |
| 38 | 2g | 82 | GLY | 3.0 |
| 40 | 1i | 104 | ARG | 3.0 |
| 34 | 1c | 87 | LEU | 3.0 |
| 1 | 1A | 1096 | A | 3.0 |
| 34 | 2c | 189 | ALA | 3.0 |
| 44 | 2m | 123 | ALA | 3.0 |
| 20 | 2Y | 1 | MET | 3.0 |
| 1 | 1A | 1093 | G | 3.0 |
| 54 | 2x | 70 | G | 3.0 |
| 1 | 1A | 2178 | C | 3.0 |
| 1 | 2A | 2107 | C | 3.0 |
| 11 | 2P | 79 | ARG | 3.0 |
| 26 | 24 | 54 | GLY | 3.0 |
| 32 | 2a | 1029 | C | 3.0 |
| 32 | 2a | 1030 | C | 3.0 |
| 45 | 2n | 51 | GLY | 3.0 |
| 9 | 2N | 10 | GLU | 3.0 |
| 40 | 1i | 2 | GLU | 3.0 |
| 41 | 2j | 41 | PRO | 3.0 |
| 47 | 1p | 41 | PRO | 3.0 |
| 33 | 2b | 48 | MET | 3.0 |
| 40 | 1i | 26 | VAL | 3.0 |
| 45 | 2n | 21 | TYR | 3.0 |
| 45 | 2n | 29 | ARG | 3.0 |
| 47 | 1p | 39 | TYR | 3.0 |
| 34 | 2c | 182 | ILE | 3.0 |
| 8 | 2I | 106 | GLY | 3.0 |
| 34 | 1c | 185 | GLY | 3.0 |
| 45 | 2n | 44 | LEU | 3.0 |
| 51 | 1t | 69 | GLY | 3.0 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 6 | 1G | 48 | GLU | 3.0 |
| 8 | 2I | 85 | GLU | 3.0 |
| 6 | 1G | 73 | ALA | 3.0 |
| 34 | 2c | 160 | ALA | 3.0 |
| 33 | 1b | 229 | VAL | 3.0 |
| 14 | 2S | 34 | HIS | 3.0 |
| 40 | 2i | 33 | PHE | 3.0 |
| 41 | 2j | 54 | PHE | 3.0 |
| 3 | 2D | 275 | LYS | 2.9 |
| 40 | 1i | 66 | ARG | 2.9 |
| 32 | 1a | 1286 | A | 2.9 |
| 32 | 2a | 1286 | A | 2.9 |
| 41 | 2j | 74 | ILE | 2.9 |
| 33 | 1b | 9 | GLU | 2.9 |
| 41 | 2j | 58 | ASP | 2.9 |
| 45 | 2n | 5 | ALA | 2.9 |
| 8 | 2I | 51 | ILE | 2.9 |
| 47 | 1p | 19 | ILE | 2.9 |
| 37 | 2f | 45 | LEU | 2.9 |
| 38 | 1g | 85 | TYR | 2.9 |
| 8 | 2I | 80 | PRO | 2.9 |
| 32 | 1a | 1001 | A | 2.9 |
| 51 | 1t | 70 | SER | 2.9 |
| 26 | 14 | 56 | VAL | 2.9 |
| 12 | 2Q | 60 | ARG | 2.9 |
| 41 | 1j | 98 | ILE | 2.9 |
| 33 | 2b | 232 | PRO | 2.9 |
| 40 | 1i | 91 | ASP | 2.9 |
| 8 | 2I | 146 | ALA | 2.9 |
| 34 | 2c | 207 | VAL | 2.9 |
| 18 | 2W | 92 | ARG | 2.9 |
| 52 | 2u | 17 | THR | 2.9 |
| 14 | 2S | 58 | LEU | 2.9 |
| 21 | 2Z | 155 | LEU | 2.9 |
| 1 | 1A | 2175 | C | 2.9 |
| 1 | 1A | 2144 | U | 2.9 |
| 1 | 2A | 2150 | U | 2.9 |
| 1 | 2A | 2104 | G | 2.9 |
| 20 | 2Y | 5 | MET | 2.9 |
| 35 | 1d | 154 | ASN | 2.9 |
| 32 | 2a | 1492 | A | 2.9 |
| 33 | 2b | 221 | LEU | 2.9 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 41 | 2j | 10 | GLY | 2.8 |
| 1 | 2A | 2188 | C | 2.8 |
| 52 | 2u | 3 | LYS | 2.8 |
| 1 | 1A | 2148 | G | 2.8 |
| 1 | 2A | 2127 | G | 2.8 |
| 50 | 2s | 41 | VAL | 2.8 |
| 35 | 1d | 152 | SER | 2.8 |
| 44 | 2m | 105 | THR | 2.8 |
| 1 | 1A | 1070 | A | 2.8 |
| 1 | 1A | 2130 | U | 2.8 |
| 21 | 1Z | 141 | VAL | 2.8 |
| 45 | 2n | 30 | ALA | 2.8 |
| 53 | 1v | 21 | C | 2.8 |
| 26 | 24 | 51 | ASP | 2.8 |
| 32 | 1a | 1353 | G | 2.8 |
| 45 | 2n | 15 | LYS | 2.8 |
| 8 | 2I | 104 | GLN | 2.8 |
| 41 | 2j | 37 | PRO | 2.8 |
| 33 | 1b | 134 | GLU | 2.8 |
| 46 | 1o | 69 | TYR | 2.8 |
| 1 | 1A | 1065 | U | 2.8 |
| 33 | 2b | 123 | ALA | 2.8 |
| 8 | 1I | 118 | LYS | 2.8 |
| 29 | 27 | 48 | LYS | 2.8 |
| 44 | 2m | 31 | LYS | 2.8 |
| 1 | 1A | 2123 | G | 2.8 |
| 1 | 2A | 2134 | A | 2.8 |
| 32 | 2a | 1035 | A | 2.8 |
| 40 | 1i | 42 | ARG | 2.8 |
| 19 | 2X | 69 | TYR | 2.8 |
| 35 | 1d | 149 | ALA | 2.8 |
| 36 | 2e | 21 | ALA | 2.8 |
| 8 | 2I | 114 | LEU | 2.8 |
| 45 | 1n | 50 | LYS | 2.8 |
| 1 | 2A | 2175 | C | 2.8 |
| 33 | 2b | 233 | SER | 2.8 |
| 34 | 2c | 9 | GLY | 2.8 |
| 51 | 2t | 103 | GLY | 2.8 |
| 35 | 1d | 37 | PRO | 2.8 |
| 7 | 2H | 107 | VAL | 2.7 |
| 1 | 1A | 1099 | G | 2.7 |
| 32 | 1a | 1531 | A | 2.7 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 32 | 2a | 971 | G | 2.7 |
| 33 | 1b | 214 | ILE | 2.7 |
| 42 | 1k | 25 | TYR | 2.7 |
| 47 | 1p | 45 | THR | 2.7 |
| 7 | 2H | 22 | GLY | 2.7 |
| 45 | 2n | 32 | SER | 2.7 |
| 20 | 2Y | 57 | GLN | 2.7 |
| 8 | 2I | 60 | GLU | 2.7 |
| 40 | 2i | 14 | VAL | 2.7 |
| 41 | 2j | 6 | ILE | 2.7 |
| 1 | 1A | 2167 | U | 2.7 |
| 6 | 2G | 115 | ARG | 2.7 |
| 11 | 1P | 70 | GLN | 2.7 |
| 29 | 17 | 46 | VAL | 2.7 |
| 8 | 2I | 58 | LEU | 2.7 |
| 12 | 2Q | 114 | ALA | 2.7 |
| 32 | 1a | 1029 | C | 2.7 |
| 33 | 1b | 196 | LEU | 2.7 |
| 35 | 2d | 78 | LEU | 2.7 |
| 44 | 2m | 66 | LEU | 2.7 |
| 45 | 2n | 2 | ALA | 2.7 |
| 12 | 2Q | 22 | LYS | 2.7 |
| 34 | 1c | 184 | TYR | 2.7 |
| 1 | 1A | 1094 | U | 2.7 |
| 32 | 1a | 204 | U | 2.7 |
| 53 | 1v | 20 | U | 2.7 |
| 14 | 2S | 20 | ARG | 2.7 |
| 15 | 2T | 93 | ARG | 2.7 |
| 16 | 2U | 12 | ARG | 2.7 |
| 33 | 1b | 131 | PRO | 2.7 |
| 44 | 2m | 104 | ARG | 2.7 |
| 1 | 1A | 2101 | G | 2.7 |
| 1 | 2A | 2124 | G | 2.7 |
| 32 | 1a | 1030(C) | G | 2.7 |
| 8 | 2I | 125 | GLU | 2.7 |
| 33 | 1b | 230 | VAL | 2.7 |
| 6 | 2G | 19 | LEU | 2.7 |
| 14 | 2S | 54 | LEU | 2.7 |
| 37 | 2f | 21 | LEU | 2.7 |
| 37 | 2f | 89 | MET | 2.7 |
| 22 | 20 | 10 | THR | 2.7 |
| 8 | 2I | 122 | GLU | 2.7 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 34 | 2c | 75 | VAL | 2.7 |
| 50 | 1s | 9 | VAL | 2.7 |
| 5 | 2F | 82 | ILE | 2.6 |
| 33 | 2b | 163 | PHE | 2.6 |
| 35 | 1d | 169 | LYS | 2.6 |
| 40 | 2i | 127 | LYS | 2.6 |
| 40 | 2i | 122 | ALA | 2.6 |
| 1 | 1A | 2133 | G | 2.6 |
| 47 | 1p | 17 | TYR | 2.6 |
| 41 | 2j | 36 | GLY | 2.6 |
| 1 | 1A | 2132 | U | 2.6 |
| 4 | 2E | 195 | LEU | 2.6 |
| 8 | 2I | 20 | ASP | 2.6 |
| 51 | 1t | 10 | LEU | 2.6 |
| 44 | 2m | 4 | ILE | 2.6 |
| 44 | 2m | 78 | ILE | 2.6 |
| 53 | 1v | 13 | A | 2.6 |
| 40 | 2i | 15 | ALA | 2.6 |
| 40 | 2i | 10 | ARG | 2.6 |
| 42 | 2k | 25 | TYR | 2.6 |
| 45 | 2n | 23 | ARG | 2.6 |
| 39 | 2h | 72 | PRO | 2.6 |
| 1 | 2A | 2164 | C | 2.6 |
| 34 | 1c | 52 | LEU | 2.6 |
| 34 | 2c | 47 | LEU | 2.6 |
| 41 | 2j | 90 | LEU | 2.6 |
| 8 | 2I | 96 | ASP | 2.6 |
| 1 | 2A | 2158 | A | 2.6 |
| 40 | 2i | 117 | HIS | 2.6 |
| 26 | 24 | 67 | TYR | 2.6 |
| 35 | 1d | 7 | PRO | 2.6 |
| 52 | 2u | 4 | GLY | 2.6 |
| 6 | 1G | 75 | LYS | 2.6 |
| 8 | 2I | 78 | THR | 2.6 |
| 19 | 1X | 95 | LEU | 2.6 |
| 7 | 2H | 89 | ILE | 2.6 |
| 26 | 24 | 50 | VAL | 2.6 |
| 33 | 1b | 223 | ILE | 2.6 |
| 42 | 1k | 92 | GLU | 2.6 |
| 33 | 1b | 163 | PHE | 2.6 |
| 36 | 1e | 138 | ALA | 2.6 |
| 1 | 1A | 1060 | U | 2.6 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 8 | 2I | 50 | ARG | 2.6 |
| 44 | 2m | 94 | ARG | 2.6 |
| 14 | 2S | 33 | LYS | 2.6 |
| 45 | 2n | 34 | TYR | 2.6 |
| 21 | 2Z | 139 | VAL | 2.6 |
| 41 | 2j | 34 | VAL | 2.6 |
| 52 | 1u | 17 | THR | 2.6 |
| 40 | 2i | 124 | GLN | 2.6 |
| 3 | 1D | 93 | ALA | 2.6 |
| 20 | 2Y | 107 | ASP | 2.6 |
| 1 | 2A | 2173 | A | 2.5 |
| 7 | 2H | 14 | GLY | 2.5 |
| 26 | 14 | 54 | GLY | 2.5 |
| 34 | 1c | 2 | GLY | 2.5 |
| 26 | 24 | 63 | TYR | 2.5 |
| 47 | 2p | 82 | GLN | 2.5 |
| 8 | 2I | 59 | ALA | 2.5 |
| 14 | 2S | 6 | ALA | 2.5 |
| 32 | 2a | 1032 | G | 2.5 |
| 1 | 1A | 2164 | C | 2.5 |
| 34 | 2c | 188 | LEU | 2.5 |
| 39 | 1h | 89 | PRO | 2.5 |
| 36 | 2e | 74 | GLY | 2.5 |
| 50 | 1s | 15 | LEU | 2.5 |
| 14 | 2S | 7 | TYR | 2.5 |
| 33 | 2b | 136 | VAL | 2.5 |
| 33 | 2b | 229 | VAL | 2.5 |
| 43 | 2l | 69 | TYR | 2.5 |
| 34 | 2c | 60 | ALA | 2.5 |
| 45 | 1n | 20 | ALA | 2.5 |
| 41 | 1j | 46 | ARG | 2.5 |
| 46 | 2o | 68 | ARG | 2.5 |
| 52 | 2u | 22 | ARG | 2.5 |
| 10 | 1O | 81 | ASP | 2.5 |
| 50 | 1s | 13 | ASP | 2.5 |
| 1 | 2A | 2189 | U | 2.5 |
| 33 | 2b | 121 | LEU | 2.5 |
| 34 | 1c | 178 | LEU | 2.5 |
| 41 | 2j | 93 | GLY | 2.5 |
| 41 | 1j | 34 | VAL | 2.5 |
| 47 | 1p | 79 | VAL | 2.5 |
| 1 | 1A | 2140 | C | 2.5 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 32 | 2a | 1366 | C | 2.5 |
| 32 | 2a | 1036 | G | 2.5 |
| 32 | 2a | 1202 | G | 2.5 |
| 44 | 1m | 2 | ALA | 2.5 |
| 41 | 2j | 7 | LYS | 2.5 |
| 43 | 1l | 91 | LYS | 2.5 |
| 40 | 2i | 79 | LEU | 2.5 |
| 7 | 2H | 39 | PRO | 2.5 |
| 1 | 1A | 2189 | U | 2.5 |
| 22 | 20 | 8 | GLY | 2.5 |
| 41 | 1j | 96 | ILE | 2.5 |
| 37 | 2f | 6 | VAL | 2.5 |
| 7 | 2H | 159 | GLU | 2.5 |
| 33 | 2b | 70 | PHE | 2.5 |
| 35 | 1d | 138 | TYR | 2.5 |
| 40 | 2i | 36 | TYR | 2.5 |
| 19 | 2X | 68 | ARG | 2.5 |
| 21 | 1Z | 51 | ALA | 2.5 |
| 1 | 1A | 2138 | C | 2.5 |
| 1 | 2A | 1536 | C | 2.5 |
| 1 | 2A | 2137 | C | 2.5 |
| 34 | 2c | 177 | THR | 2.5 |
| 47 | 1p | 7 | ALA | 2.5 |
| 44 | 2m | 120 | LYS | 2.5 |
| 45 | 2n | 50 | LYS | 2.5 |
| 1 | 2A | 2154 | G | 2.5 |
| 1 | 2A | 2893 | G | 2.5 |
| 22 | 10 | 3 | HIS | 2.5 |
| 7 | 2H | 88 | LEU | 2.4 |
| 37 | 1f | 55 | ASP | 2.4 |
| 40 | 2i | 96 | LEU | 2.4 |
| 42 | 1k | 98 | LEU | 2.4 |
| 38 | 2g | 21 | VAL | 2.4 |
| 44 | 1m | 15 | VAL | 2.4 |
| 52 | 2u | 16 | GLY | 2.4 |
| 38 | 2g | 4 | ARG | 2.4 |
| 40 | 1i | 10 | ARG | 2.4 |
| 40 | 1i | 107 | ARG | 2.4 |
| 47 | 2p | 26 | ARG | 2.4 |
| 5 | 2F | 80 | ALA | 2.4 |
| 7 | 2H | 94 | TYR | 2.4 |
| 36 | 2e | 94 | ALA | 2.4 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 40 | 2i | 82 | ALA | 2.4 |
| 41 | 1j | 42 | THR | 2.4 |
| 26 | 24 | 40 | HIS | 2.4 |
| 8 | 2I | 75 | LEU | 2.4 |
| 40 | 2i | 19 | LEU | 2.4 |
| 1 | 2A | 1171 | G | 2.4 |
| 32 | 1a | 102 | G | 2.4 |
| 32 | 1a | 630 | G | 2.4 |
| 41 | 2j | 77 | PRO | 2.4 |
| 26 | 14 | 45 | GLY | 2.4 |
| 33 | 1b | 165 | VAL | 2.4 |
| 34 | 2c | 68 | VAL | 2.4 |
| 8 | 2I | 91 | SER | 2.4 |
| 12 | 1Q | 60 | ARG | 2.4 |
| 26 | 24 | 57 | GLU | 2.4 |
| 32 | 1a | 1532 | U | 2.4 |
| 43 | 1l | 64 | TYR | 2.4 |
| 22 | 10 | 10 | THR | 2.4 |
| 41 | 2j | 67 | THR | 2.4 |
| 21 | 2Z | 144 | LEU | 2.4 |
| 41 | 1j | 65 | LEU | 2.4 |
| 41 | 2j | 65 | LEU | 2.4 |
| 1 | 2A | 2163 | C | 2.4 |
| 1 | 2A | 2179 | C | 2.4 |
| 21 | 2Z | 165 | VAL | 2.4 |
| 1 | 2A | 2176 | A | 2.4 |
| 53 | 1v | 14 | A | 2.4 |
| 6 | 1G | 51 | ARG | 2.4 |
| 22 | 20 | 5 | LYS | 2.4 |
| 45 | 2n | 17 | LYS | 2.4 |
| 51 | 1t | 14 | LYS | 2.4 |
| 6 | 1G | 35 | GLU | 2.4 |
| 14 | 2S | 29 | PHE | 2.4 |
| 32 | 2a | 1156 | G | 2.4 |
| 33 | 2b | 55 | PHE | 2.4 |
| 33 | 2b | 231 | GLU | 2.4 |
| 44 | 2m | 67 | GLU | 2.4 |
| 47 | 2p | 9 | PHE | 2.4 |
| 12 | 2Q | 28 | ALA | 2.4 |
| 34 | 2c | 137 | ALA | 2.4 |
| 2 | 2B | 55 | U | 2.4 |
| 44 | 2m | 103 | THR | 2.4 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 14 | 2S | 59 | LYS | 2.4 |
| 36 | 2e | 85 | GLY | 2.4 |
| 35 | 1d | 153 | ARG | 2.4 |
| 45 | 2n | 3 | ARG | 2.4 |
| 1 | 1A | 2142 | C | 2.4 |
| 8 | 2I | 55 | ALA | 2.4 |
| 33 | 2b | 13 | ALA | 2.4 |
| 35 | 1d | 195 | ALA | 2.4 |
| 42 | 1k | 68 | ALA | 2.4 |
| 45 | 1n | 59 | ALA | 2.4 |
| 11 | 2P | 70 | GLN | 2.4 |
| 35 | 1d | 83 | SER | 2.4 |
| 1 | 1A | 2166 | G | 2.4 |
| 27 | 25 | 29 | THR | 2.4 |
| 35 | 1d | 181 | MET | 2.4 |
| 23 | 21 | 46 | LEU | 2.4 |
| 33 | 2b | 215 | LEU | 2.4 |
| 41 | 2j | 71 | LEU | 2.4 |
| 44 | 1m | 96 | LEU | 2.4 |
| 51 | 1t | 13 | LEU | 2.4 |
| 40 | 2i | 123 | PRO | 2.4 |
| 3 | 1D | 276 | LYS | 2.3 |
| 8 | 2I | 113 | ARG | 2.3 |
| 21 | 2Z | 141 | VAL | 2.3 |
| 40 | 1i | 78 | LYS | 2.3 |
| 19 | 2X | 86 | GLY | 2.3 |
| 41 | 2j | 46 | ARG | 2.3 |
| 45 | 2n | 12 | ARG | 2.3 |
| 45 | 2n | 28 | GLY | 2.3 |
| 44 | 2m | 75 | ALA | 2.3 |
| 1 | 2A | 34 | C | 2.3 |
| 2 | 1B | 88 | C | 2.3 |
| 11 | 2P | 68 | GLN | 2.3 |
| 47 | 1p | 82 | GLN | 2.3 |
| 33 | 2b | 54 | THR | 2.3 |
| 34 | 1c | 12 | LEU | 2.3 |
| 45 | 1n | 7 | ILE | 2.3 |
| 47 | 1p | 33 | ILE | 2.3 |
| 17 | 2V | 76 | LYS | 2.3 |
| 33 | 2b | 8 | LYS | 2.3 |
| 41 | 2j | 39 | PRO | 2.3 |
| 1 | 1A | 2116 | G | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | 2A | 11 | G | 2.3 |
| 1 | 2A | 2106 | G | 2.3 |
| 8 | 2I | 3 | VAL | 2.3 |
| 12 | 2Q | 109 | VAL | 2.3 |
| 26 | 24 | 58 | ARG | 2.3 |
| 45 | 1n | 18 | VAL | 2.3 |
| 33 | 2b | 38 | GLY | 2.3 |
| 40 | 2i | 59 | PHE | 2.3 |
| 8 | 2I | 135 | GLU | 2.3 |
| 8 | 2I | 68 | LEU | 2.3 |
| 34 | 1c | 47 | LEU | 2.3 |
| 39 | 1h | 2 | LEU | 2.3 |
| 39 | 2h | 2 | LEU | 2.3 |
| 41 | 2j | 88 | LEU | 2.3 |
| 45 | 1n | 61 | TRP | 2.3 |
| 1 | 2A | 2136 | C | 2.3 |
| 2 | 2B | 6 | C | 2.3 |
| 42 | 2k | 31 | THR | 2.3 |
| 32 | 2a | 1225 | A | 2.3 |
| 8 | 2I | 95 | LYS | 2.3 |
| 29 | 17 | 48 | LYS | 2.3 |
| 33 | 2b | 96 | ARG | 2.3 |
| 35 | 2d | 132 | ARG | 2.3 |
| 7 | 2H | 169 | VAL | 2.3 |
| 8 | 2I | 81 | VAL | 2.3 |
| 27 | 15 | 60 | VAL | 2.3 |
| 50 | 2s | 9 | VAL | 2.3 |
| 34 | 2c | 155 | GLY | 2.3 |
| 49 | 2r | 43 | PHE | 2.3 |
| 1 | 2A | 2100 | G | 2.3 |
| 1 | 2A | 2125 | G | 2.3 |
| 10 | 2O | 108 | GLU | 2.3 |
| 22 | 10 | 2 | ALA | 2.3 |
| 32 | 1a | 1001(A) | G | 2.3 |
| 32 | 1a | 1024 | G | 2.3 |
| 32 | 1a | 1036 | G | 2.3 |
| 32 | 2a | 1031 | G | 2.3 |
| 40 | 2i | 2 | GLU | 2.3 |
| 41 | 1j | 25 | GLU | 2.3 |
| 4 | 2E | 127 | ASP | 2.3 |
| 22 | 20 | 84 | LEU | 2.3 |
| 37 | 1f | 21 | LEU | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 47 | 1p | 6 | LEU | 2.3 |
| 47 | 2p | 73 | LEU | 2.3 |
| 33 | 2b | 214 | ILE | 2.3 |
| 38 | 1g | 153 | HIS | 2.3 |
| 35 | 2d | 208 | SER | 2.3 |
| 48 | 2q | 99 | SER | 2.3 |
| 48 | 2q | 100 | LYS | 2.3 |
| 52 | 1u | 14 | TRP | 2.3 |
| 5 | 2F | 6 | VAL | 2.3 |
| 36 | 2e | 128 | PRO | 2.3 |
| 50 | 2s | 2 | PRO | 2.3 |
| 32 | 1a | 1352 | C | 2.3 |
| 32 | 2a | 1027 | C | 2.3 |
| 35 | 1d | 23 | GLY | 2.3 |
| 52 | 2u | 11 | GLY | 2.3 |
| 33 | 1b | 12 | GLU | 2.3 |
| 45 | 2n | 8 | GLU | 2.3 |
| 20 | 2Y | 90 | LEU | 2.3 |
| 33 | 1b | 221 | LEU | 2.3 |
| 52 | 2u | 5 | ASP | 2.3 |
| 45 | 1n | 17 | LYS | 2.3 |
| 32 | 1a | 1023 | G | 2.3 |
| 35 | 1d | 115 | ARG | 2.3 |
| 48 | 1q | 99 | SER | 2.3 |
| 7 | 2H | 10 | PRO | 2.3 |
| 34 | 2c | 48 | TYR | 2.3 |
| 35 | 1d | 170 | VAL | 2.3 |
| 40 | 2i | 69 | GLY | 2.3 |
| 41 | 1j | 52 | GLY | 2.3 |
| 1 | 2A | 2105 | C | 2.2 |
| 1 | 2A | 2135 | A | 2.2 |
| 1 | 2A | 2789 | C | 2.2 |
| 2 | 2B | 88 | C | 2.2 |
| 38 | 1g | 26 | PHE | 2.2 |
| 45 | 1n | 16 | PHE | 2.2 |
| 8 | 2I | 53 | ALA | 2.2 |
| 33 | 1b | 77 | ALA | 2.2 |
| 41 | 1j | 55 | LYS | 2.2 |
| 41 | 1j | 75 | ILE | 2.2 |
| 35 | 2d | 49 | ARG | 2.2 |
| 33 | 1b | 97 | TRP | 2.2 |
| 35 | 1d | 136 | PRO | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 40 | 2i | 92 | TYR | 2.2 |
| 1 | 1A | 2159 | G | 2.2 |
| 44 | 1m | 100 | GLY | 2.2 |
| 34 | 1c | 203 | PHE | 2.2 |
| 38 | 1g | 43 | PHE | 2.2 |
| 45 | 2n | 37 | PHE | 2.2 |
| 1 | 2A | 2172 | U | 2.2 |
| 32 | 1a | 1000 | U | 2.2 |
| 6 | 2G | 50 | ALA | 2.2 |
| 33 | 2b | 12 | GLU | 2.2 |
| 1 | 1A | 2129 | C | 2.2 |
| 1 | 1A | 2804 | C | 2.2 |
| 1 | 2A | 277 | C | 2.2 |
| 32 | 1a | 1492 | A | 2.2 |
| 32 | 2a | 1447 | A | 2.2 |
| 35 | 2d | 21 | LEU | 2.2 |
| 41 | 2j | 85 | LEU | 2.2 |
| 48 | 2q | 98 | LEU | 2.2 |
| 7 | 2H | 60 | ARG | 2.2 |
| 15 | 2T | 108 | ARG | 2.2 |
| 21 | 2Z | 154 | ASP | 2.2 |
| 29 | 27 | 47 | ARG | 2.2 |
| 6 | 2G | 142 | PRO | 2.2 |
| 8 | 2I | 137 | PRO | 2.2 |
| 34 | 2c | 191 | THR | 2.2 |
| 35 | 2d | 88 | VAL | 2.2 |
| 45 | 1n | 14 | PRO | 2.2 |
| 47 | 1p | 22 | THR | 2.2 |
| 21 | 2Z | 106 | GLY | 2.2 |
| 36 | 2e | 22 | GLY | 2.2 |
| 35 | 1d | 110 | PHE | 2.2 |
| 1 | 1A | 1059 | G | 2.2 |
| 1 | 1A | 1062 | G | 2.2 |
| 1 | 1A | 2151 | G | 2.2 |
| 1 | 2A | 2181 | G | 2.2 |
| 6 | 1G | 50 | ALA | 2.2 |
| 32 | 2a | 1190 | G | 2.2 |
| 32 | 2a | 1365 | G | 2.2 |
| 33 | 2b | 11 | LEU | 2.2 |
| 34 | 2c | 87 | LEU | 2.2 |
| 40 | 1i | 19 | LEU | 2.2 |
| 45 | 2n | 39 | LEU | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 42 | 1k | 117 | ASN | 2.2 |
| 39 | 2h | 80 | ILE | 2.2 |
| 44 | 2m | 101 | GLN | 2.2 |
| 47 | 1p | 75 | ARG | 2.2 |
| 48 | 1q | 91 | ARG | 2.2 |
| 32 | 2a | 1236 | A | 2.2 |
| 32 | 1a | 1028 | C | 2.2 |
| 50 | 2s | 12 | ASP | 2.2 |
| 33 | 2b | 15 | VAL | 2.2 |
| 33 | 2b | 93 | VAL | 2.2 |
| 11 | 2P | 34 | GLY | 2.2 |
| 21 | 2Z | 99 | TYR | 2.2 |
| 40 | 1i | 8 | GLY | 2.2 |
| 52 | 2u | 2 | GLY | 2.2 |
| 45 | 2n | 4 | LYS | 2.2 |
| 8 | 2I | 47 | LEU | 2.2 |
| 17 | 2V | 71 | LEU | 2.2 |
| 33 | 1b | 11 | LEU | 2.2 |
| 38 | 2g | 12 | LEU | 2.2 |
| 27 | 25 | 19 | ARG | 2.2 |
| 41 | 2j | 98 | ILE | 2.2 |
| 37 | 1f | 18 | GLN | 2.2 |
| 41 | 2j | 69 | ASN | 2.2 |
| 1 | 1A | 1058 | G | 2.2 |
| 35 | 1d | 102 | ASP | 2.2 |
| 50 | 2s | 76 | PRO | 2.2 |
| 54 | 1x | 76 | A | 2.2 |
| 1 | 2A | 2177 | C | 2.2 |
| 8 | 2I | 130 | TYR | 2.2 |
| 14 | 2S | 92 | TYR | 2.2 |
| 26 | 14 | 59 | PHE | 2.2 |
| 40 | 2i | 62 | TYR | 2.2 |
| 47 | 1p | 80 | PHE | 2.2 |
| 47 | 1p | 74 | LEU | 2.2 |
| 48 | 2q | 31 | LEU | 2.2 |
| 8 | 2I | 115 | ALA | 2.2 |
| 34 | 2c | 168 | ALA | 2.2 |
| 35 | 2d | 158 | ILE | 2.1 |
| 41 | 2j | 60 | ARG | 2.1 |
| 44 | 2m | 9 | ILE | 2.1 |
| 41 | 2j | 76 | ASN | 2.1 |
| 8 | 2I | 136 | VAL | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 23 | 21 | 62 | VAL | 2.1 |
| 33 | 2b | 71 | VAL | 2.1 |
| 6 | 1G | 49 | ASP | 2.1 |
| 15 | 1T | 107 | ASP | 2.1 |
| 1 | 1A | 2131 | G | 2.1 |
| 45 | 1n | 11 | LYS | 2.1 |
| 1 | 1A | 2177 | C | 2.1 |
| 35 | 1d | 194 | LEU | 2.1 |
| 49 | 1r | 31 | LEU | 2.1 |
| 21 | 2Z | 149 | SER | 2.1 |
| 40 | 1i | 43 | ALA | 2.1 |
| 14 | 2S | 3 | ARG | 2.1 |
| 24 | 22 | 69 | ARG | 2.1 |
| 40 | 2i | 66 | ARG | 2.1 |
| 41 | 2j | 83 | GLU | 2.1 |
| 47 | 1p | 5 | ARG | 2.1 |
| 40 | 2i | 81 | ILE | 2.1 |
| 44 | 2m | 22 | ILE | 2.1 |
| 7 | 2H | 15 | VAL | 2.1 |
| 7 | 2H | 113 | VAL | 2.1 |
| 34 | 2c | 66 | VAL | 2.1 |
| 24 | 22 | 1 | MET | 2.1 |
| 41 | 1j | 39 | PRO | 2.1 |
| 41 | 2j | 72 | VAL | 2.1 |
| 20 | 2Y | 54 | LYS | 2.1 |
| 43 | 1l | 21 | LYS | 2.1 |
| 45 | 2n | 9 | LYS | 2.1 |
| 51 | 1t | 21 | LYS | 2.1 |
| 3 | 2D | 55 | GLY | 2.1 |
| 17 | 2V | 42 | GLY | 2.1 |
| 40 | 1i | 6 | GLY | 2.1 |
| 45 | 1n | 51 | GLY | 2.1 |
| 33 | 1b | 10 | LEU | 2.1 |
| 35 | 2d | 162 | LEU | 2.1 |
| 1 | 1A | 1069 | A | 2.1 |
| 2 | 2B | 53 | A | 2.1 |
| 6 | 2G | 146 | TYR | 2.1 |
| 8 | 2I | 46 | ALA | 2.1 |
| 29 | 17 | 45 | ALA | 2.1 |
| 33 | 2b | 21 | ARG | 2.1 |
| 34 | 2c | 24 | ALA | 2.1 |
| 1 | 2A | 2318 | G | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 2 | 2B | 23 | G | 2.1 |
| 11 | 2P | 74 | GLU | 2.1 |
| 34 | 1c | 8 | ILE | 2.1 |
| 45 | 2n | 7 | ILE | 2.1 |
| 1 | 2A | 2178 | C | 2.1 |
| 6 | 1G | 76 | SER | 2.1 |
| 7 | 2H | 2 | SER | 2.1 |
| 22 | 20 | 9 | SER | 2.1 |
| 39 | 2h | 70 | GLN | 2.1 |
| 50 | 2s | 14 | HIS | 2.1 |
| 6 | 1G | 182 | LYS | 2.1 |
| 41 | 1j | 86 | MET | 2.1 |
| 44 | 1m | 106 | ASN | 2.1 |
| 1 | 1A | 2150 | U | 2.1 |
| 33 | 2b | 61 | LEU | 2.1 |
| 35 | 1d | 101 | LEU | 2.1 |
| 20 | 2Y | 12 | THR | 2.1 |
| 36 | 2e | 5 | ASP | 2.1 |
| 8 | 2I | 82 | ARG | 2.1 |
| 33 | 1b | 36 | ARG | 2.1 |
| 52 | 2u | 7 | ARG | 2.1 |
| 21 | 2Z | 146 | ILE | 2.1 |
| 21 | 2Z | 173 | ALA | 2.1 |
| 33 | 1b | 62 | ALA | 2.1 |
| 34 | 1c | 61 | ALA | 2.1 |
| 46 | 2o | 6 | GLU | 2.1 |
| 47 | 2p | 38 | TYR | 2.1 |
| 1 | 1A | 2173 | A | 2.1 |
| 1 | 2A | 899 | A | 2.1 |
| 2 | 2B | 59 | A | 2.1 |
| 32 | 2a | 1363(A) | A | 2.1 |
| 41 | 2j | 35 | SER | 2.1 |
| 37 | 2f | 27 | GLN | 2.1 |
| 1 | 2A | 2129 | C | 2.1 |
| 20 | 1Y | 1 | MET | 2.1 |
| 32 | 1a | 1002 | G | 2.1 |
| 32 | 1a | 1003 | G | 2.1 |
| 32 | 1a | 1039 | C | 2.1 |
| 32 | 2a | 972 | C | 2.1 |
| 32 | 2a | 995 | C | 2.1 |
| 32 | 2a | 1019 | C | 2.1 |
| 35 | 1d | 84 | LYS | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 40 | 1i | 117 | HIS | 2.1 |
| 33 | 1b | 167 | PRO | 2.1 |
| 39 | 2h | 67 | PRO | 2.1 |
| 21 | 1Z | 150 | LEU | 2.1 |
| 26 | 24 | 45 | GLY | 2.1 |
| 34 | 1c | 13 | GLY | 2.1 |
| 40 | 1i | 37 | PHE | 2.1 |
| 47 | 2p | 78 | GLY | 2.1 |
| 50 | 2s | 84 | GLY | 2.1 |
| 6 | 2G | 51 | ARG | 2.1 |
| 11 | 1P | 15 | ARG | 2.1 |
| 40 | 2i | 83 | ARG | 2.1 |
| 51 | 1t | 17 | ARG | 2.1 |
| 40 | 2i | 84 | ALA | 2.1 |
| 41 | 2j | 38 | ILE | 2.1 |
| 34 | 1c | 201 | TYR | 2.1 |
| 6 | 2G | 76 | SER | 2.0 |
| 7 | 2H | 38 | SER | 2.0 |
| 8 | 2I | 56 | LYS | 2.0 |
| 22 | 20 | 53 | MET | 2.0 |
| 41 | 1j | 35 | SER | 2.0 |
| 48 | 1q | 62 | SER | 2.0 |
| 41 | 1j | 33 | GLN | 2.0 |
| 51 | 1t | 74 | LYS | 2.0 |
| 51 | 2t | 73 | HIS | 2.0 |
| 21 | 2Z | 128 | VAL | 2.0 |
| 32 | 2a | 1531 | A | 2.0 |
| 34 | 1c | 207 | VAL | 2.0 |
| 42 | 1k | 30 | VAL | 2.0 |
| 45 | 2n | 18 | VAL | 2.0 |
| 33 | 1b | 234 | PRO | 2.0 |
| 44 | 1m | 97 | PRO | 2.0 |
| 52 | 2u | 23 | PRO | 2.0 |
| 1 | 1A | 154(A) | C | 2.0 |
| 14 | 2S | 78 | LEU | 2.0 |
| 34 | 2c | 94 | LEU | 2.0 |
| 35 | 1d | 19 | LEU | 2.0 |
| 40 | 2i | 99 | LEU | 2.0 |
| 1 | 1A | 2125 | G | 2.0 |
| 1 | 1A | 2165 | G | 2.0 |
| 15 | 1T | 115 | ARG | 2.0 |
| 33 | 2b | 89 | GLY | 2.0 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 35 | 2d | 209 | ARG | 2.0 |
| 43 | 2l | 14 | GLY | 2.0 |
| 45 | 2n | 16 | PHE | 2.0 |
| 6 | 2G | 161 | THR | 2.0 |
| 34 | 1c | 152 | ILE | 2.0 |
| 49 | 2r | 82 | THR | 2.0 |
| 51 | 1t | 55 | ILE | 2.0 |
| 12 | 1Q | 28 | ALA | 2.0 |
| 21 | 2Z | 152 | ALA | 2.0 |
| 50 | 2s | 80 | TYR | 2.0 |
| 10 | 2O | 1 | MET | 2.0 |
| 33 | 2b | 83 | MET | 2.0 |
| 8 | 2I | 105 | HIS | 2.0 |
| 20 | 2Y | 45 | VAL | 2.0 |
| 38 | 1g | 13 | GLN | 2.0 |
| 19 | 2X | 95 | LEU | 2.0 |
| 34 | 2c | 52 | LEU | 2.0 |
| 15 | 1T | 104 | ASN | 2.0 |
| 28 | 26 | 6 | ARG | 2.0 |
| 35 | 1d | 122 | ARG | 2.0 |
| 35 | 2d | 199 | ASN | 2.0 |
| 50 | 1s | 29 | ARG | 2.0 |
| 50 | 2s | 78 | ARG | 2.0 |
| 3 | 2D | 256 | GLY | 2.0 |
| 12 | 2Q | 61 | GLY | 2.0 |
| 44 | 2m | 100 | GLY | 2.0 |
| 1 | 1A | 2185 | C | 2.0 |
| 32 | 2a | 1367 | C | 2.0 |
| 36 | 2e | 120 | THR | 2.0 |
| 40 | 2i | 64 | THR | 2.0 |
| 46 | 1o | 4 | THR | 2.0 |
| 47 | 1p | 69 | THR | 2.0 |
| 1 | 1A | 12 | U | 2.0 |
| 54 | 2x | 47 | U | 2.0 |
| 1 | 1A | 2157 | G | 2.0 |
| 1 | 2A | 2319 | G | 2.0 |
| 3 | 1D | 275 | LYS | 2.0 |
| 26 | 24 | 53 | GLU | 2.0 |
| 32 | 2a | 1002 | G | 2.0 |
| 33 | 2b | 22 | LYS | 2.0 |
| 35 | 1d | 30 | LYS | 2.0 |
| 40 | 2i | 125 | TYR | 2.0 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 44 | 2m | 15 | VAL | 2.0 |

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, $95^{th}$ 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 |
|---|---|---|---|---|---|---|---|---|
| 1 | 5MU | 2A | 1915 | 21/22 | 0.73 | 0.12 | 74,81,86,91 | 0 |
| 54 | PSU | 2x | 55 | 20/21 | 0.78 | 0.12 | 72,78,85,91 | 0 |
| 32 | PSU | 2a | 516 | 20/21 | 0.86 | 0.12 | 70,76,79,84 | 0 |
| 32 | 5MC | 2a | 1400 | 21/22 | 0.86 | 0.15 | 65,72,79,81 | 0 |
| 54 | 4SU | 2x | 8 | 20/21 | 0.86 | 0.11 | 72,83,87,87 | 0 |
| 1 | 5MU | 1A | 1915 | 21/22 | 0.86 | 0.11 | 58,70,76,89 | 0 |
| 32 | 2MG | 2a | 1207 | 24/25 | 0.87 | 0.11 | 77,83,89,92 | 0 |
| 43 | 0TD | 2l | 92 | 10/11 | 0.87 | 0.15 | 57,66,71,84 | 0 |
| 54 | PSU | 1x | 55 | 20/21 | 0.88 | 0.10 | 61,67,75,78 | 0 |
| 54 | 5MC | 2x | 32 | 21/22 | 0.89 | 0.15 | 61,79,80,82 | 0 |
| 32 | PSU | 1a | 516 | 20/21 | 0.89 | 0.10 | 65,70,76,78 | 0 |
| 32 | 7MG | 2a | 527 | 24/25 | 0.90 | 0.11 | 59,66,71,72 | 0 |
| 54 | 5MC | 1x | 32 | 21/22 | 0.90 | 0.13 | 52,64,68,76 | 0 |
| 1 | PSU | 2A | 1911 | 20/21 | 0.90 | 0.10 | 57,65,72,79 | 0 |
| 32 | 4OC | 2a | 1402 | 22/23 | 0.90 | 0.13 | 55,63,68,75 | 0 |
| 32 | M2G | 2a | 966 | 25/26 | 0.91 | 0.14 | 63,69,81,83 | 0 |
| 32 | 2MG | 1a | 1207 | 24/25 | 0.91 | 0.09 | 60,76,82,87 | 0 |
| 43 | 0TD | 1l | 92 | 10/11 | 0.91 | 0.11 | 52,57,60,75 | 0 |
| 54 | 5MU | 2x | 54 | 21/22 | 0.91 | 0.09 | 72,79,82,87 | 0 |
| 54 | 4SU | 1x | 8 | 20/21 | 0.91 | 0.10 | 58,68,74,78 | 0 |
| 54 | 5MU | 1x | 54 | 21/22 | 0.92 | 0.10 | 64,69,77,83 | 0 |
| 32 | 5MC | 2a | 967 | 21/22 | 0.93 | 0.14 | 67,72,79,80 | 0 |
| 1 | PSU | 2A | 1917 | 20/21 | 0.93 | 0.08 | 60,70,75,77 | 0 |
| 32 | M2G | 1a | 966 | 25/26 | 0.93 | 0.13 | 51,59,65,73 | 0 |
| 1 | 5MC | 2A | 1962 | 21/22 | 0.94 | 0.09 | 40,53,61,65 | 0 |
| 1 | 2MA | 2A | 2503 | 23/24 | 0.94 | 0.10 | 30,34,39,42 | 0 |
| 32 | 5MC | 2a | 1404 | 21/22 | 0.94 | 0.09 | 45,57,67,68 | 0 |
| 32 | UR3 | 2a | 1498 | 21/22 | 0.94 | 0.10 | 52,59,63,70 | 0 |
| 32 | MA6 | 2a | 1518 | 24/25 | 0.94 | 0.12 | 55,62,66,67 | 0 |
| 32 | 5MC | 1a | 1404 | 21/22 | 0.94 | 0.10 | 34,46,49,51 | 0 |
| 1 | PSU | 1A | 1917 | 20/21 | 0.94 | 0.08 | 50,59,68,74 | 0 |
| 32 | 7MG | 1a | 527 | 24/25 | 0.94 | 0.10 | 51,57,63,66 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 1 | 4OC | 2A | 1920 | 21/23 | 0.94 | 0.10 | 53,65,68,71 | 0 |
| 1 | 5MU | 2A | 1939 | 21/22 | 0.94 | 0.10 | 39,43,47,50 | 0 |
| 32 | 5MC | 1a | 967 | 21/22 | 0.95 | 0.10 | 54,62,71,74 | 0 |
| 1 | OMG | 2A | 2251 | 24/25 | 0.95 | 0.10 | 30,40,46,46 | 0 |
| 32 | 5MC | 1a | 1407 | 21/22 | 0.95 | 0.09 | 41,43,48,52 | 0 |
| 1 | PSU | 1A | 1911 | 20/21 | 0.95 | 0.08 | 42,49,56,58 | 0 |
| 32 | 4OC | 1a | 1402 | 22/23 | 0.95 | 0.10 | 49,53,59,62 | 0 |
| 1 | 5MC | 2A | 1942 | 21/22 | 0.95 | 0.08 | 47,55,60,63 | 0 |
| 32 | 5MC | 2a | 1407 | 21/22 | 0.96 | 0.09 | 51,57,62,64 | 0 |
| 1 | 5MC | 1A | 1942 | 21/22 | 0.96 | 0.08 | 28,34,40,43 | 0 |
| 1 | 4OC | 1A | 1920 | 21/23 | 0.96 | 0.08 | 34,46,49,54 | 0 |
| 32 | MA6 | 2a | 1519 | 24/25 | 0.96 | 0.11 | 56,60,65,67 | 0 |
| 32 | 5MC | 1a | 1400 | 21/22 | 0.96 | 0.09 | 36,57,61,62 | 0 |
| 32 | MA6 | 1a | 1518 | 24/25 | 0.96 | 0.10 | 35,43,48,52 | 0 |
| 1 | 2MU | 2A | 2552 | 21/23 | 0.96 | 0.07 | 34,38,44,47 | 0 |
| 1 | PSU | 2A | 2605 | 20/21 | 0.96 | 0.09 | 28,38,44,46 | 0 |
| 32 | MA6 | 1a | 1519 | 24/25 | 0.96 | 0.10 | 38,43,48,51 | 0 |
| 32 | UR3 | 1a | 1498 | 21/22 | 0.97 | 0.07 | 39,46,49,52 | 0 |
| 1 | 5MU | 1A | 1939 | 21/22 | 0.97 | 0.07 | 22,27,32,34 | 0 |
| 1 | OMG | 1A | 2251 | 24/25 | 0.97 | 0.08 | 23,29,33,35 | 0 |
| 1 | PSU | 1A | 2605 | 20/21 | 0.97 | 0.07 | 20,27,29,31 | 0 |
| 1 | 2MA | 1A | 2503 | 23/24 | 0.98 | 0.06 | 14,21,24,25 | 0 |
| 1 | 2MU | 1A | 2552 | 21/23 | 0.98 | 0.07 | 26,29,34,37 | 0 |
| 1 | 5MC | 1A | 1962 | 21/22 | 0.98 | 0.07 | 28,37,44,54 | 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 |
|---|---|---|---|---|---|---|---|---|
| 55 | MG | 2a | 3173 | 1/1 | 0.30 | 0.26 | 76,76,76,76 | 0 |
| 55 | MG | 1B | 232 | 1/1 | 0.43 | 0.27 | 65,65,65,65 | 0 |
| 55 | MG | 1a | 1765 | 1/1 | 0.45 | 0.17 | 90,90,90,90 | 0 |
| 55 | MG | 1B | 230 | 1/1 | 0.56 | 0.24 | 82,82,82,82 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 55 | MG | 1a | 1678 | 1/1 | 0.56 | 0.23 | 85,85,85,85 | 0 |
| 55 | MG | 2A | 3464 | 1/1 | 0.58 | 0.30 | 77,77,77,77 | 0 |
| 55 | MG | 2A | 3741 | 1/1 | 0.58 | 0.22 | 72,72,72,72 | 0 |
| 55 | MG | 1A | 3624 | 1/1 | 0.58 | 0.29 | 81,81,81,81 | 0 |
| 55 | MG | 1B | 229 | 1/1 | 0.59 | 0.42 | 72,72,72,72 | 0 |
| 55 | MG | 2A | 3735 | 1/1 | 0.59 | 0.17 | 60,60,60,60 | 0 |
| 55 | MG | 2a | 3024 | 1/1 | 0.60 | 0.35 | 77,77,77,77 | 0 |
| 55 | MG | 1A | 3541 | 1/1 | 0.61 | 0.58 | 67,67,67,67 | 0 |
| 55 | MG | 2A | 3270 | 1/1 | 0.62 | 0.27 | 70,70,70,70 | 0 |
| 55 | MG | 2B | 213 | 1/1 | 0.62 | 0.31 | 76,76,76,76 | 0 |
| 55 | MG | 1a | 1677 | 1/1 | 0.62 | 0.30 | 75,75,75,75 | 0 |
| 55 | MG | 1x | 113 | 1/1 | 0.62 | 0.16 | 68,68,68,68 | 0 |
| 55 | MG | 2A | 3854 | 1/1 | 0.63 | 0.28 | 68,68,68,68 | 0 |
| 55 | MG | 2a | 3128 | 1/1 | 0.64 | 0.17 | 90,90,90,90 | 0 |
| 55 | MG | 2a | 3139 | 1/1 | 0.64 | 0.21 | 69,69,69,69 | 0 |
| 55 | MG | 2A | 3222 | 1/1 | 0.64 | 0.21 | 68,68,68,68 | 0 |
| 55 | MG | 2A | 3377 | 1/1 | 0.67 | 0.13 | 65,65,65,65 | 0 |
| 55 | MG | 1a | 1662 | 1/1 | 0.67 | 0.45 | 69,69,69,69 | 0 |
| 55 | MG | 1a | 1638 | 1/1 | 0.68 | 0.17 | 55,55,55,55 | 0 |
| 55 | MG | 1A | 3347 | 1/1 | 0.68 | 0.31 | 60,60,60,60 | 0 |
| 55 | MG | 2a | 3082 | 1/1 | 0.68 | 0.26 | 75,75,75,75 | 0 |
| 55 | MG | 2A | 3289 | 1/1 | 0.68 | 0.34 | 75,75,75,75 | 0 |
| 55 | MG | 2A | 3830 | 1/1 | 0.68 | 0.16 | 76,76,76,76 | 0 |
| 55 | MG | 1U | 207 | 1/1 | 0.68 | 0.43 | 54,54,54,54 | 0 |
| 55 | MG | 2A | 3653 | 1/1 | 0.69 | 0.20 | 72,72,72,72 | 0 |
| 55 | MG | 2a | 3083 | 1/1 | 0.69 | 0.12 | 64,64,64,64 | 0 |
| 55 | MG | 2A | 3690 | 1/1 | 0.69 | 0.12 | 64,64,64,64 | 0 |
| 55 | MG | 1a | 1681 | 1/1 | 0.69 | 0.21 | 76,76,76,76 | 0 |
| 55 | MG | 1a | 1789 | 1/1 | 0.69 | 0.19 | 79,79,79,79 | 0 |
| 55 | MG | 1a | 1715 | 1/1 | 0.70 | 0.15 | 53,53,53,53 | 0 |
| 55 | MG | 2A | 3294 | 1/1 | 0.70 | 0.22 | 61,61,61,61 | 0 |
| 55 | MG | 2A | 3317 | 1/1 | 0.70 | 0.12 | 78,78,78,78 | 0 |
| 55 | MG | 2a | 3180 | 1/1 | 0.70 | 0.27 | 63,63,63,63 | 0 |
| 55 | MG | 1a | 1769 | 1/1 | 0.71 | 0.19 | 71,71,71,71 | 0 |
| 55 | MG | 1a | 1718 | 1/1 | 0.71 | 0.33 | 68,68,68,68 | 0 |
| 55 | MG | 2a | 3050 | 1/1 | 0.71 | 0.33 | 79,79,79,79 | 0 |
| 55 | MG | 2a | 3040 | 1/1 | 0.72 | 0.15 | 55,55,55,55 | 0 |
| 55 | MG | 1a | 1719 | 1/1 | 0.73 | 0.36 | 61,61,61,61 | 0 |
| 55 | MG | 1a | 1612 | 1/1 | 0.73 | 0.12 | 57,57,57,57 | 0 |
| 55 | MG | 2d | 302 | 1/1 | 0.73 | 0.19 | 73,73,73,73 | 0 |
| 55 | MG | 2B | 216 | 1/1 | 0.74 | 0.21 | 65,65,65,65 | 0 |
| 55 | MG | 1A | 3219 | 1/1 | 0.74 | 0.29 | 68,68,68,68 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 55 | MG | 2a | 3029 | 1/1 | 0.74 | 0.37 | 78,78,78,78 | 0 |
| 55 | MG | 1A | 3248 | 1/1 | 0.74 | 0.22 | 66,66,66,66 | 0 |
| 55 | MG | 2i | 201 | 1/1 | 0.74 | 0.57 | 82,82,82,82 | 0 |
| 55 | MG | 2x | 101 | 1/1 | 0.74 | 0.21 | 84,84,84,84 | 0 |
| 55 | MG | 2A | 3498 | 1/1 | 0.75 | 0.39 | 74,74,74,74 | 0 |
| 55 | MG | 2a | 3174 | 1/1 | 0.75 | 0.20 | 75,75,75,75 | 0 |
| 55 | MG | 1A | 3499 | 1/1 | 0.75 | 0.35 | 65,65,65,65 | 0 |
| 55 | MG | 2a | 3206 | 1/1 | 0.75 | 0.23 | 78,78,78,78 | 0 |
| 55 | MG | 2a | 3092 | 1/1 | 0.75 | 0.42 | 68,68,68,68 | 0 |
| 55 | MG | 1A | 4023 | 1/1 | 0.75 | 0.10 | 73,73,73,73 | 0 |
| 55 | MG | 2j | 202 | 1/1 | 0.75 | 0.18 | 74,74,74,74 | 0 |
| 55 | MG | 2T | 201 | 1/1 | 0.75 | 0.31 | 65,65,65,65 | 0 |
| 55 | MG | 2A | 3252 | 1/1 | 0.76 | 0.10 | 50,50,50,50 | 0 |
| 55 | MG | 2a | 3190 | 1/1 | 0.76 | 0.22 | 66,66,66,66 | 0 |
| 55 | MG | 2a | 3130 | 1/1 | 0.76 | 0.35 | 69,69,69,69 | 0 |
| 55 | MG | 1A | 3926 | 1/1 | 0.76 | 0.11 | 45,45,45,45 | 0 |
| 55 | MG | 2a | 3158 | 1/1 | 0.76 | 0.19 | 70,70,70,70 | 0 |
| 55 | MG | 1A | 3851 | 1/1 | 0.76 | 0.15 | 49,49,49,49 | 0 |
| 55 | MG | 2A | 3229 | 1/1 | 0.76 | 0.17 | 59,59,59,59 | 0 |
| 55 | MG | 2A | 3092 | 1/1 | 0.77 | 0.29 | 62,62,62,62 | 0 |
| 55 | MG | 2A | 3163 | 1/1 | 0.77 | 0.22 | 64,64,64,64 | 0 |
| 55 | MG | 2a | 3105 | 1/1 | 0.77 | 0.22 | 80,80,80,80 | 0 |
| 55 | MG | 2a | 3117 | 1/1 | 0.77 | 0.31 | 49,49,49,49 | 0 |
| 55 | MG | 2A | 3760 | 1/1 | 0.77 | 0.10 | 76,76,76,76 | 0 |
| 55 | MG | 2A | 3346 | 1/1 | 0.77 | 0.11 | 67,67,67,67 | 0 |
| 55 | MG | 2A | 3359 | 1/1 | 0.77 | 0.20 | 63,63,63,63 | 0 |
| 55 | MG | 2B | 204 | 1/1 | 0.77 | 0.20 | 75,75,75,75 | 0 |
| 55 | MG | 2A | 3361 | 1/1 | 0.77 | 0.19 | 64,64,64,64 | 0 |
| 55 | MG | 1a | 1702 | 1/1 | 0.77 | 0.25 | 60,60,60,60 | 0 |
| 55 | MG | 2A | 3441 | 1/1 | 0.77 | 0.14 | 63,63,63,63 | 0 |
| 55 | MG | 1A | 3947 | 1/1 | 0.77 | 0.12 | 23,23,23,23 | 0 |
| 55 | MG | 2a | 3205 | 1/1 | 0.77 | 0.22 | 59,59,59,59 | 0 |
| 55 | MG | 1A | 3450 | 1/1 | 0.77 | 0.18 | 74,74,74,74 | 0 |
| 55 | MG | 1A | 3741 | 1/1 | 0.77 | 0.10 | 56,56,56,56 | 0 |
| 55 | MG | 2A | 3089 | 1/1 | 0.77 | 0.20 | 72,72,72,72 | 0 |
| 55 | MG | 2a | 3061 | 1/1 | 0.77 | 0.23 | 68,68,68,68 | 0 |
| 55 | MG | 2A | 3715 | 1/1 | 0.77 | 0.14 | 66,66,66,66 | 0 |
| 55 | MG | 2x | 104 | 1/1 | 0.77 | 0.17 | 70,70,70,70 | 0 |
| 55 | MG | 2A | 3365 | 1/1 | 0.78 | 0.18 | 66,66,66,66 | 0 |
| 55 | MG | 2A | 3080 | 1/1 | 0.78 | 0.21 | 67,67,67,67 | 0 |
| 55 | MG | 2A | 3258 | 1/1 | 0.78 | 0.25 | 64,64,64,64 | 0 |
| 55 | MG | 1a | 1750 | 1/1 | 0.78 | 0.15 | 77,77,77,77 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 55 | MG | 18 | 105 | 1/1 | 0.78 | 0.22 | 75,75,75,75 | 0 |
| 55 | MG | 2a | 3145 | 1/1 | 0.78 | 0.39 | 67,67,67,67 | 0 |
| 55 | MG | 2B | 214 | 1/1 | 0.78 | 0.37 | 82,82,82,82 | 0 |
| 55 | MG | 2A | 3612 | 1/1 | 0.78 | 0.30 | 53,53,53,53 | 0 |
| 55 | MG | 1A | 3988 | 1/1 | 0.78 | 0.12 | 50,50,50,50 | 0 |
| 55 | MG | 2A | 3689 | 1/1 | 0.78 | 0.12 | 71,71,71,71 | 0 |
| 55 | MG | 1A | 3549 | 1/1 | 0.78 | 0.29 | 45,45,45,45 | 0 |
| 55 | MG | 2A | 3707 | 1/1 | 0.78 | 0.13 | 56,56,56,56 | 0 |
| 55 | MG | 2A | 3227 | 1/1 | 0.78 | 0.21 | 69,69,69,69 | 0 |
| 55 | MG | 2A | 3725 | 1/1 | 0.78 | 0.29 | 68,68,68,68 | 0 |
| 55 | MG | 1a | 1642 | 1/1 | 0.78 | 0.27 | 67,67,67,67 | 0 |
| 55 | MG | 2A | 3740 | 1/1 | 0.78 | 0.20 | 68,68,68,68 | 0 |
| 55 | MG | 2a | 3091 | 1/1 | 0.78 | 0.26 | 71,71,71,71 | 0 |
| 55 | MG | 2A | 3230 | 1/1 | 0.78 | 0.10 | 78,78,78,78 | 0 |
| 55 | MG | 1A | 3346 | 1/1 | 0.79 | 0.15 | 55,55,55,55 | 0 |
| 55 | MG | 2a | 3110 | 1/1 | 0.79 | 0.18 | 61,61,61,61 | 0 |
| 55 | MG | 2B | 206 | 1/1 | 0.79 | 0.21 | 57,57,57,57 | 0 |
| 55 | MG | 2A | 3654 | 1/1 | 0.79 | 0.12 | 63,63,63,63 | 0 |
| 55 | MG | 2a | 3129 | 1/1 | 0.79 | 0.40 | 64,64,64,64 | 0 |
| 55 | MG | 1a | 1636 | 1/1 | 0.79 | 0.22 | 63,63,63,63 | 0 |
| 55 | MG | 1A | 3464 | 1/1 | 0.79 | 0.08 | 40,40,40,40 | 0 |
| 55 | MG | 2F | 306 | 1/1 | 0.79 | 0.14 | 62,62,62,62 | 0 |
| 55 | MG | 1A | 3303 | 1/1 | 0.79 | 0.13 | 62,62,62,62 | 0 |
| 55 | MG | 2U | 201 | 1/1 | 0.79 | 0.27 | 58,58,58,58 | 0 |
| 55 | MG | 1A | 3683 | 1/1 | 0.79 | 0.09 | 53,53,53,53 | 0 |
| 55 | MG | 1a | 1748 | 1/1 | 0.79 | 0.13 | 63,63,63,63 | 0 |
| 55 | MG | 2A | 3094 | 1/1 | 0.79 | 0.14 | 67,67,67,67 | 0 |
| 55 | MG | 2A | 3484 | 1/1 | 0.79 | 0.58 | 58,58,58,58 | 0 |
| 55 | MG | 1A | 3527 | 1/1 | 0.79 | 0.29 | 53,53,53,53 | 0 |
| 55 | MG | 2a | 3069 | 1/1 | 0.79 | 0.28 | 57,57,57,57 | 0 |
| 55 | MG | 2A | 3551 | 1/1 | 0.79 | 0.15 | 42,42,42,42 | 0 |
| 55 | MG | 2A | 3827 | 1/1 | 0.79 | 0.16 | 64,64,64,64 | 0 |
| 55 | MG | 2A | 3570 | 1/1 | 0.79 | 0.19 | 65,65,65,65 | 0 |
| 55 | MG | 1a | 1601 | 1/1 | 0.79 | 0.12 | 63,63,63,63 | 0 |
| 55 | MG | 2A | 3158 | 1/1 | 0.80 | 0.21 | 51,51,51,51 | 0 |
| 55 | MG | 1a | 1773 | 1/1 | 0.80 | 0.21 | 70,70,70,70 | 0 |
| 55 | MG | 2A | 3170 | 1/1 | 0.80 | 0.31 | 65,65,65,65 | 0 |
| 55 | MG | 2B | 210 | 1/1 | 0.80 | 0.19 | 59,59,59,59 | 0 |
| 55 | MG | 1A | 3284 | 1/1 | 0.80 | 0.09 | 37,37,37,37 | 0 |
| 55 | MG | 1A | 3742 | 1/1 | 0.80 | 0.18 | 51,51,51,51 | 0 |
| 55 | MG | 1a | 1618 | 1/1 | 0.80 | 0.12 | 51,51,51,51 | 0 |
| 55 | MG | 1A | 3305 | 1/1 | 0.80 | 0.25 | 51,51,51,51 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 55 | MG | 2A | 3369 | 1/1 | 0.80 | 0.18 | 78,78,78,78 | 0 |
| 55 | MG | 2A | 3090 | 1/1 | 0.80 | 0.23 | 57,57,57,57 | 0 |
| 55 | MG | 2a | 3162 | 1/1 | 0.80 | 0.22 | 61,61,61,61 | 0 |
| 55 | MG | 2a | 3021 | 1/1 | 0.80 | 0.12 | 55,55,55,55 | 0 |
| 55 | MG | 1A | 3858 | 1/1 | 0.80 | 0.16 | 69,69,69,69 | 0 |
| 55 | MG | 2a | 3175 | 1/1 | 0.80 | 0.15 | 70,70,70,70 | 0 |
| 55 | MG | 2A | 3454 | 1/1 | 0.80 | 0.14 | 47,47,47,47 | 0 |
| 55 | MG | 2A | 3461 | 1/1 | 0.80 | 0.19 | 60,60,60,60 | 0 |
| 55 | MG | 2A | 3260 | 1/1 | 0.80 | 0.25 | 60,60,60,60 | 0 |
| 55 | MG | 2A | 3475 | 1/1 | 0.80 | 0.19 | 67,67,67,67 | 0 |
| 55 | MG | 2a | 3063 | 1/1 | 0.80 | 0.33 | 69,69,69,69 | 0 |
| 55 | MG | 2A | 3778 | 1/1 | 0.80 | 0.11 | 63,63,63,63 | 0 |
| 55 | MG | 1B | 223 | 1/1 | 0.80 | 0.15 | 56,56,56,56 | 0 |
| 55 | MG | 2A | 3285 | 1/1 | 0.80 | 0.14 | 52,52,52,52 | 0 |
| 55 | MG | 2A | 3852 | 1/1 | 0.80 | 0.20 | 61,61,61,61 | 0 |
| 55 | MG | 1a | 1803 | 1/1 | 0.81 | 0.11 | 66,66,66,66 | 0 |
| 55 | MG | 1a | 1834 | 1/1 | 0.81 | 0.37 | 68,68,68,68 | 0 |
| 55 | MG | 1t | 201 | 1/1 | 0.81 | 0.28 | 59,59,59,59 | 0 |
| 55 | MG | 1v | 102 | 1/1 | 0.81 | 0.18 | 74,74,74,74 | 0 |
| 55 | MG | 1x | 109 | 1/1 | 0.81 | 0.22 | 73,73,73,73 | 0 |
| 55 | MG | 1A | 3824 | 1/1 | 0.81 | 0.29 | 47,47,47,47 | 0 |
| 55 | MG | 2A | 3049 | 1/1 | 0.81 | 0.15 | 68,68,68,68 | 0 |
| 55 | MG | 2A | 3465 | 1/1 | 0.81 | 0.28 | 54,54,54,54 | 0 |
| 55 | MG | 1A | 3212 | 1/1 | 0.81 | 0.19 | 53,53,53,53 | 0 |
| 55 | MG | 1Y | 203 | 1/1 | 0.81 | 0.07 | 68,68,68,68 | 0 |
| 55 | MG | 1A | 3120 | 1/1 | 0.81 | 0.13 | 49,49,49,49 | 0 |
| 55 | MG | 2a | 3135 | 1/1 | 0.81 | 0.31 | 64,64,64,64 | 0 |
| 55 | MG | 2A | 3516 | 1/1 | 0.81 | 0.28 | 60,60,60,60 | 0 |
| 55 | MG | 2A | 3521 | 1/1 | 0.81 | 0.14 | 55,55,55,55 | 0 |
| 55 | MG | 2A | 3527 | 1/1 | 0.81 | 0.15 | 54,54,54,54 | 0 |
| 55 | MG | 1B | 207 | 1/1 | 0.81 | 0.16 | 49,49,49,49 | 0 |
| 55 | MG | 2A | 3554 | 1/1 | 0.81 | 0.23 | 67,67,67,67 | 0 |
| 55 | MG | 2D | 303 | 1/1 | 0.81 | 0.15 | 62,62,62,62 | 0 |
| 55 | MG | 2A | 3290 | 1/1 | 0.81 | 0.36 | 68,68,68,68 | 0 |
| 55 | MG | 2a | 3176 | 1/1 | 0.81 | 0.25 | 67,67,67,67 | 0 |
| 55 | MG | 2A | 3596 | 1/1 | 0.81 | 0.11 | 48,48,48,48 | 0 |
| 55 | MG | 1A | 3861 | 1/1 | 0.81 | 0.08 | 48,48,48,48 | 0 |
| 55 | MG | 2A | 3645 | 1/1 | 0.81 | 0.22 | 54,54,54,54 | 0 |
| 55 | MG | 2A | 3118 | 1/1 | 0.81 | 0.18 | 59,59,59,59 | 0 |
| 55 | MG | 2A | 3323 | 1/1 | 0.81 | 0.21 | 67,67,67,67 | 0 |
| 55 | MG | 2A | 3130 | 1/1 | 0.81 | 0.25 | 57,57,57,57 | 0 |
| 55 | MG | 2A | 3348 | 1/1 | 0.81 | 0.30 | 64,64,64,64 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 55 | MG | 1A | 3873 | 1/1 | 0.81 | 0.20 | 75,75,75,75 | 0 |
| 55 | MG | 1A | 3131 | 1/1 | 0.81 | 0.09 | 73,73,73,73 | 0 |
| 55 | MG | 2a | 3101 | 1/1 | 0.82 | 0.19 | 73,73,73,73 | 0 |
| 55 | MG | 2A | 3068 | 1/1 | 0.82 | 0.34 | 69,69,69,69 | 0 |
| 55 | MG | 2A | 3310 | 1/1 | 0.82 | 0.20 | 66,66,66,66 | 0 |
| 55 | MG | 2a | 3116 | 1/1 | 0.82 | 0.21 | 54,54,54,54 | 0 |
| 55 | MG | 2A | 3666 | 1/1 | 0.82 | 0.23 | 72,72,72,72 | 0 |
| 55 | MG | 2a | 3125 | 1/1 | 0.82 | 0.29 | 61,61,61,61 | 0 |
| 55 | MG | 2A | 3678 | 1/1 | 0.82 | 0.11 | 79,79,79,79 | 0 |
| 55 | MG | 1a | 1671 | 1/1 | 0.82 | 0.29 | 63,63,63,63 | 0 |
| 55 | MG | 2A | 3234 | 1/1 | 0.82 | 0.24 | 61,61,61,61 | 0 |
| 55 | MG | 2A | 3704 | 1/1 | 0.82 | 0.12 | 53,53,53,53 | 0 |
| 55 | MG | 1a | 1787 | 1/1 | 0.82 | 0.12 | 73,73,73,73 | 0 |
| 55 | MG | 2A | 3710 | 1/1 | 0.82 | 0.15 | 50,50,50,50 | 0 |
| 55 | MG | 2a | 3150 | 1/1 | 0.82 | 0.29 | 71,71,71,71 | 0 |
| 55 | MG | 2A | 3253 | 1/1 | 0.82 | 0.08 | 64,64,64,64 | 0 |
| 55 | MG | 2a | 3004 | 1/1 | 0.82 | 0.33 | 65,65,65,65 | 0 |
| 55 | MG | 2a | 3164 | 1/1 | 0.82 | 0.15 | 66,66,66,66 | 0 |
| 55 | MG | 2A | 3355 | 1/1 | 0.82 | 0.19 | 61,61,61,61 | 0 |
| 55 | MG | 2A | 3730 | 1/1 | 0.82 | 0.10 | 60,60,60,60 | 0 |
| 55 | MG | 1A | 3680 | 1/1 | 0.82 | 0.18 | 33,33,33,33 | 0 |
| 55 | MG | 2a | 3037 | 1/1 | 0.82 | 0.22 | 80,80,80,80 | 0 |
| 55 | MG | 2A | 3166 | 1/1 | 0.82 | 0.26 | 71,71,71,71 | 0 |
| 55 | MG | 2A | 3266 | 1/1 | 0.82 | 0.15 | 59,59,59,59 | 0 |
| 55 | MG | 2a | 3191 | 1/1 | 0.82 | 0.26 | 55,55,55,55 | 0 |
| 55 | MG | 1A | 3879 | 1/1 | 0.82 | 0.14 | 64,64,64,64 | 0 |
| 55 | MG | 2A | 3201 | 1/1 | 0.82 | 0.17 | 66,66,66,66 | 0 |
| 55 | MG | 2a | 3208 | 1/1 | 0.82 | 0.20 | 58,58,58,58 | 0 |
| 55 | MG | 2a | 3209 | 1/1 | 0.82 | 0.24 | 63,63,63,63 | 0 |
| 55 | MG | 2A | 3582 | 1/1 | 0.82 | 0.13 | 56,56,56,56 | 0 |
| 55 | MG | 2A | 3384 | 1/1 | 0.82 | 0.21 | 68,68,68,68 | 0 |
| 55 | MG | 2A | 3836 | 1/1 | 0.82 | 0.15 | 49,49,49,49 | 0 |
| 55 | MG | 1A | 3603 | 1/1 | 0.82 | 0.32 | 53,53,53,53 | 0 |
| 55 | MG | 2A | 3111 | 1/1 | 0.82 | 0.17 | 65,65,65,65 | 0 |
| 55 | MG | 1a | 1727 | 1/1 | 0.83 | 0.35 | 67,67,67,67 | 0 |
| 55 | MG | 1A | 3302 | 1/1 | 0.83 | 0.17 | 45,45,45,45 | 0 |
| 55 | MG | 2A | 3070 | 1/1 | 0.83 | 0.12 | 60,60,60,60 | 0 |
| 55 | MG | 1A | 3488 | 1/1 | 0.83 | 0.11 | 58,58,58,58 | 0 |
| 55 | MG | 2A | 3082 | 1/1 | 0.83 | 0.26 | 57,57,57,57 | 0 |
| 55 | MG | 1A | 3895 | 1/1 | 0.83 | 0.13 | 41,41,41,41 | 0 |
| 55 | MG | 1A | 3901 | 1/1 | 0.83 | 0.13 | 48,48,48,48 | 0 |
| 55 | MG | 2A | 3486 | 1/1 | 0.83 | 0.30 | 50,50,50,50 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 55 | MG | 2a | 3108 | 1/1 | 0.83 | 0.23 | 72,72,72,72 | 0 |
| 55 | MG | 2A | 3773 | 1/1 | 0.83 | 0.19 | 62,62,62,62 | 0 |
| 55 | MG | 1a | 1670 | 1/1 | 0.83 | 0.10 | 67,67,67,67 | 0 |
| 55 | MG | 2A | 3817 | 1/1 | 0.83 | 0.16 | 40,40,40,40 | 0 |
| 55 | MG | 1A | 3156 | 1/1 | 0.83 | 0.25 | 36,36,36,36 | 0 |
| 55 | MG | 2a | 3127 | 1/1 | 0.83 | 0.23 | 60,60,60,60 | 0 |
| 55 | MG | 2A | 3095 | 1/1 | 0.83 | 0.30 | 65,65,65,65 | 0 |
| 55 | MG | 1D | 310 | 1/1 | 0.83 | 0.15 | 40,40,40,40 | 0 |
| 55 | MG | 2A | 3536 | 1/1 | 0.83 | 0.32 | 58,58,58,58 | 0 |
| 55 | MG | 2A | 3540 | 1/1 | 0.83 | 0.15 | 40,40,40,40 | 0 |
| 55 | MG | 2B | 201 | 1/1 | 0.83 | 0.13 | 68,68,68,68 | 0 |
| 55 | MG | 1A | 3940 | 1/1 | 0.83 | 0.15 | 52,52,52,52 | 0 |
| 55 | MG | 1a | 1807 | 1/1 | 0.83 | 0.15 | 63,63,63,63 | 0 |
| 55 | MG | 2A | 3151 | 1/1 | 0.83 | 0.17 | 68,68,68,68 | 0 |
| 55 | MG | 2a | 3159 | 1/1 | 0.83 | 0.15 | 53,53,53,53 | 0 |
| 55 | MG | 1a | 1815 | 1/1 | 0.83 | 0.23 | 63,63,63,63 | 0 |
| 55 | MG | 1a | 1829 | 1/1 | 0.83 | 0.16 | 79,79,79,79 | 0 |
| 55 | MG | 2A | 3165 | 1/1 | 0.83 | 0.11 | 60,60,60,60 | 0 |
| 55 | MG | 2A | 3615 | 1/1 | 0.83 | 0.27 | 67,67,67,67 | 0 |
| 55 | MG | 1A | 3509 | 1/1 | 0.83 | 0.20 | 32,32,32,32 | 0 |
| 55 | MG | 2G | 201 | 1/1 | 0.83 | 0.16 | 68,68,68,68 | 0 |
| 55 | MG | 1A | 3523 | 1/1 | 0.83 | 0.17 | 47,47,47,47 | 0 |
| 55 | MG | 2A | 3177 | 1/1 | 0.83 | 0.35 | 56,56,56,56 | 0 |
| 55 | MG | 20 | 101 | 1/1 | 0.83 | 0.14 | 65,65,65,65 | 0 |
| 55 | MG | 2a | 3197 | 1/1 | 0.83 | 0.20 | 57,57,57,57 | 0 |
| 55 | MG | 2A | 3189 | 1/1 | 0.83 | 0.10 | 55,55,55,55 | 0 |
| 55 | MG | 2A | 3669 | 1/1 | 0.83 | 0.26 | 52,52,52,52 | 0 |
| 55 | MG | 2A | 3676 | 1/1 | 0.83 | 0.11 | 69,69,69,69 | 0 |
| 55 | MG | 2a | 3028 | 1/1 | 0.83 | 0.22 | 70,70,70,70 | 0 |
| 55 | MG | 2A | 3190 | 1/1 | 0.83 | 0.31 | 65,65,65,65 | 0 |
| 55 | MG | 1A | 3223 | 1/1 | 0.83 | 0.24 | 55,55,55,55 | 0 |
| 55 | MG | 2j | 201 | 1/1 | 0.83 | 0.08 | 71,71,71,71 | 0 |
| 55 | MG | 1A | 4027 | 1/1 | 0.83 | 0.10 | 21,21,21,21 | 0 |
| 55 | MG | 2A | 3378 | 1/1 | 0.83 | 0.10 | 67,67,67,67 | 0 |
| 55 | MG | 1A | 4107 | 1/1 | 0.83 | 0.16 | 63,63,63,63 | 0 |
| 55 | MG | 2A | 3320 | 1/1 | 0.84 | 0.11 | 64,64,64,64 | 0 |
| 55 | MG | 2A | 3083 | 1/1 | 0.84 | 0.11 | 35,35,35,35 | 0 |
| 55 | MG | 1a | 1714 | 1/1 | 0.84 | 0.15 | 51,51,51,51 | 0 |
| 55 | MG | 2A | 3781 | 1/1 | 0.84 | 0.15 | 62,62,62,62 | 0 |
| 55 | MG | 1A | 3620 | 1/1 | 0.84 | 0.24 | 38,38,38,38 | 0 |
| 55 | MG | 2A | 3563 | 1/1 | 0.84 | 0.12 | 41,41,41,41 | 0 |
| 55 | MG | 1a | 1639 | 1/1 | 0.84 | 0.29 | 73,73,73,73 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 55 | MG | 15 | 105 | 1/1 | 0.84 | 0.10 | 43,43,43,43 | 0 |
| 55 | MG | 1a | 1831 | 1/1 | 0.84 | 0.29 | 70,70,70,70 | 0 |
| 55 | MG | 2A | 3853 | 1/1 | 0.84 | 0.07 | 64,64,64,64 | 0 |
| 55 | MG | 2A | 3605 | 1/1 | 0.84 | 0.14 | 34,34,34,34 | 0 |
| 55 | MG | 1A | 3385 | 1/1 | 0.84 | 0.13 | 48,48,48,48 | 0 |
| 55 | MG | 2A | 3244 | 1/1 | 0.84 | 0.20 | 51,51,51,51 | 0 |
| 55 | MG | 2B | 205 | 1/1 | 0.84 | 0.13 | 64,64,64,64 | 0 |
| 55 | MG | 2A | 3374 | 1/1 | 0.84 | 0.13 | 65,65,65,65 | 0 |
| 55 | MG | 2A | 3646 | 1/1 | 0.84 | 0.20 | 70,70,70,70 | 0 |
| 55 | MG | 1A | 3654 | 1/1 | 0.84 | 0.13 | 36,36,36,36 | 0 |
| 55 | MG | 1a | 1604 | 1/1 | 0.84 | 0.19 | 65,65,65,65 | 0 |
| 55 | MG | 2A | 3141 | 1/1 | 0.84 | 0.30 | 69,69,69,69 | 0 |
| 55 | MG | 1A | 3804 | 1/1 | 0.84 | 0.12 | 24,24,24,24 | 0 |
| 55 | MG | 2A | 3674 | 1/1 | 0.84 | 0.15 | 57,57,57,57 | 0 |
| 55 | MG | 1a | 1614 | 1/1 | 0.84 | 0.10 | 69,69,69,69 | 0 |
| 55 | MG | 2A | 3161 | 1/1 | 0.84 | 0.30 | 50,50,50,50 | 0 |
| 55 | MG | 2A | 3685 | 1/1 | 0.84 | 0.11 | 68,68,68,68 | 0 |
| 55 | MG | 2A | 3462 | 1/1 | 0.84 | 0.24 | 60,60,60,60 | 0 |
| 55 | MG | 28 | 103 | 1/1 | 0.84 | 0.30 | 67,67,67,67 | 0 |
| 55 | MG | 2A | 3274 | 1/1 | 0.84 | 0.09 | 54,54,54,54 | 0 |
| 55 | MG | 2a | 3017 | 1/1 | 0.84 | 0.14 | 49,49,49,49 | 0 |
| 55 | MG | 2A | 3280 | 1/1 | 0.84 | 0.17 | 70,70,70,70 | 0 |
| 55 | MG | 1A | 4113 | 1/1 | 0.84 | 0.16 | 57,57,57,57 | 0 |
| 55 | MG | 1a | 1775 | 1/1 | 0.84 | 0.18 | 59,59,59,59 | 0 |
| 55 | MG | 1a | 1783 | 1/1 | 0.84 | 0.18 | 61,61,61,61 | 0 |
| 55 | MG | 2A | 3716 | 1/1 | 0.84 | 0.10 | 64,64,64,64 | 0 |
| 55 | MG | 2A | 3720 | 1/1 | 0.84 | 0.20 | 53,53,53,53 | 0 |
| 55 | MG | 2a | 3041 | 1/1 | 0.84 | 0.10 | 55,55,55,55 | 0 |
| 55 | MG | 2A | 3492 | 1/1 | 0.84 | 0.24 | 49,49,49,49 | 0 |
| 55 | MG | 2A | 3077 | 1/1 | 0.84 | 0.13 | 64,64,64,64 | 0 |
| 55 | MG | 1a | 1686 | 1/1 | 0.84 | 0.22 | 67,67,67,67 | 0 |
| 55 | MG | 2t | 201 | 1/1 | 0.84 | 0.18 | 62,62,62,62 | 0 |
| 55 | MG | 1A | 3465 | 1/1 | 0.84 | 0.24 | 57,57,57,57 | 0 |
| 55 | MG | 2A | 3318 | 1/1 | 0.84 | 0.33 | 81,81,81,81 | 0 |
| 55 | MG | 2a | 3030 | 1/1 | 0.85 | 0.17 | 60,60,60,60 | 0 |
| 55 | MG | 1a | 1643 | 1/1 | 0.85 | 0.09 | 65,65,65,65 | 0 |
| 55 | MG | 1a | 1753 | 1/1 | 0.85 | 0.20 | 67,67,67,67 | 0 |
| 55 | MG | 1a | 1763 | 1/1 | 0.85 | 0.14 | 59,59,59,59 | 0 |
| 55 | MG | 2a | 3044 | 1/1 | 0.85 | 0.12 | 78,78,78,78 | 0 |
| 55 | MG | 2a | 3048 | 1/1 | 0.85 | 0.18 | 68,68,68,68 | 0 |
| 55 | MG | 1a | 1644 | 1/1 | 0.85 | 0.14 | 72,72,72,72 | 0 |
| 55 | MG | 2a | 3052 | 1/1 | 0.85 | 0.27 | 62,62,62,62 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 55 | MG | 1a | 1656 | 1/1 | 0.85 | 0.18 | 59,59,59,59 | 0 |
| 55 | MG | 2A | 3259 | 1/1 | 0.85 | 0.20 | 61,61,61,61 | 0 |
| 55 | MG | 1A | 3912 | 1/1 | 0.85 | 0.13 | 27,27,27,27 | 0 |
| 55 | MG | 2A | 3485 | 1/1 | 0.85 | 0.12 | 60,60,60,60 | 0 |
| 55 | MG | 1A | 4038 | 1/1 | 0.85 | 0.09 | 73,73,73,73 | 0 |
| 55 | MG | 2a | 3088 | 1/1 | 0.85 | 0.22 | 61,61,61,61 | 0 |
| 55 | MG | 2a | 3090 | 1/1 | 0.85 | 0.12 | 72,72,72,72 | 0 |
| 55 | MG | 1A | 4098 | 1/1 | 0.85 | 0.10 | 57,57,57,57 | 0 |
| 55 | MG | 1A | 3239 | 1/1 | 0.85 | 0.18 | 35,35,35,35 | 0 |
| 55 | MG | 1A | 3928 | 1/1 | 0.85 | 0.09 | 44,44,44,44 | 0 |
| 55 | MG | 2A | 3115 | 1/1 | 0.85 | 0.16 | 42,42,42,42 | 0 |
| 55 | MG | 1a | 1792 | 1/1 | 0.85 | 0.19 | 84,84,84,84 | 0 |
| 55 | MG | 2A | 3806 | 1/1 | 0.85 | 0.22 | 37,37,37,37 | 0 |
| 55 | MG | 2a | 3111 | 1/1 | 0.85 | 0.20 | 47,47,47,47 | 0 |
| 55 | MG | 1A | 3930 | 1/1 | 0.85 | 0.20 | 53,53,53,53 | 0 |
| 55 | MG | 2A | 3136 | 1/1 | 0.85 | 0.20 | 59,59,59,59 | 0 |
| 55 | MG | 2a | 3124 | 1/1 | 0.85 | 0.24 | 49,49,49,49 | 0 |
| 55 | MG | 1A | 3495 | 1/1 | 0.85 | 0.13 | 60,60,60,60 | 0 |
| 55 | MG | 2A | 3315 | 1/1 | 0.85 | 0.10 | 69,69,69,69 | 0 |
| 55 | MG | 2A | 3844 | 1/1 | 0.85 | 0.30 | 73,73,73,73 | 0 |
| 55 | MG | 2A | 3847 | 1/1 | 0.85 | 0.18 | 72,72,72,72 | 0 |
| 55 | MG | 1A | 3384 | 1/1 | 0.85 | 0.14 | 37,37,37,37 | 0 |
| 55 | MG | 1a | 1703 | 1/1 | 0.85 | 0.19 | 66,66,66,66 | 0 |
| 55 | MG | 1a | 1708 | 1/1 | 0.85 | 0.24 | 58,58,58,58 | 0 |
| 55 | MG | 2A | 3861 | 1/1 | 0.85 | 0.12 | 50,50,50,50 | 0 |
| 55 | MG | 2a | 3147 | 1/1 | 0.85 | 0.29 | 56,56,56,56 | 0 |
| 55 | MG | 1a | 1832 | 1/1 | 0.85 | 0.14 | 61,61,61,61 | 0 |
| 55 | MG | 2B | 202 | 1/1 | 0.85 | 0.15 | 43,43,43,43 | 0 |
| 55 | MG | 2A | 3332 | 1/1 | 0.85 | 0.18 | 61,61,61,61 | 0 |
| 55 | MG | 2A | 3342 | 1/1 | 0.85 | 0.07 | 47,47,47,47 | 0 |
| 55 | MG | 1A | 3900 | 1/1 | 0.85 | 0.13 | 50,50,50,50 | 0 |
| 55 | MG | 2A | 3618 | 1/1 | 0.85 | 0.23 | 28,28,28,28 | 0 |
| 55 | MG | 1f | 201 | 1/1 | 0.85 | 0.24 | 64,64,64,64 | 0 |
| 55 | MG | 1n | 102 | 1/1 | 0.85 | 0.13 | 66,66,66,66 | 0 |
| 55 | MG | 2A | 3647 | 1/1 | 0.85 | 0.12 | 74,74,74,74 | 0 |
| 55 | MG | 1a | 1621 | 1/1 | 0.85 | 0.22 | 72,72,72,72 | 0 |
| 55 | MG | 2A | 3185 | 1/1 | 0.85 | 0.09 | 55,55,55,55 | 0 |
| 55 | MG | 1v | 101 | 1/1 | 0.85 | 0.29 | 71,71,71,71 | 0 |
| 55 | MG | 1a | 1717 | 1/1 | 0.85 | 0.13 | 62,62,62,62 | 0 |
| 55 | MG | 1A | 3992 | 1/1 | 0.85 | 0.18 | 58,58,58,58 | 0 |
| 55 | MG | 2X | 101 | 1/1 | 0.85 | 0.21 | 63,63,63,63 | 0 |
| 55 | MG | 2A | 3675 | 1/1 | 0.85 | 0.28 | 58,58,58,58 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 55 | MG | 23 | 101 | 1/1 | 0.85 | 0.13 | 58,58,58,58 | 0 |
| 55 | MG | 2A | 3375 | 1/1 | 0.85 | 0.20 | 65,65,65,65 | 0 |
| 55 | MG | 1A | 3872 | 1/1 | 0.85 | 0.12 | 52,52,52,52 | 0 |
| 55 | MG | 1a | 1726 | 1/1 | 0.85 | 0.22 | 54,54,54,54 | 0 |
| 55 | MG | 1P | 202 | 1/1 | 0.85 | 0.17 | 59,59,59,59 | 0 |
| 55 | MG | 2r | 101 | 1/1 | 0.85 | 0.24 | 66,66,66,66 | 0 |
| 55 | MG | 2A | 3414 | 1/1 | 0.85 | 0.45 | 52,52,52,52 | 0 |
| 55 | MG | 2A | 3698 | 1/1 | 0.85 | 0.23 | 64,64,64,64 | 0 |
| 55 | MG | 1U | 202 | 1/1 | 0.85 | 0.52 | 49,49,49,49 | 0 |
| 55 | MG | 2A | 3238 | 1/1 | 0.86 | 0.20 | 56,56,56,56 | 0 |
| 55 | MG | 1a | 1668 | 1/1 | 0.86 | 0.09 | 62,62,62,62 | 0 |
| 55 | MG | 1A | 3554 | 1/1 | 0.86 | 0.10 | 49,49,49,49 | 0 |
| 55 | MG | 1A | 4104 | 1/1 | 0.86 | 0.12 | 46,46,46,46 | 0 |
| 55 | MG | 2A | 3717 | 1/1 | 0.86 | 0.17 | 65,65,65,65 | 0 |
| 55 | MG | 1a | 1673 | 1/1 | 0.86 | 0.28 | 59,59,59,59 | 0 |
| 55 | MG | 1a | 1676 | 1/1 | 0.86 | 0.28 | 59,59,59,59 | 0 |
| 55 | MG | 2A | 3472 | 1/1 | 0.86 | 0.29 | 60,60,60,60 | 0 |
| 55 | MG | 1A | 3717 | 1/1 | 0.86 | 0.13 | 41,41,41,41 | 0 |
| 55 | MG | 1A | 4109 | 1/1 | 0.86 | 0.12 | 50,50,50,50 | 0 |
| 55 | MG | 1a | 1602 | 1/1 | 0.86 | 0.24 | 64,64,64,64 | 0 |
| 55 | MG | 1A | 3938 | 1/1 | 0.86 | 0.23 | 28,28,28,28 | 0 |
| 55 | MG | 1a | 1814 | 1/1 | 0.86 | 0.11 | 71,71,71,71 | 0 |
| 55 | MG | 2A | 3776 | 1/1 | 0.86 | 0.14 | 59,59,59,59 | 0 |
| 55 | MG | 2A | 3493 | 1/1 | 0.86 | 0.14 | 55,55,55,55 | 0 |
| 55 | MG | 1a | 1608 | 1/1 | 0.86 | 0.14 | 57,57,57,57 | 0 |
| 55 | MG | 2A | 3784 | 1/1 | 0.86 | 0.12 | 39,39,39,39 | 0 |
| 55 | MG | 2A | 3499 | 1/1 | 0.86 | 0.22 | 59,59,59,59 | 0 |
| 55 | MG | 2A | 3288 | 1/1 | 0.86 | 0.11 | 72,72,72,72 | 0 |
| 55 | MG | 2A | 3133 | 1/1 | 0.86 | 0.12 | 62,62,62,62 | 0 |
| 55 | MG | 1A | 3576 | 1/1 | 0.86 | 0.13 | 54,54,54,54 | 0 |
| 55 | MG | 1a | 1704 | 1/1 | 0.86 | 0.41 | 59,59,59,59 | 0 |
| 55 | MG | 2A | 3296 | 1/1 | 0.86 | 0.15 | 47,47,47,47 | 0 |
| 55 | MG | 2A | 3299 | 1/1 | 0.86 | 0.20 | 53,53,53,53 | 0 |
| 55 | MG | 2A | 3300 | 1/1 | 0.86 | 0.29 | 53,53,53,53 | 0 |
| 55 | MG | 2A | 3142 | 1/1 | 0.86 | 0.28 | 54,54,54,54 | 0 |
| 55 | MG | 2A | 3147 | 1/1 | 0.86 | 0.19 | 60,60,60,60 | 0 |
| 55 | MG | 1A | 3512 | 1/1 | 0.86 | 0.10 | 56,56,56,56 | 0 |
| 55 | MG | 2A | 3595 | 1/1 | 0.86 | 0.34 | 51,51,51,51 | 0 |
| 55 | MG | 1B | 226 | 1/1 | 0.86 | 0.20 | 68,68,68,68 | 0 |
| 55 | MG | 2A | 3598 | 1/1 | 0.86 | 0.15 | 59,59,59,59 | 0 |
| 55 | MG | 1b | 301 | 1/1 | 0.86 | 0.15 | 74,74,74,74 | 0 |
| 55 | MG | 2a | 3148 | 1/1 | 0.86 | 0.39 | 69,69,69,69 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 55 | MG | 1A | 3982 | 1/1 | 0.86 | 0.11 | 26,26,26,26 | 0 |
| 55 | MG | 1A | 3394 | 1/1 | 0.86 | 0.27 | 65,65,65,65 | 0 |
| 55 | MG | 2B | 211 | 1/1 | 0.86 | 0.26 | 63,63,63,63 | 0 |
| 55 | MG | 2a | 3160 | 1/1 | 0.86 | 0.09 | 81,81,81,81 | 0 |
| 55 | MG | 1A | 3991 | 1/1 | 0.86 | 0.10 | 53,53,53,53 | 0 |
| 55 | MG | 2A | 3625 | 1/1 | 0.86 | 0.11 | 41,41,41,41 | 0 |
| 55 | MG | 2a | 3165 | 1/1 | 0.86 | 0.12 | 77,77,77,77 | 0 |
| 55 | MG | 2A | 3630 | 1/1 | 0.86 | 0.38 | 54,54,54,54 | 0 |
| 55 | MG | 1A | 3264 | 1/1 | 0.86 | 0.08 | 41,41,41,41 | 0 |
| 55 | MG | 2E | 304 | 1/1 | 0.86 | 0.25 | 60,60,60,60 | 0 |
| 55 | MG | 1A | 3165 | 1/1 | 0.86 | 0.17 | 51,51,51,51 | 0 |
| 55 | MG | 2A | 3350 | 1/1 | 0.86 | 0.16 | 55,55,55,55 | 0 |
| 55 | MG | 1x | 101 | 1/1 | 0.86 | 0.26 | 59,59,59,59 | 0 |
| 55 | MG | 1T | 203 | 1/1 | 0.86 | 0.14 | 56,56,56,56 | 0 |
| 55 | MG | 2A | 3660 | 1/1 | 0.86 | 0.19 | 54,54,54,54 | 0 |
| 55 | MG | 2a | 3198 | 1/1 | 0.86 | 0.17 | 66,66,66,66 | 0 |
| 55 | MG | 1a | 1741 | 1/1 | 0.86 | 0.26 | 58,58,58,58 | 0 |
| 55 | MG | 2A | 3364 | 1/1 | 0.86 | 0.23 | 56,56,56,56 | 0 |
| 55 | MG | 2A | 3192 | 1/1 | 0.86 | 0.22 | 70,70,70,70 | 0 |
| 55 | MG | 2A | 3043 | 1/1 | 0.86 | 0.12 | 49,49,49,49 | 0 |
| 55 | MG | 2a | 3012 | 1/1 | 0.86 | 0.15 | 63,63,63,63 | 0 |
| 55 | MG | 1A | 3857 | 1/1 | 0.86 | 0.14 | 42,42,42,42 | 0 |
| 55 | MG | 1a | 1654 | 1/1 | 0.86 | 0.13 | 42,42,42,42 | 0 |
| 55 | MG | 1A | 3231 | 1/1 | 0.86 | 0.13 | 55,55,55,55 | 0 |
| 55 | MG | 2p | 101 | 1/1 | 0.86 | 0.14 | 51,51,51,51 | 0 |
| 55 | MG | 1V | 204 | 1/1 | 0.86 | 0.14 | 65,65,65,65 | 0 |
| 55 | MG | 2A | 3380 | 1/1 | 0.86 | 0.18 | 74,74,74,74 | 0 |
| 55 | MG | 2A | 3232 | 1/1 | 0.86 | 0.15 | 58,58,58,58 | 0 |
| 55 | MG | 1a | 1663 | 1/1 | 0.86 | 0.10 | 65,65,65,65 | 0 |
| 55 | MG | 1A | 3788 | 1/1 | 0.87 | 0.17 | 51,51,51,51 | 0 |
| 55 | MG | 1a | 1679 | 1/1 | 0.87 | 0.18 | 64,64,64,64 | 0 |
| 55 | MG | 1A | 3539 | 1/1 | 0.87 | 0.20 | 48,48,48,48 | 0 |
| 55 | MG | 28 | 101 | 1/1 | 0.87 | 0.16 | 63,63,63,63 | 0 |
| 55 | MG | 2A | 3322 | 1/1 | 0.87 | 0.24 | 57,57,57,57 | 0 |
| 55 | MG | 2A | 3150 | 1/1 | 0.87 | 0.21 | 66,66,66,66 | 0 |
| 55 | MG | 2a | 3005 | 1/1 | 0.87 | 0.21 | 53,53,53,53 | 0 |
| 55 | MG | 2A | 3327 | 1/1 | 0.87 | 0.30 | 53,53,53,53 | 0 |
| 55 | MG | 2A | 3330 | 1/1 | 0.87 | 0.12 | 63,63,63,63 | 0 |
| 55 | MG | 1A | 3810 | 1/1 | 0.87 | 0.10 | 52,52,52,52 | 0 |
| 55 | MG | 2A | 3341 | 1/1 | 0.87 | 0.14 | 56,56,56,56 | 0 |
| 55 | MG | 2A | 3157 | 1/1 | 0.87 | 0.12 | 60,60,60,60 | 0 |
| 55 | MG | 1A | 3819 | 1/1 | 0.87 | 0.14 | 52,52,52,52 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 55 | MG | 1A | 4008 | 1/1 | 0.87 | 0.16 | 25,25,25,25 | 0 |
| 55 | MG | 2a | 3032 | 1/1 | 0.87 | 0.24 | 58,58,58,58 | 0 |
| 55 | MG | 2a | 3034 | 1/1 | 0.87 | 0.27 | 56,56,56,56 | 0 |
| 55 | MG | 1A | 4018 | 1/1 | 0.87 | 0.38 | 57,57,57,57 | 0 |
| 55 | MG | 1A | 3298 | 1/1 | 0.87 | 0.20 | 42,42,42,42 | 0 |
| 55 | MG | 1n | 101 | 1/1 | 0.87 | 0.49 | 78,78,78,78 | 0 |
| 55 | MG | 1A | 3839 | 1/1 | 0.87 | 0.20 | 64,64,64,64 | 0 |
| 55 | MG | 2A | 3362 | 1/1 | 0.87 | 0.13 | 57,57,57,57 | 0 |
| 55 | MG | 1A | 3431 | 1/1 | 0.87 | 0.07 | 36,36,36,36 | 0 |
| 55 | MG | 2A | 3183 | 1/1 | 0.87 | 0.21 | 53,53,53,53 | 0 |
| 55 | MG | 1A | 3016 | 1/1 | 0.87 | 0.17 | 55,55,55,55 | 0 |
| 55 | MG | 1A | 3241 | 1/1 | 0.87 | 0.12 | 42,42,42,42 | 0 |
| 55 | MG | 1A | 3585 | 1/1 | 0.87 | 0.21 | 44,44,44,44 | 0 |
| 55 | MG | 2A | 3376 | 1/1 | 0.87 | 0.20 | 60,60,60,60 | 0 |
| 55 | MG | 2A | 3191 | 1/1 | 0.87 | 0.10 | 62,62,62,62 | 0 |
| 55 | MG | 2a | 3087 | 1/1 | 0.87 | 0.25 | 61,61,61,61 | 0 |
| 55 | MG | 1x | 107 | 1/1 | 0.87 | 0.18 | 66,66,66,66 | 0 |
| 55 | MG | 2A | 3200 | 1/1 | 0.87 | 0.25 | 66,66,66,66 | 0 |
| 55 | MG | 2A | 3382 | 1/1 | 0.87 | 0.14 | 66,66,66,66 | 0 |
| 55 | MG | 1a | 1723 | 1/1 | 0.87 | 0.23 | 49,49,49,49 | 0 |
| 55 | MG | 2a | 3098 | 1/1 | 0.87 | 0.25 | 62,62,62,62 | 0 |
| 55 | MG | 2A | 3718 | 1/1 | 0.87 | 0.17 | 57,57,57,57 | 0 |
| 55 | MG | 2A | 3202 | 1/1 | 0.87 | 0.13 | 55,55,55,55 | 0 |
| 55 | MG | 2A | 3423 | 1/1 | 0.87 | 0.21 | 48,48,48,48 | 0 |
| 55 | MG | 1A | 3592 | 1/1 | 0.87 | 0.17 | 50,50,50,50 | 0 |
| 55 | MG | 2A | 3445 | 1/1 | 0.87 | 0.15 | 52,52,52,52 | 0 |
| 55 | MG | 2A | 3036 | 1/1 | 0.87 | 0.10 | 49,49,49,49 | 0 |
| 55 | MG | 2A | 3457 | 1/1 | 0.87 | 0.21 | 62,62,62,62 | 0 |
| 55 | MG | 2A | 3039 | 1/1 | 0.87 | 0.13 | 49,49,49,49 | 0 |
| 55 | MG | 2A | 3766 | 1/1 | 0.87 | 0.19 | 47,47,47,47 | 0 |
| 55 | MG | 2A | 3768 | 1/1 | 0.87 | 0.15 | 58,58,58,58 | 0 |
| 55 | MG | 1A | 3060 | 1/1 | 0.87 | 0.29 | 46,46,46,46 | 0 |
| 55 | MG | 1A | 3329 | 1/1 | 0.87 | 0.24 | 58,58,58,58 | 0 |
| 55 | MG | 2A | 3063 | 1/1 | 0.87 | 0.25 | 50,50,50,50 | 0 |
| 55 | MG | 1A | 3256 | 1/1 | 0.87 | 0.16 | 37,37,37,37 | 0 |
| 55 | MG | 2A | 3069 | 1/1 | 0.87 | 0.10 | 41,41,41,41 | 0 |
| 55 | MG | 2a | 3143 | 1/1 | 0.87 | 0.27 | 56,56,56,56 | 0 |
| 55 | MG | 2A | 3250 | 1/1 | 0.87 | 0.10 | 56,56,56,56 | 0 |
| 55 | MG | 1A | 3081 | 1/1 | 0.87 | 0.11 | 57,57,57,57 | 0 |
| 55 | MG | 2A | 3071 | 1/1 | 0.87 | 0.17 | 55,55,55,55 | 0 |
| 55 | MG | 1a | 1650 | 1/1 | 0.87 | 0.24 | 69,69,69,69 | 0 |
| 55 | MG | 2a | 3152 | 1/1 | 0.87 | 0.23 | 45,45,45,45 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 55 | MG | 1A | 3655 | 1/1 | 0.87 | 0.09 | 30,30,30,30 | 0 |
| 55 | MG | 2A | 3841 | 1/1 | 0.87 | 0.10 | 57,57,57,57 | 0 |
| 55 | MG | 1A | 3904 | 1/1 | 0.87 | 0.14 | 20,20,20,20 | 0 |
| 55 | MG | 1B | 231 | 1/1 | 0.87 | 0.13 | 30,30,30,30 | 0 |
| 55 | MG | 2A | 3505 | 1/1 | 0.87 | 0.18 | 48,48,48,48 | 0 |
| 55 | MG | 2A | 3085 | 1/1 | 0.87 | 0.11 | 60,60,60,60 | 0 |
| 55 | MG | 2A | 3520 | 1/1 | 0.87 | 0.12 | 44,44,44,44 | 0 |
| 55 | MG | 2A | 3856 | 1/1 | 0.87 | 0.30 | 63,63,63,63 | 0 |
| 55 | MG | 1a | 1770 | 1/1 | 0.87 | 0.13 | 65,65,65,65 | 0 |
| 55 | MG | 1A | 3502 | 1/1 | 0.87 | 0.10 | 45,45,45,45 | 0 |
| 55 | MG | 2a | 3177 | 1/1 | 0.87 | 0.10 | 64,64,64,64 | 0 |
| 55 | MG | 1a | 1667 | 1/1 | 0.87 | 0.17 | 61,61,61,61 | 0 |
| 55 | MG | 2a | 3185 | 1/1 | 0.87 | 0.12 | 58,58,58,58 | 0 |
| 55 | MG | 1A | 3350 | 1/1 | 0.87 | 0.20 | 62,62,62,62 | 0 |
| 55 | MG | 2A | 3550 | 1/1 | 0.87 | 0.20 | 37,37,37,37 | 0 |
| 55 | MG | 2a | 3193 | 1/1 | 0.87 | 0.19 | 47,47,47,47 | 0 |
| 55 | MG | 1a | 1786 | 1/1 | 0.87 | 0.18 | 74,74,74,74 | 0 |
| 55 | MG | 2A | 3106 | 1/1 | 0.87 | 0.10 | 62,62,62,62 | 0 |
| 55 | MG | 1A | 3376 | 1/1 | 0.87 | 0.10 | 39,39,39,39 | 0 |
| 55 | MG | 2A | 3568 | 1/1 | 0.87 | 0.15 | 38,38,38,38 | 0 |
| 55 | MG | 1A | 3737 | 1/1 | 0.87 | 0.11 | 23,23,23,23 | 0 |
| 55 | MG | 2A | 3571 | 1/1 | 0.87 | 0.17 | 69,69,69,69 | 0 |
| 55 | MG | 1A | 3282 | 1/1 | 0.87 | 0.24 | 58,58,58,58 | 0 |
| 55 | MG | 2A | 3586 | 1/1 | 0.87 | 0.13 | 66,66,66,66 | 0 |
| 55 | MG | 2F | 302 | 1/1 | 0.87 | 0.11 | 43,43,43,43 | 0 |
| 55 | MG | 1a | 1795 | 1/1 | 0.87 | 0.13 | 79,79,79,79 | 0 |
| 55 | MG | 1A | 3088 | 1/1 | 0.87 | 0.23 | 35,35,35,35 | 0 |
| 55 | MG | 1A | 3776 | 1/1 | 0.87 | 0.10 | 60,60,60,60 | 0 |
| 55 | MG | 2A | 3599 | 1/1 | 0.87 | 0.19 | 60,60,60,60 | 0 |
| 55 | MG | 2W | 201 | 1/1 | 0.87 | 0.09 | 36,36,36,36 | 0 |
| 55 | MG | 2W | 202 | 1/1 | 0.87 | 0.21 | 52,52,52,52 | 0 |
| 57 | V7A | 1a | 1835 | 35/35 | 0.87 | 0.16 | 65,73,81,85 | 0 |
| 57 | V7A | 2a | 3210 | 35/35 | 0.87 | 0.17 | 68,82,90,91 | 0 |
| 55 | MG | 1A | 4084 | 1/1 | 0.88 | 0.13 | 43,43,43,43 | 0 |
| 55 | MG | 1A | 4088 | 1/1 | 0.88 | 0.12 | 28,28,28,28 | 0 |
| 55 | MG | 2A | 3333 | 1/1 | 0.88 | 0.20 | 58,58,58,58 | 0 |
| 55 | MG | 2A | 3627 | 1/1 | 0.88 | 0.19 | 39,39,39,39 | 0 |
| 55 | MG | 1A | 3170 | 1/1 | 0.88 | 0.16 | 47,47,47,47 | 0 |
| 55 | MG | 1A | 3505 | 1/1 | 0.88 | 0.22 | 65,65,65,65 | 0 |
| 55 | MG | 1a | 1657 | 1/1 | 0.88 | 0.26 | 56,56,56,56 | 0 |
| 55 | MG | 2a | 3018 | 1/1 | 0.88 | 0.10 | 60,60,60,60 | 0 |
| 55 | MG | 2A | 3152 | 1/1 | 0.88 | 0.18 | 59,59,59,59 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 55 | MG | 2a | 3023 | 1/1 | 0.88 | 0.27 | 60,60,60,60 | 0 |
| 55 | MG | 1A | 3877 | 1/1 | 0.88 | 0.18 | 40,40,40,40 | 0 |
| 55 | MG | 2A | 3353 | 1/1 | 0.88 | 0.12 | 61,61,61,61 | 0 |
| 55 | MG | 1A | 3262 | 1/1 | 0.88 | 0.09 | 54,54,54,54 | 0 |
| 55 | MG | 1a | 1666 | 1/1 | 0.88 | 0.23 | 69,69,69,69 | 0 |
| 55 | MG | 2A | 3162 | 1/1 | 0.88 | 0.29 | 66,66,66,66 | 0 |
| 55 | MG | 2A | 3671 | 1/1 | 0.88 | 0.32 | 60,60,60,60 | 0 |
| 55 | MG | 1a | 1825 | 1/1 | 0.88 | 0.19 | 58,58,58,58 | 0 |
| 55 | MG | 1A | 3028 | 1/1 | 0.88 | 0.13 | 65,65,65,65 | 0 |
| 55 | MG | 1A | 3708 | 1/1 | 0.88 | 0.16 | 25,25,25,25 | 0 |
| 55 | MG | 1A | 3413 | 1/1 | 0.88 | 0.11 | 55,55,55,55 | 0 |
| 55 | MG | 2a | 3047 | 1/1 | 0.88 | 0.37 | 67,67,67,67 | 0 |
| 55 | MG | 2A | 3681 | 1/1 | 0.88 | 0.10 | 37,37,37,37 | 0 |
| 55 | MG | 2a | 3049 | 1/1 | 0.88 | 0.21 | 67,67,67,67 | 0 |
| 55 | MG | 2A | 3174 | 1/1 | 0.88 | 0.34 | 58,58,58,58 | 0 |
| 55 | MG | 1B | 224 | 1/1 | 0.88 | 0.11 | 53,53,53,53 | 0 |
| 55 | MG | 2a | 3056 | 1/1 | 0.88 | 0.21 | 47,47,47,47 | 0 |
| 55 | MG | 2a | 3058 | 1/1 | 0.88 | 0.14 | 52,52,52,52 | 0 |
| 55 | MG | 1A | 3735 | 1/1 | 0.88 | 0.12 | 58,58,58,58 | 0 |
| 55 | MG | 1A | 3268 | 1/1 | 0.88 | 0.11 | 46,46,46,46 | 0 |
| 55 | MG | 1A | 3915 | 1/1 | 0.88 | 0.11 | 25,25,25,25 | 0 |
| 55 | MG | 2a | 3076 | 1/1 | 0.88 | 0.20 | 50,50,50,50 | 0 |
| 55 | MG | 1A | 3434 | 1/1 | 0.88 | 0.21 | 51,51,51,51 | 0 |
| 55 | MG | 1A | 3436 | 1/1 | 0.88 | 0.17 | 45,45,45,45 | 0 |
| 55 | MG | 1A | 3445 | 1/1 | 0.88 | 0.24 | 51,51,51,51 | 0 |
| 55 | MG | 2A | 3403 | 1/1 | 0.88 | 0.17 | 55,55,55,55 | 0 |
| 55 | MG | 1a | 1684 | 1/1 | 0.88 | 0.22 | 49,49,49,49 | 0 |
| 55 | MG | 2A | 3422 | 1/1 | 0.88 | 0.13 | 51,51,51,51 | 0 |
| 55 | MG | 1G | 203 | 1/1 | 0.88 | 0.14 | 50,50,50,50 | 0 |
| 55 | MG | 2a | 3093 | 1/1 | 0.88 | 0.14 | 51,51,51,51 | 0 |
| 55 | MG | 2A | 3432 | 1/1 | 0.88 | 0.22 | 50,50,50,50 | 0 |
| 55 | MG | 2A | 3729 | 1/1 | 0.88 | 0.27 | 51,51,51,51 | 0 |
| 55 | MG | 2a | 3102 | 1/1 | 0.88 | 0.20 | 67,67,67,67 | 0 |
| 55 | MG | 2a | 3103 | 1/1 | 0.88 | 0.22 | 54,54,54,54 | 0 |
| 55 | MG | 1O | 202 | 1/1 | 0.88 | 0.13 | 56,56,56,56 | 0 |
| 55 | MG | 2A | 3205 | 1/1 | 0.88 | 0.19 | 51,51,51,51 | 0 |
| 55 | MG | 2A | 3738 | 1/1 | 0.88 | 0.10 | 50,50,50,50 | 0 |
| 55 | MG | 2A | 3447 | 1/1 | 0.88 | 0.29 | 71,71,71,71 | 0 |
| 55 | MG | 2A | 3448 | 1/1 | 0.88 | 0.14 | 49,49,49,49 | 0 |
| 55 | MG | 2A | 3219 | 1/1 | 0.88 | 0.07 | 50,50,50,50 | 0 |
| 55 | MG | 1A | 3096 | 1/1 | 0.88 | 0.18 | 60,60,60,60 | 0 |
| 55 | MG | 1A | 3567 | 1/1 | 0.88 | 0.15 | 31,31,31,31 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 55 | MG | 2A | 3771 | 1/1 | 0.88 | 0.14 | 56,56,56,56 | 0 |
| 55 | MG | 2A | 3003 | 1/1 | 0.88 | 0.20 | 50,50,50,50 | 0 |
| 55 | MG | 1A | 3946 | 1/1 | 0.88 | 0.10 | 50,50,50,50 | 0 |
| 55 | MG | 2A | 3231 | 1/1 | 0.88 | 0.17 | 65,65,65,65 | 0 |
| 55 | MG | 2a | 3134 | 1/1 | 0.88 | 0.27 | 47,47,47,47 | 0 |
| 55 | MG | 2A | 3467 | 1/1 | 0.88 | 0.35 | 64,64,64,64 | 0 |
| 55 | MG | 1A | 3569 | 1/1 | 0.88 | 0.29 | 40,40,40,40 | 0 |
| 55 | MG | 2a | 3140 | 1/1 | 0.88 | 0.41 | 59,59,59,59 | 0 |
| 55 | MG | 2a | 3141 | 1/1 | 0.88 | 0.22 | 66,66,66,66 | 0 |
| 55 | MG | 2A | 3793 | 1/1 | 0.88 | 0.13 | 49,49,49,49 | 0 |
| 55 | MG | 1V | 203 | 1/1 | 0.88 | 0.14 | 47,47,47,47 | 0 |
| 55 | MG | 2A | 3813 | 1/1 | 0.88 | 0.13 | 52,52,52,52 | 0 |
| 55 | MG | 2A | 3044 | 1/1 | 0.88 | 0.26 | 66,66,66,66 | 0 |
| 55 | MG | 1A | 3039 | 1/1 | 0.88 | 0.12 | 57,57,57,57 | 0 |
| 55 | MG | 1A | 3984 | 1/1 | 0.88 | 0.19 | 53,53,53,53 | 0 |
| 55 | MG | 2a | 3157 | 1/1 | 0.88 | 0.12 | 61,61,61,61 | 0 |
| 55 | MG | 11 | 104 | 1/1 | 0.88 | 0.16 | 62,62,62,62 | 0 |
| 55 | MG | 1A | 3288 | 1/1 | 0.88 | 0.13 | 40,40,40,40 | 0 |
| 55 | MG | 1A | 3989 | 1/1 | 0.88 | 0.15 | 36,36,36,36 | 0 |
| 55 | MG | 1A | 3589 | 1/1 | 0.88 | 0.15 | 28,28,28,28 | 0 |
| 55 | MG | 1a | 1730 | 1/1 | 0.88 | 0.37 | 60,60,60,60 | 0 |
| 55 | MG | 1a | 1731 | 1/1 | 0.88 | 0.25 | 63,63,63,63 | 0 |
| 55 | MG | 1A | 3847 | 1/1 | 0.88 | 0.10 | 35,35,35,35 | 0 |
| 55 | MG | 2A | 3855 | 1/1 | 0.88 | 0.15 | 52,52,52,52 | 0 |
| 55 | MG | 1a | 1744 | 1/1 | 0.88 | 0.15 | 50,50,50,50 | 0 |
| 55 | MG | 2A | 3860 | 1/1 | 0.88 | 0.10 | 43,43,43,43 | 0 |
| 55 | MG | 1a | 1745 | 1/1 | 0.88 | 0.21 | 62,62,62,62 | 0 |
| 55 | MG | 2A | 3086 | 1/1 | 0.88 | 0.25 | 66,66,66,66 | 0 |
| 55 | MG | 1A | 3850 | 1/1 | 0.88 | 0.09 | 56,56,56,56 | 0 |
| 55 | MG | 1a | 1749 | 1/1 | 0.88 | 0.14 | 56,56,56,56 | 0 |
| 55 | MG | 1A | 3361 | 1/1 | 0.88 | 0.12 | 56,56,56,56 | 0 |
| 55 | MG | 2A | 3552 | 1/1 | 0.88 | 0.17 | 38,38,38,38 | 0 |
| 55 | MG | 2A | 3293 | 1/1 | 0.88 | 0.19 | 68,68,68,68 | 0 |
| 55 | MG | 2A | 3558 | 1/1 | 0.88 | 0.12 | 36,36,36,36 | 0 |
| 55 | MG | 2a | 3202 | 1/1 | 0.88 | 0.37 | 76,76,76,76 | 0 |
| 55 | MG | 1A | 3489 | 1/1 | 0.88 | 0.31 | 40,40,40,40 | 0 |
| 55 | MG | 1A | 3369 | 1/1 | 0.88 | 0.12 | 49,49,49,49 | 0 |
| 55 | MG | 2a | 3207 | 1/1 | 0.88 | 0.21 | 53,53,53,53 | 0 |
| 55 | MG | 1A | 3255 | 1/1 | 0.88 | 0.14 | 53,53,53,53 | 0 |
| 55 | MG | 2A | 3107 | 1/1 | 0.88 | 0.11 | 74,74,74,74 | 0 |
| 55 | MG | 2A | 3108 | 1/1 | 0.88 | 0.09 | 61,61,61,61 | 0 |
| 55 | MG | 1A | 4041 | 1/1 | 0.88 | 0.09 | 74,74,74,74 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 55 | MG | 1A | 4045 | 1/1 | 0.88 | 0.09 | 49,49,49,49 | 0 |
| 55 | MG | 1A | 4050 | 1/1 | 0.88 | 0.31 | 70,70,70,70 | 0 |
| 55 | MG | 2N | 201 | 1/1 | 0.88 | 0.29 | 62,62,62,62 | 0 |
| 55 | MG | 2q | 201 | 1/1 | 0.88 | 0.21 | 67,67,67,67 | 0 |
| 55 | MG | 1A | 4061 | 1/1 | 0.88 | 0.16 | 62,62,62,62 | 0 |
| 55 | MG | 2A | 3131 | 1/1 | 0.88 | 0.07 | 64,64,64,64 | 0 |
| 55 | MG | 1A | 4076 | 1/1 | 0.88 | 0.10 | 61,61,61,61 | 0 |
| 55 | MG | 2A | 3606 | 1/1 | 0.88 | 0.23 | 39,39,39,39 | 0 |
| 55 | MG | 2A | 3607 | 1/1 | 0.88 | 0.22 | 49,49,49,49 | 0 |
| 55 | MG | 1A | 4081 | 1/1 | 0.88 | 0.15 | 43,43,43,43 | 0 |
| 55 | MG | 2A | 3617 | 1/1 | 0.89 | 0.10 | 23,23,23,23 | 0 |
| 55 | MG | 1x | 105 | 1/1 | 0.89 | 0.24 | 65,65,65,65 | 0 |
| 55 | MG | 2A | 3347 | 1/1 | 0.89 | 0.10 | 46,46,46,46 | 0 |
| 55 | MG | 1A | 3897 | 1/1 | 0.89 | 0.25 | 28,28,28,28 | 0 |
| 55 | MG | 1A | 4062 | 1/1 | 0.89 | 0.08 | 37,37,37,37 | 0 |
| 55 | MG | 1x | 111 | 1/1 | 0.89 | 0.17 | 65,65,65,65 | 0 |
| 55 | MG | 2A | 3172 | 1/1 | 0.89 | 0.23 | 41,41,41,41 | 0 |
| 55 | MG | 2a | 3019 | 1/1 | 0.89 | 0.25 | 60,60,60,60 | 0 |
| 55 | MG | 1A | 3419 | 1/1 | 0.89 | 0.10 | 46,46,46,46 | 0 |
| 55 | MG | 2A | 3648 | 1/1 | 0.89 | 0.16 | 55,55,55,55 | 0 |
| 55 | MG | 1A | 3785 | 1/1 | 0.89 | 0.15 | 46,46,46,46 | 0 |
| 55 | MG | 2A | 3005 | 1/1 | 0.89 | 0.11 | 38,38,38,38 | 0 |
| 55 | MG | 2A | 3659 | 1/1 | 0.89 | 0.36 | 44,44,44,44 | 0 |
| 55 | MG | 2A | 3020 | 1/1 | 0.89 | 0.15 | 54,54,54,54 | 0 |
| 55 | MG | 2A | 3021 | 1/1 | 0.89 | 0.13 | 40,40,40,40 | 0 |
| 55 | MG | 2A | 3025 | 1/1 | 0.89 | 0.15 | 56,56,56,56 | 0 |
| 55 | MG | 2a | 3035 | 1/1 | 0.89 | 0.13 | 63,63,63,63 | 0 |
| 55 | MG | 2A | 3372 | 1/1 | 0.89 | 0.25 | 59,59,59,59 | 0 |
| 55 | MG | 1A | 3601 | 1/1 | 0.89 | 0.13 | 56,56,56,56 | 0 |
| 55 | MG | 1A | 3481 | 1/1 | 0.89 | 0.14 | 56,56,56,56 | 0 |
| 55 | MG | 2a | 3043 | 1/1 | 0.89 | 0.13 | 60,60,60,60 | 0 |
| 55 | MG | 2A | 3199 | 1/1 | 0.89 | 0.09 | 52,52,52,52 | 0 |
| 55 | MG | 2a | 3046 | 1/1 | 0.89 | 0.08 | 56,56,56,56 | 0 |
| 55 | MG | 1a | 1624 | 1/1 | 0.89 | 0.10 | 59,59,59,59 | 0 |
| 55 | MG | 1A | 3808 | 1/1 | 0.89 | 0.15 | 40,40,40,40 | 0 |
| 55 | MG | 1A | 3919 | 1/1 | 0.89 | 0.09 | 33,33,33,33 | 0 |
| 55 | MG | 1A | 4105 | 1/1 | 0.89 | 0.11 | 53,53,53,53 | 0 |
| 55 | MG | 2A | 3215 | 1/1 | 0.89 | 0.16 | 69,69,69,69 | 0 |
| 55 | MG | 2A | 3218 | 1/1 | 0.89 | 0.24 | 49,49,49,49 | 0 |
| 55 | MG | 2A | 3405 | 1/1 | 0.89 | 0.24 | 57,57,57,57 | 0 |
| 55 | MG | 2A | 3406 | 1/1 | 0.89 | 0.24 | 45,45,45,45 | 0 |
| 55 | MG | 2A | 3066 | 1/1 | 0.89 | 0.15 | 43,43,43,43 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 55 | MG | 2A | 3418 | 1/1 | 0.89 | 0.16 | 56,56,56,56 | 0 |
| 55 | MG | 1A | 3922 | 1/1 | 0.89 | 0.11 | 38,38,38,38 | 0 |
| 55 | MG | 2a | 3079 | 1/1 | 0.89 | 0.40 | 61,61,61,61 | 0 |
| 55 | MG | 1A | 3609 | 1/1 | 0.89 | 0.15 | 27,27,27,27 | 0 |
| 55 | MG | 2A | 3425 | 1/1 | 0.89 | 0.19 | 43,43,43,43 | 0 |
| 55 | MG | 2A | 3427 | 1/1 | 0.89 | 0.36 | 54,54,54,54 | 0 |
| 55 | MG | 2A | 3721 | 1/1 | 0.89 | 0.16 | 48,48,48,48 | 0 |
| 55 | MG | 1A | 3818 | 1/1 | 0.89 | 0.14 | 40,40,40,40 | 0 |
| 55 | MG | 1A | 3486 | 1/1 | 0.89 | 0.15 | 56,56,56,56 | 0 |
| 55 | MG | 2A | 3076 | 1/1 | 0.89 | 0.11 | 75,75,75,75 | 0 |
| 55 | MG | 2A | 3732 | 1/1 | 0.89 | 0.14 | 44,44,44,44 | 0 |
| 55 | MG | 2A | 3734 | 1/1 | 0.89 | 0.17 | 42,42,42,42 | 0 |
| 55 | MG | 1B | 209 | 1/1 | 0.89 | 0.25 | 53,53,53,53 | 0 |
| 55 | MG | 1B | 214 | 1/1 | 0.89 | 0.22 | 51,51,51,51 | 0 |
| 55 | MG | 2A | 3081 | 1/1 | 0.89 | 0.22 | 69,69,69,69 | 0 |
| 55 | MG | 1A | 3932 | 1/1 | 0.89 | 0.35 | 38,38,38,38 | 0 |
| 55 | MG | 2a | 3107 | 1/1 | 0.89 | 0.24 | 65,65,65,65 | 0 |
| 55 | MG | 2A | 3743 | 1/1 | 0.89 | 0.17 | 69,69,69,69 | 0 |
| 55 | MG | 2A | 3754 | 1/1 | 0.89 | 0.27 | 48,48,48,48 | 0 |
| 55 | MG | 2A | 3758 | 1/1 | 0.89 | 0.12 | 53,53,53,53 | 0 |
| 55 | MG | 2A | 3459 | 1/1 | 0.89 | 0.43 | 52,52,52,52 | 0 |
| 55 | MG | 1A | 3524 | 1/1 | 0.89 | 0.26 | 59,59,59,59 | 0 |
| 55 | MG | 1A | 3644 | 1/1 | 0.89 | 0.14 | 21,21,21,21 | 0 |
| 55 | MG | 1A | 3842 | 1/1 | 0.89 | 0.43 | 35,35,35,35 | 0 |
| 55 | MG | 2A | 3254 | 1/1 | 0.89 | 0.16 | 49,49,49,49 | 0 |
| 55 | MG | 2A | 3255 | 1/1 | 0.89 | 0.17 | 61,61,61,61 | 0 |
| 55 | MG | 1A | 3371 | 1/1 | 0.89 | 0.14 | 40,40,40,40 | 0 |
| 55 | MG | 1A | 3185 | 1/1 | 0.89 | 0.22 | 50,50,50,50 | 0 |
| 55 | MG | 1A | 3492 | 1/1 | 0.89 | 0.10 | 47,47,47,47 | 0 |
| 55 | MG | 2A | 3265 | 1/1 | 0.89 | 0.19 | 56,56,56,56 | 0 |
| 55 | MG | 1A | 3852 | 1/1 | 0.89 | 0.08 | 39,39,39,39 | 0 |
| 55 | MG | 2A | 3807 | 1/1 | 0.89 | 0.12 | 36,36,36,36 | 0 |
| 55 | MG | 2A | 3268 | 1/1 | 0.89 | 0.12 | 68,68,68,68 | 0 |
| 55 | MG | 2a | 3142 | 1/1 | 0.89 | 0.19 | 54,54,54,54 | 0 |
| 55 | MG | 2A | 3816 | 1/1 | 0.89 | 0.26 | 54,54,54,54 | 0 |
| 55 | MG | 2A | 3269 | 1/1 | 0.89 | 0.11 | 55,55,55,55 | 0 |
| 55 | MG | 2A | 3494 | 1/1 | 0.89 | 0.15 | 64,64,64,64 | 0 |
| 55 | MG | 2A | 3496 | 1/1 | 0.89 | 0.10 | 53,53,53,53 | 0 |
| 55 | MG | 2a | 3149 | 1/1 | 0.89 | 0.10 | 59,59,59,59 | 0 |
| 55 | MG | 1F | 310 | 1/1 | 0.89 | 0.21 | 46,46,46,46 | 0 |
| 55 | MG | 1A | 3493 | 1/1 | 0.89 | 0.15 | 45,45,45,45 | 0 |
| 55 | MG | 2A | 3275 | 1/1 | 0.89 | 0.10 | 64,64,64,64 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 55 | MG | 2A | 3513 | 1/1 | 0.89 | 0.12 | 43,43,43,43 | 0 |
| 55 | MG | 2A | 3276 | 1/1 | 0.89 | 0.26 | 60,60,60,60 | 0 |
| 55 | MG | 1a | 1804 | 1/1 | 0.89 | 0.14 | 49,49,49,49 | 0 |
| 55 | MG | 1a | 1806 | 1/1 | 0.89 | 0.14 | 43,43,43,43 | 0 |
| 55 | MG | 1A | 3027 | 1/1 | 0.89 | 0.26 | 55,55,55,55 | 0 |
| 55 | MG | 1A | 3496 | 1/1 | 0.89 | 0.16 | 59,59,59,59 | 0 |
| 55 | MG | 2A | 3858 | 1/1 | 0.89 | 0.13 | 68,68,68,68 | 0 |
| 55 | MG | 2A | 3859 | 1/1 | 0.89 | 0.20 | 53,53,53,53 | 0 |
| 55 | MG | 1A | 3862 | 1/1 | 0.89 | 0.11 | 52,52,52,52 | 0 |
| 55 | MG | 2A | 3548 | 1/1 | 0.89 | 0.12 | 39,39,39,39 | 0 |
| 55 | MG | 2A | 3291 | 1/1 | 0.89 | 0.21 | 47,47,47,47 | 0 |
| 55 | MG | 2a | 3179 | 1/1 | 0.89 | 0.19 | 54,54,54,54 | 0 |
| 55 | MG | 1A | 4012 | 1/1 | 0.89 | 0.18 | 47,47,47,47 | 0 |
| 55 | MG | 2a | 3183 | 1/1 | 0.89 | 0.15 | 53,53,53,53 | 0 |
| 55 | MG | 1A | 3497 | 1/1 | 0.89 | 0.11 | 31,31,31,31 | 0 |
| 55 | MG | 1A | 4019 | 1/1 | 0.89 | 0.11 | 28,28,28,28 | 0 |
| 55 | MG | 1a | 1692 | 1/1 | 0.89 | 0.16 | 55,55,55,55 | 0 |
| 55 | MG | 1a | 1698 | 1/1 | 0.89 | 0.20 | 51,51,51,51 | 0 |
| 55 | MG | 1A | 3002 | 1/1 | 0.89 | 0.11 | 49,49,49,49 | 0 |
| 55 | MG | 2A | 3145 | 1/1 | 0.89 | 0.31 | 51,51,51,51 | 0 |
| 55 | MG | 2A | 3146 | 1/1 | 0.89 | 0.18 | 42,42,42,42 | 0 |
| 55 | MG | 1Y | 201 | 1/1 | 0.89 | 0.08 | 48,48,48,48 | 0 |
| 55 | MG | 2A | 3148 | 1/1 | 0.89 | 0.07 | 48,48,48,48 | 0 |
| 55 | MG | 2E | 301 | 1/1 | 0.89 | 0.20 | 55,55,55,55 | 0 |
| 55 | MG | 2A | 3321 | 1/1 | 0.89 | 0.06 | 70,70,70,70 | 0 |
| 55 | MG | 2F | 301 | 1/1 | 0.89 | 0.12 | 49,49,49,49 | 0 |
| 55 | MG | 2A | 3149 | 1/1 | 0.89 | 0.12 | 61,61,61,61 | 0 |
| 55 | MG | 2e | 201 | 1/1 | 0.89 | 0.07 | 80,80,80,80 | 0 |
| 55 | MG | 1l | 202 | 1/1 | 0.89 | 0.18 | 61,61,61,61 | 0 |
| 55 | MG | 1A | 3180 | 1/1 | 0.89 | 0.15 | 49,49,49,49 | 0 |
| 55 | MG | 1A | 3290 | 1/1 | 0.89 | 0.25 | 48,48,48,48 | 0 |
| 55 | MG | 1A | 3883 | 1/1 | 0.89 | 0.21 | 30,30,30,30 | 0 |
| 55 | MG | 2T | 202 | 1/1 | 0.89 | 0.18 | 59,59,59,59 | 0 |
| 55 | MG | 1A | 3892 | 1/1 | 0.89 | 0.14 | 36,36,36,36 | 0 |
| 55 | MG | 2A | 3609 | 1/1 | 0.89 | 0.22 | 33,33,33,33 | 0 |
| 55 | MG | 2A | 3610 | 1/1 | 0.89 | 0.17 | 59,59,59,59 | 0 |
| 55 | MG | 1A | 3764 | 1/1 | 0.89 | 0.09 | 45,45,45,45 | 0 |
| 55 | MG | 2x | 105 | 1/1 | 0.89 | 0.24 | 67,67,67,67 | 0 |
| 55 | MG | 2A | 3613 | 1/1 | 0.89 | 0.11 | 40,40,40,40 | 0 |
| 55 | MG | 1A | 4058 | 1/1 | 0.89 | 0.13 | 38,38,38,38 | 0 |
| 55 | MG | 1A | 3466 | 1/1 | 0.90 | 0.09 | 50,50,50,50 | 0 |
| 55 | MG | 1a | 1820 | 1/1 | 0.90 | 0.20 | 66,66,66,66 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 55 | MG | 2A | 3611 | 1/1 | 0.90 | 0.10 | 47,47,47,47 | 0 |
| 55 | MG | 2A | 3334 | 1/1 | 0.90 | 0.19 | 64,64,64,64 | 0 |
| 55 | MG | 2A | 3338 | 1/1 | 0.90 | 0.07 | 52,52,52,52 | 0 |
| 55 | MG | 28 | 102 | 1/1 | 0.90 | 0.41 | 59,59,59,59 | 0 |
| 55 | MG | 2A | 3614 | 1/1 | 0.90 | 0.23 | 44,44,44,44 | 0 |
| 55 | MG | 1a | 1824 | 1/1 | 0.90 | 0.15 | 64,64,64,64 | 0 |
| 55 | MG | 1A | 3476 | 1/1 | 0.90 | 0.10 | 45,45,45,45 | 0 |
| 55 | MG | 2a | 3006 | 1/1 | 0.90 | 0.21 | 57,57,57,57 | 0 |
| 55 | MG | 2A | 3344 | 1/1 | 0.90 | 0.24 | 45,45,45,45 | 0 |
| 55 | MG | 2a | 3013 | 1/1 | 0.90 | 0.17 | 56,56,56,56 | 0 |
| 55 | MG | 2a | 3015 | 1/1 | 0.90 | 0.19 | 55,55,55,55 | 0 |
| 55 | MG | 1a | 1826 | 1/1 | 0.90 | 0.23 | 45,45,45,45 | 0 |
| 55 | MG | 2A | 3156 | 1/1 | 0.90 | 0.12 | 58,58,58,58 | 0 |
| 55 | MG | 2A | 3628 | 1/1 | 0.90 | 0.16 | 33,33,33,33 | 0 |
| 55 | MG | 1a | 1827 | 1/1 | 0.90 | 0.20 | 48,48,48,48 | 0 |
| 55 | MG | 1a | 1828 | 1/1 | 0.90 | 0.09 | 50,50,50,50 | 0 |
| 55 | MG | 1A | 3740 | 1/1 | 0.90 | 0.10 | 34,34,34,34 | 0 |
| 55 | MG | 2a | 3025 | 1/1 | 0.90 | 0.21 | 55,55,55,55 | 0 |
| 55 | MG | 2a | 3027 | 1/1 | 0.90 | 0.29 | 50,50,50,50 | 0 |
| 55 | MG | 1A | 3326 | 1/1 | 0.90 | 0.16 | 40,40,40,40 | 0 |
| 55 | MG | 1A | 3516 | 1/1 | 0.90 | 0.17 | 69,69,69,69 | 0 |
| 55 | MG | 2A | 3650 | 1/1 | 0.90 | 0.10 | 56,56,56,56 | 0 |
| 55 | MG | 2A | 3360 | 1/1 | 0.90 | 0.20 | 56,56,56,56 | 0 |
| 55 | MG | 1a | 1833 | 1/1 | 0.90 | 0.16 | 61,61,61,61 | 0 |
| 55 | MG | 1E | 306 | 1/1 | 0.90 | 0.14 | 22,22,22,22 | 0 |
| 55 | MG | 1a | 1675 | 1/1 | 0.90 | 0.25 | 57,57,57,57 | 0 |
| 55 | MG | 1A | 4011 | 1/1 | 0.90 | 0.12 | 57,57,57,57 | 0 |
| 55 | MG | 2A | 3173 | 1/1 | 0.90 | 0.13 | 44,44,44,44 | 0 |
| 55 | MG | 2A | 3670 | 1/1 | 0.90 | 0.20 | 49,49,49,49 | 0 |
| 55 | MG | 1A | 3748 | 1/1 | 0.90 | 0.18 | 45,45,45,45 | 0 |
| 55 | MG | 1G | 204 | 1/1 | 0.90 | 0.11 | 50,50,50,50 | 0 |
| 55 | MG | 1O | 201 | 1/1 | 0.90 | 0.31 | 45,45,45,45 | 0 |
| 55 | MG | 1A | 4015 | 1/1 | 0.90 | 0.13 | 39,39,39,39 | 0 |
| 55 | MG | 1a | 1683 | 1/1 | 0.90 | 0.22 | 46,46,46,46 | 0 |
| 55 | MG | 1A | 3762 | 1/1 | 0.90 | 0.10 | 54,54,54,54 | 0 |
| 55 | MG | 2A | 3682 | 1/1 | 0.90 | 0.14 | 59,59,59,59 | 0 |
| 55 | MG | 2A | 3683 | 1/1 | 0.90 | 0.08 | 79,79,79,79 | 0 |
| 55 | MG | 1Q | 203 | 1/1 | 0.90 | 0.09 | 55,55,55,55 | 0 |
| 55 | MG | 2a | 3060 | 1/1 | 0.90 | 0.31 | 63,63,63,63 | 0 |
| 55 | MG | 1T | 202 | 1/1 | 0.90 | 0.07 | 44,44,44,44 | 0 |
| 55 | MG | 1A | 3878 | 1/1 | 0.90 | 0.16 | 57,57,57,57 | 0 |
| 55 | MG | 2a | 3064 | 1/1 | 0.90 | 0.16 | 46,46,46,46 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 55 | MG | 2a | 3066 | 1/1 | 0.90 | 0.14 | 61,61,61,61 | 0 |
| 55 | MG | 2A | 3392 | 1/1 | 0.90 | 0.21 | 31,31,31,31 | 0 |
| 55 | MG | 2a | 3075 | 1/1 | 0.90 | 0.12 | 59,59,59,59 | 0 |
| 55 | MG | 2A | 3402 | 1/1 | 0.90 | 0.24 | 47,47,47,47 | 0 |
| 55 | MG | 1a | 1701 | 1/1 | 0.90 | 0.17 | 54,54,54,54 | 0 |
| 55 | MG | 1A | 3602 | 1/1 | 0.90 | 0.14 | 39,39,39,39 | 0 |
| 55 | MG | 1A | 3775 | 1/1 | 0.90 | 0.09 | 19,19,19,19 | 0 |
| 55 | MG | 2A | 3412 | 1/1 | 0.90 | 0.22 | 55,55,55,55 | 0 |
| 55 | MG | 2A | 3002 | 1/1 | 0.90 | 0.17 | 53,53,53,53 | 0 |
| 55 | MG | 2a | 3089 | 1/1 | 0.90 | 0.14 | 59,59,59,59 | 0 |
| 55 | MG | 1A | 4029 | 1/1 | 0.90 | 0.07 | 42,42,42,42 | 0 |
| 55 | MG | 2A | 3719 | 1/1 | 0.90 | 0.16 | 70,70,70,70 | 0 |
| 55 | MG | 1A | 3890 | 1/1 | 0.90 | 0.11 | 52,52,52,52 | 0 |
| 55 | MG | 2A | 3013 | 1/1 | 0.90 | 0.13 | 51,51,51,51 | 0 |
| 55 | MG | 2a | 3096 | 1/1 | 0.90 | 0.07 | 44,44,44,44 | 0 |
| 55 | MG | 1a | 1710 | 1/1 | 0.90 | 0.06 | 53,53,53,53 | 0 |
| 55 | MG | 2a | 3099 | 1/1 | 0.90 | 0.19 | 66,66,66,66 | 0 |
| 55 | MG | 1A | 3519 | 1/1 | 0.90 | 0.09 | 48,48,48,48 | 0 |
| 55 | MG | 2A | 3228 | 1/1 | 0.90 | 0.09 | 58,58,58,58 | 0 |
| 55 | MG | 2A | 3023 | 1/1 | 0.90 | 0.10 | 49,49,49,49 | 0 |
| 55 | MG | 1A | 3182 | 1/1 | 0.90 | 0.07 | 38,38,38,38 | 0 |
| 55 | MG | 1a | 1716 | 1/1 | 0.90 | 0.28 | 56,56,56,56 | 0 |
| 55 | MG | 2A | 3737 | 1/1 | 0.90 | 0.19 | 50,50,50,50 | 0 |
| 55 | MG | 1A | 3095 | 1/1 | 0.90 | 0.20 | 51,51,51,51 | 0 |
| 55 | MG | 1A | 3796 | 1/1 | 0.90 | 0.10 | 34,34,34,34 | 0 |
| 55 | MG | 17 | 101 | 1/1 | 0.90 | 0.21 | 54,54,54,54 | 0 |
| 55 | MG | 2A | 3045 | 1/1 | 0.90 | 0.17 | 57,57,57,57 | 0 |
| 55 | MG | 1A | 3800 | 1/1 | 0.90 | 0.10 | 22,22,22,22 | 0 |
| 55 | MG | 1a | 1724 | 1/1 | 0.90 | 0.18 | 49,49,49,49 | 0 |
| 55 | MG | 2A | 3463 | 1/1 | 0.90 | 0.22 | 25,25,25,25 | 0 |
| 55 | MG | 1A | 3084 | 1/1 | 0.90 | 0.21 | 33,33,33,33 | 0 |
| 55 | MG | 2A | 3067 | 1/1 | 0.90 | 0.13 | 53,53,53,53 | 0 |
| 55 | MG | 1A | 3109 | 1/1 | 0.90 | 0.22 | 50,50,50,50 | 0 |
| 55 | MG | 2A | 3468 | 1/1 | 0.90 | 0.35 | 51,51,51,51 | 0 |
| 55 | MG | 2A | 3775 | 1/1 | 0.90 | 0.16 | 74,74,74,74 | 0 |
| 55 | MG | 2a | 3137 | 1/1 | 0.90 | 0.17 | 58,58,58,58 | 0 |
| 55 | MG | 1A | 4079 | 1/1 | 0.90 | 0.20 | 61,61,61,61 | 0 |
| 55 | MG | 1A | 3914 | 1/1 | 0.90 | 0.12 | 35,35,35,35 | 0 |
| 55 | MG | 1a | 1740 | 1/1 | 0.90 | 0.32 | 42,42,42,42 | 0 |
| 55 | MG | 2A | 3783 | 1/1 | 0.90 | 0.09 | 72,72,72,72 | 0 |
| 55 | MG | 2A | 3264 | 1/1 | 0.90 | 0.31 | 55,55,55,55 | 0 |
| 55 | MG | 1A | 3292 | 1/1 | 0.90 | 0.24 | 29,29,29,29 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 55 | MG | 2A | 3801 | 1/1 | 0.90 | 0.14 | 51,51,51,51 | 0 |
| 55 | MG | 2A | 3488 | 1/1 | 0.90 | 0.20 | 73,73,73,73 | 0 |
| 55 | MG | 1A | 3367 | 1/1 | 0.90 | 0.13 | 34,34,34,34 | 0 |
| 55 | MG | 1A | 4089 | 1/1 | 0.90 | 0.26 | 39,39,39,39 | 0 |
| 55 | MG | 1a | 1619 | 1/1 | 0.90 | 0.10 | 70,70,70,70 | 0 |
| 55 | MG | 2a | 3154 | 1/1 | 0.90 | 0.19 | 47,47,47,47 | 0 |
| 55 | MG | 1A | 3662 | 1/1 | 0.90 | 0.10 | 42,42,42,42 | 0 |
| 55 | MG | 2A | 3826 | 1/1 | 0.90 | 0.14 | 72,72,72,72 | 0 |
| 55 | MG | 1A | 4102 | 1/1 | 0.90 | 0.09 | 38,38,38,38 | 0 |
| 55 | MG | 1a | 1625 | 1/1 | 0.90 | 0.13 | 58,58,58,58 | 0 |
| 55 | MG | 2A | 3834 | 1/1 | 0.90 | 0.10 | 29,29,29,29 | 0 |
| 55 | MG | 1a | 1758 | 1/1 | 0.90 | 0.12 | 51,51,51,51 | 0 |
| 55 | MG | 1A | 3668 | 1/1 | 0.90 | 0.11 | 49,49,49,49 | 0 |
| 55 | MG | 2a | 3167 | 1/1 | 0.90 | 0.11 | 50,50,50,50 | 0 |
| 55 | MG | 2A | 3282 | 1/1 | 0.90 | 0.12 | 72,72,72,72 | 0 |
| 55 | MG | 2A | 3283 | 1/1 | 0.90 | 0.39 | 54,54,54,54 | 0 |
| 55 | MG | 1A | 3833 | 1/1 | 0.90 | 0.14 | 52,52,52,52 | 0 |
| 55 | MG | 1a | 1766 | 1/1 | 0.90 | 0.19 | 49,49,49,49 | 0 |
| 55 | MG | 1A | 3221 | 1/1 | 0.90 | 0.18 | 54,54,54,54 | 0 |
| 55 | MG | 2A | 3537 | 1/1 | 0.90 | 0.28 | 54,54,54,54 | 0 |
| 55 | MG | 1a | 1641 | 1/1 | 0.90 | 0.21 | 60,60,60,60 | 0 |
| 55 | MG | 2A | 3541 | 1/1 | 0.90 | 0.13 | 40,40,40,40 | 0 |
| 55 | MG | 2A | 3543 | 1/1 | 0.90 | 0.11 | 35,35,35,35 | 0 |
| 55 | MG | 2a | 3188 | 1/1 | 0.90 | 0.26 | 60,60,60,60 | 0 |
| 55 | MG | 2A | 3545 | 1/1 | 0.90 | 0.16 | 45,45,45,45 | 0 |
| 55 | MG | 2A | 3099 | 1/1 | 0.90 | 0.13 | 54,54,54,54 | 0 |
| 55 | MG | 2A | 3292 | 1/1 | 0.90 | 0.12 | 45,45,45,45 | 0 |
| 55 | MG | 1A | 3117 | 1/1 | 0.90 | 0.17 | 31,31,31,31 | 0 |
| 55 | MG | 1A | 3844 | 1/1 | 0.90 | 0.07 | 45,45,45,45 | 0 |
| 55 | MG | 2a | 3199 | 1/1 | 0.90 | 0.30 | 69,69,69,69 | 0 |
| 55 | MG | 1A | 3703 | 1/1 | 0.90 | 0.11 | 41,41,41,41 | 0 |
| 55 | MG | 1a | 1645 | 1/1 | 0.90 | 0.18 | 70,70,70,70 | 0 |
| 55 | MG | 1a | 1649 | 1/1 | 0.90 | 0.30 | 61,61,61,61 | 0 |
| 55 | MG | 2A | 3567 | 1/1 | 0.90 | 0.18 | 38,38,38,38 | 0 |
| 55 | MG | 1A | 3229 | 1/1 | 0.90 | 0.09 | 51,51,51,51 | 0 |
| 55 | MG | 2A | 3312 | 1/1 | 0.90 | 0.09 | 51,51,51,51 | 0 |
| 55 | MG | 1B | 210 | 1/1 | 0.90 | 0.18 | 50,50,50,50 | 0 |
| 55 | MG | 2A | 3581 | 1/1 | 0.90 | 0.13 | 55,55,55,55 | 0 |
| 55 | MG | 2g | 201 | 1/1 | 0.90 | 0.08 | 73,73,73,73 | 0 |
| 55 | MG | 1A | 3715 | 1/1 | 0.90 | 0.11 | 40,40,40,40 | 0 |
| 55 | MG | 1A | 3949 | 1/1 | 0.90 | 0.14 | 56,56,56,56 | 0 |
| 55 | MG | 1a | 1658 | 1/1 | 0.90 | 0.23 | 76,76,76,76 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 55 | MG | 1A | 3024 | 1/1 | 0.90 | 0.12 | 23,23,23,23 | 0 |
| 55 | MG | 1A | 3854 | 1/1 | 0.90 | 0.11 | 33,33,33,33 | 0 |
| 55 | MG | 1a | 1808 | 1/1 | 0.90 | 0.11 | 67,67,67,67 | 0 |
| 55 | MG | 2A | 3601 | 1/1 | 0.90 | 0.09 | 57,57,57,57 | 0 |
| 55 | MG | 2O | 201 | 1/1 | 0.90 | 0.22 | 56,56,56,56 | 0 |
| 55 | MG | 2x | 102 | 1/1 | 0.90 | 0.16 | 73,73,73,73 | 0 |
| 55 | MG | 2A | 3602 | 1/1 | 0.90 | 0.10 | 65,65,65,65 | 0 |
| 55 | MG | 1a | 1812 | 1/1 | 0.90 | 0.15 | 71,71,71,71 | 0 |
| 55 | MG | 1a | 1664 | 1/1 | 0.90 | 0.18 | 68,68,68,68 | 0 |
| 55 | MG | 2A | 3331 | 1/1 | 0.90 | 0.26 | 64,64,64,64 | 0 |
| 55 | MG | 1A | 3579 | 1/1 | 0.91 | 0.17 | 45,45,45,45 | 0 |
| 55 | MG | 1A | 3583 | 1/1 | 0.91 | 0.17 | 36,36,36,36 | 0 |
| 55 | MG | 2V | 201 | 1/1 | 0.91 | 0.38 | 62,62,62,62 | 0 |
| 55 | MG | 1a | 1606 | 1/1 | 0.91 | 0.11 | 49,49,49,49 | 0 |
| 55 | MG | 1a | 1607 | 1/1 | 0.91 | 0.08 | 75,75,75,75 | 0 |
| 55 | MG | 1a | 1784 | 1/1 | 0.91 | 0.19 | 58,58,58,58 | 0 |
| 55 | MG | 1A | 3234 | 1/1 | 0.91 | 0.14 | 29,29,29,29 | 0 |
| 55 | MG | 2A | 3339 | 1/1 | 0.91 | 0.27 | 60,60,60,60 | 0 |
| 55 | MG | 1a | 1611 | 1/1 | 0.91 | 0.07 | 43,43,43,43 | 0 |
| 55 | MG | 1A | 4016 | 1/1 | 0.91 | 0.13 | 22,22,22,22 | 0 |
| 55 | MG | 1A | 3286 | 1/1 | 0.91 | 0.18 | 40,40,40,40 | 0 |
| 55 | MG | 1a | 1794 | 1/1 | 0.91 | 0.08 | 50,50,50,50 | 0 |
| 55 | MG | 1A | 3590 | 1/1 | 0.91 | 0.07 | 31,31,31,31 | 0 |
| 55 | MG | 1A | 3834 | 1/1 | 0.91 | 0.16 | 33,33,33,33 | 0 |
| 55 | MG | 2a | 3007 | 1/1 | 0.91 | 0.26 | 59,59,59,59 | 0 |
| 55 | MG | 2a | 3008 | 1/1 | 0.91 | 0.13 | 62,62,62,62 | 0 |
| 55 | MG | 2A | 3349 | 1/1 | 0.91 | 0.08 | 45,45,45,45 | 0 |
| 55 | MG | 1A | 3482 | 1/1 | 0.91 | 0.11 | 50,50,50,50 | 0 |
| 55 | MG | 2A | 3632 | 1/1 | 0.91 | 0.11 | 53,53,53,53 | 0 |
| 55 | MG | 2A | 3638 | 1/1 | 0.91 | 0.19 | 53,53,53,53 | 0 |
| 55 | MG | 2A | 3639 | 1/1 | 0.91 | 0.15 | 67,67,67,67 | 0 |
| 55 | MG | 2A | 3352 | 1/1 | 0.91 | 0.23 | 43,43,43,43 | 0 |
| 55 | MG | 1A | 3596 | 1/1 | 0.91 | 0.18 | 43,43,43,43 | 0 |
| 55 | MG | 1A | 4034 | 1/1 | 0.91 | 0.20 | 57,57,57,57 | 0 |
| 55 | MG | 2A | 3357 | 1/1 | 0.91 | 0.07 | 44,44,44,44 | 0 |
| 55 | MG | 1a | 1626 | 1/1 | 0.91 | 0.10 | 48,48,48,48 | 0 |
| 55 | MG | 1A | 3103 | 1/1 | 0.91 | 0.29 | 58,58,58,58 | 0 |
| 55 | MG | 1A | 4040 | 1/1 | 0.91 | 0.09 | 57,57,57,57 | 0 |
| 55 | MG | 1A | 3487 | 1/1 | 0.91 | 0.11 | 44,44,44,44 | 0 |
| 55 | MG | 1A | 3190 | 1/1 | 0.91 | 0.73 | 34,34,34,34 | 0 |
| 55 | MG | 2a | 3031 | 1/1 | 0.91 | 0.17 | 51,51,51,51 | 0 |
| 55 | MG | 2A | 3662 | 1/1 | 0.91 | 0.12 | 63,63,63,63 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 55 | MG | 1a | 1821 | 1/1 | 0.91 | 0.11 | 53,53,53,53 | 0 |
| 55 | MG | 1A | 3208 | 1/1 | 0.91 | 0.14 | 64,64,64,64 | 0 |
| 55 | MG | 2A | 3371 | 1/1 | 0.91 | 0.16 | 68,68,68,68 | 0 |
| 55 | MG | 1A | 3610 | 1/1 | 0.91 | 0.15 | 44,44,44,44 | 0 |
| 55 | MG | 1A | 3853 | 1/1 | 0.91 | 0.12 | 30,30,30,30 | 0 |
| 55 | MG | 1A | 3380 | 1/1 | 0.91 | 0.21 | 38,38,38,38 | 0 |
| 55 | MG | 1A | 4072 | 1/1 | 0.91 | 0.09 | 47,47,47,47 | 0 |
| 55 | MG | 1A | 3250 | 1/1 | 0.91 | 0.10 | 40,40,40,40 | 0 |
| 55 | MG | 1a | 1830 | 1/1 | 0.91 | 0.14 | 59,59,59,59 | 0 |
| 55 | MG | 2A | 3179 | 1/1 | 0.91 | 0.14 | 56,56,56,56 | 0 |
| 55 | MG | 2A | 3182 | 1/1 | 0.91 | 0.11 | 63,63,63,63 | 0 |
| 55 | MG | 1A | 3627 | 1/1 | 0.91 | 0.16 | 41,41,41,41 | 0 |
| 55 | MG | 2a | 3051 | 1/1 | 0.91 | 0.16 | 45,45,45,45 | 0 |
| 55 | MG | 2A | 3391 | 1/1 | 0.91 | 0.21 | 45,45,45,45 | 0 |
| 55 | MG | 1A | 3634 | 1/1 | 0.91 | 0.36 | 55,55,55,55 | 0 |
| 55 | MG | 2a | 3057 | 1/1 | 0.91 | 0.23 | 45,45,45,45 | 0 |
| 55 | MG | 2A | 3697 | 1/1 | 0.91 | 0.14 | 57,57,57,57 | 0 |
| 55 | MG | 1A | 3641 | 1/1 | 0.91 | 0.11 | 23,23,23,23 | 0 |
| 55 | MG | 1A | 3870 | 1/1 | 0.91 | 0.14 | 46,46,46,46 | 0 |
| 55 | MG | 2A | 3706 | 1/1 | 0.91 | 0.10 | 39,39,39,39 | 0 |
| 55 | MG | 1A | 3253 | 1/1 | 0.91 | 0.19 | 55,55,55,55 | 0 |
| 55 | MG | 1e | 201 | 1/1 | 0.91 | 0.09 | 71,71,71,71 | 0 |
| 55 | MG | 2a | 3067 | 1/1 | 0.91 | 0.27 | 58,58,58,58 | 0 |
| 55 | MG | 2a | 3068 | 1/1 | 0.91 | 0.22 | 50,50,50,50 | 0 |
| 55 | MG | 2A | 3711 | 1/1 | 0.91 | 0.14 | 39,39,39,39 | 0 |
| 55 | MG | 2a | 3070 | 1/1 | 0.91 | 0.13 | 63,63,63,63 | 0 |
| 55 | MG | 2A | 3193 | 1/1 | 0.91 | 0.45 | 54,54,54,54 | 0 |
| 55 | MG | 2A | 3197 | 1/1 | 0.91 | 0.20 | 54,54,54,54 | 0 |
| 55 | MG | 1A | 3388 | 1/1 | 0.91 | 0.16 | 28,28,28,28 | 0 |
| 55 | MG | 2a | 3081 | 1/1 | 0.91 | 0.13 | 75,75,75,75 | 0 |
| 55 | MG | 1A | 4101 | 1/1 | 0.91 | 0.15 | 61,61,61,61 | 0 |
| 55 | MG | 1A | 3154 | 1/1 | 0.91 | 0.05 | 34,34,34,34 | 0 |
| 55 | MG | 2a | 3086 | 1/1 | 0.91 | 0.13 | 56,56,56,56 | 0 |
| 55 | MG | 1A | 3657 | 1/1 | 0.91 | 0.16 | 36,36,36,36 | 0 |
| 55 | MG | 2A | 3426 | 1/1 | 0.91 | 0.21 | 56,56,56,56 | 0 |
| 55 | MG | 2A | 3722 | 1/1 | 0.91 | 0.12 | 72,72,72,72 | 0 |
| 55 | MG | 1A | 3408 | 1/1 | 0.91 | 0.25 | 45,45,45,45 | 0 |
| 55 | MG | 1A | 3411 | 1/1 | 0.91 | 0.15 | 43,43,43,43 | 0 |
| 55 | MG | 1A | 4108 | 1/1 | 0.91 | 0.19 | 53,53,53,53 | 0 |
| 55 | MG | 2A | 3442 | 1/1 | 0.91 | 0.12 | 51,51,51,51 | 0 |
| 55 | MG | 2a | 3094 | 1/1 | 0.91 | 0.19 | 63,63,63,63 | 0 |
| 55 | MG | 1A | 3679 | 1/1 | 0.91 | 0.12 | 24,24,24,24 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 55 | MG | 1A | 3062 | 1/1 | 0.91 | 0.11 | 43,43,43,43 | 0 |
| 55 | MG | 1A | 3310 | 1/1 | 0.91 | 0.23 | 60,60,60,60 | 0 |
| 55 | MG | 2A | 3453 | 1/1 | 0.91 | 0.21 | 66,66,66,66 | 0 |
| 55 | MG | 1A | 3511 | 1/1 | 0.91 | 0.10 | 48,48,48,48 | 0 |
| 55 | MG | 1A | 3428 | 1/1 | 0.91 | 0.09 | 41,41,41,41 | 0 |
| 55 | MG | 2A | 3742 | 1/1 | 0.91 | 0.17 | 59,59,59,59 | 0 |
| 55 | MG | 1A | 3323 | 1/1 | 0.91 | 0.14 | 52,52,52,52 | 0 |
| 55 | MG | 2A | 3748 | 1/1 | 0.91 | 0.10 | 50,50,50,50 | 0 |
| 55 | MG | 2A | 3751 | 1/1 | 0.91 | 0.07 | 50,50,50,50 | 0 |
| 55 | MG | 2A | 3001 | 1/1 | 0.91 | 0.20 | 48,48,48,48 | 0 |
| 55 | MG | 1B | 220 | 1/1 | 0.91 | 0.09 | 40,40,40,40 | 0 |
| 55 | MG | 1A | 3903 | 1/1 | 0.91 | 0.19 | 54,54,54,54 | 0 |
| 55 | MG | 2A | 3761 | 1/1 | 0.91 | 0.12 | 49,49,49,49 | 0 |
| 55 | MG | 2A | 3765 | 1/1 | 0.91 | 0.12 | 72,72,72,72 | 0 |
| 55 | MG | 2A | 3236 | 1/1 | 0.91 | 0.12 | 51,51,51,51 | 0 |
| 55 | MG | 2A | 3237 | 1/1 | 0.91 | 0.26 | 50,50,50,50 | 0 |
| 55 | MG | 1A | 3517 | 1/1 | 0.91 | 0.08 | 50,50,50,50 | 0 |
| 55 | MG | 2A | 3012 | 1/1 | 0.91 | 0.14 | 36,36,36,36 | 0 |
| 55 | MG | 2A | 3248 | 1/1 | 0.91 | 0.27 | 58,58,58,58 | 0 |
| 55 | MG | 1A | 3907 | 1/1 | 0.91 | 0.12 | 28,28,28,28 | 0 |
| 55 | MG | 2a | 3136 | 1/1 | 0.91 | 0.41 | 59,59,59,59 | 0 |
| 55 | MG | 2A | 3478 | 1/1 | 0.91 | 0.22 | 30,30,30,30 | 0 |
| 55 | MG | 2A | 3779 | 1/1 | 0.91 | 0.19 | 73,73,73,73 | 0 |
| 55 | MG | 1A | 3723 | 1/1 | 0.91 | 0.12 | 14,14,14,14 | 0 |
| 55 | MG | 1A | 3518 | 1/1 | 0.91 | 0.09 | 50,50,50,50 | 0 |
| 55 | MG | 1A | 3110 | 1/1 | 0.91 | 0.53 | 35,35,35,35 | 0 |
| 55 | MG | 1A | 3435 | 1/1 | 0.91 | 0.09 | 47,47,47,47 | 0 |
| 55 | MG | 2a | 3144 | 1/1 | 0.91 | 0.20 | 57,57,57,57 | 0 |
| 55 | MG | 2A | 3489 | 1/1 | 0.91 | 0.12 | 49,49,49,49 | 0 |
| 55 | MG | 1A | 3055 | 1/1 | 0.91 | 0.28 | 47,47,47,47 | 0 |
| 55 | MG | 1E | 301 | 1/1 | 0.91 | 0.18 | 45,45,45,45 | 0 |
| 55 | MG | 2A | 3041 | 1/1 | 0.91 | 0.25 | 55,55,55,55 | 0 |
| 55 | MG | 1E | 302 | 1/1 | 0.91 | 0.19 | 26,26,26,26 | 0 |
| 55 | MG | 1A | 3338 | 1/1 | 0.91 | 0.20 | 46,46,46,46 | 0 |
| 55 | MG | 2A | 3824 | 1/1 | 0.91 | 0.13 | 54,54,54,54 | 0 |
| 55 | MG | 1A | 3745 | 1/1 | 0.91 | 0.14 | 48,48,48,48 | 0 |
| 55 | MG | 1G | 201 | 1/1 | 0.91 | 0.22 | 39,39,39,39 | 0 |
| 55 | MG | 2A | 3058 | 1/1 | 0.91 | 0.16 | 41,41,41,41 | 0 |
| 55 | MG | 2A | 3831 | 1/1 | 0.91 | 0.09 | 51,51,51,51 | 0 |
| 55 | MG | 2A | 3832 | 1/1 | 0.91 | 0.17 | 65,65,65,65 | 0 |
| 55 | MG | 2A | 3833 | 1/1 | 0.91 | 0.12 | 57,57,57,57 | 0 |
| 55 | MG | 1A | 3747 | 1/1 | 0.91 | 0.07 | 34,34,34,34 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 55 | MG | 2A | 3517 | 1/1 | 0.91 | 0.12 | 65,65,65,65 | 0 |
| 55 | MG | 1A | 3529 | 1/1 | 0.91 | 0.21 | 42,42,42,42 | 0 |
| 55 | MG | 1A | 3937 | 1/1 | 0.91 | 0.15 | 33,33,33,33 | 0 |
| 55 | MG | 1A | 3532 | 1/1 | 0.91 | 0.17 | 33,33,33,33 | 0 |
| 55 | MG | 1a | 1722 | 1/1 | 0.91 | 0.17 | 66,66,66,66 | 0 |
| 55 | MG | 1A | 3537 | 1/1 | 0.91 | 0.17 | 44,44,44,44 | 0 |
| 55 | MG | 1A | 3767 | 1/1 | 0.91 | 0.07 | 43,43,43,43 | 0 |
| 55 | MG | 1A | 3768 | 1/1 | 0.91 | 0.13 | 36,36,36,36 | 0 |
| 55 | MG | 1A | 3448 | 1/1 | 0.91 | 0.14 | 40,40,40,40 | 0 |
| 55 | MG | 1A | 3950 | 1/1 | 0.91 | 0.07 | 51,51,51,51 | 0 |
| 55 | MG | 2A | 3547 | 1/1 | 0.91 | 0.15 | 59,59,59,59 | 0 |
| 55 | MG | 1A | 3449 | 1/1 | 0.91 | 0.14 | 58,58,58,58 | 0 |
| 55 | MG | 1A | 3047 | 1/1 | 0.91 | 0.19 | 43,43,43,43 | 0 |
| 55 | MG | 2a | 3192 | 1/1 | 0.91 | 0.23 | 55,55,55,55 | 0 |
| 55 | MG | 1A | 3270 | 1/1 | 0.91 | 0.17 | 43,43,43,43 | 0 |
| 55 | MG | 1a | 1742 | 1/1 | 0.91 | 0.28 | 35,35,35,35 | 0 |
| 55 | MG | 2A | 3553 | 1/1 | 0.91 | 0.16 | 42,42,42,42 | 0 |
| 55 | MG | 1A | 3564 | 1/1 | 0.91 | 0.12 | 31,31,31,31 | 0 |
| 55 | MG | 2A | 3087 | 1/1 | 0.91 | 0.10 | 45,45,45,45 | 0 |
| 55 | MG | 2a | 3204 | 1/1 | 0.91 | 0.16 | 55,55,55,55 | 0 |
| 55 | MG | 1A | 3349 | 1/1 | 0.91 | 0.12 | 42,42,42,42 | 0 |
| 55 | MG | 1A | 3129 | 1/1 | 0.91 | 0.13 | 39,39,39,39 | 0 |
| 55 | MG | 2A | 3301 | 1/1 | 0.91 | 0.12 | 62,62,62,62 | 0 |
| 55 | MG | 2A | 3303 | 1/1 | 0.91 | 0.10 | 60,60,60,60 | 0 |
| 55 | MG | 2B | 215 | 1/1 | 0.91 | 0.15 | 47,47,47,47 | 0 |
| 55 | MG | 13 | 102 | 1/1 | 0.91 | 0.17 | 41,41,41,41 | 0 |
| 55 | MG | 2B | 219 | 1/1 | 0.91 | 0.27 | 60,60,60,60 | 0 |
| 55 | MG | 2f | 201 | 1/1 | 0.91 | 0.15 | 55,55,55,55 | 0 |
| 55 | MG | 15 | 101 | 1/1 | 0.91 | 0.15 | 34,34,34,34 | 0 |
| 55 | MG | 1A | 3999 | 1/1 | 0.91 | 0.14 | 64,64,64,64 | 0 |
| 55 | MG | 2E | 303 | 1/1 | 0.91 | 0.15 | 50,50,50,50 | 0 |
| 55 | MG | 1A | 4005 | 1/1 | 0.91 | 0.10 | 34,34,34,34 | 0 |
| 55 | MG | 2l | 201 | 1/1 | 0.91 | 0.28 | 76,76,76,76 | 0 |
| 55 | MG | 17 | 104 | 1/1 | 0.91 | 0.11 | 45,45,45,45 | 0 |
| 55 | MG | 1a | 1764 | 1/1 | 0.91 | 0.19 | 39,39,39,39 | 0 |
| 55 | MG | 1A | 3470 | 1/1 | 0.91 | 0.10 | 46,46,46,46 | 0 |
| 55 | MG | 19 | 101 | 1/1 | 0.91 | 0.15 | 43,43,43,43 | 0 |
| 55 | MG | 2A | 3114 | 1/1 | 0.91 | 0.08 | 46,46,46,46 | 0 |
| 55 | MG | 2A | 3325 | 1/1 | 0.91 | 0.09 | 44,44,44,44 | 0 |
| 55 | MG | 2Q | 201 | 1/1 | 0.91 | 0.16 | 57,57,57,57 | 0 |
| 55 | MG | 2Q | 202 | 1/1 | 0.91 | 0.28 | 56,56,56,56 | 0 |
| 55 | MG | 2R | 201 | 1/1 | 0.91 | 0.12 | 48,48,48,48 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 55 | MG | 1A | 4009 | 1/1 | 0.91 | 0.19 | 30,30,30,30 | 0 |
| 55 | MG | 2A | 3006 | 1/1 | 0.92 | 0.07 | 56,56,56,56 | 0 |
| 55 | MG | 2D | 302 | 1/1 | 0.92 | 0.24 | 42,42,42,42 | 0 |
| 55 | MG | 2A | 3267 | 1/1 | 0.92 | 0.11 | 66,66,66,66 | 0 |
| 55 | MG | 2A | 3008 | 1/1 | 0.92 | 0.12 | 46,46,46,46 | 0 |
| 55 | MG | 1B | 201 | 1/1 | 0.92 | 0.14 | 50,50,50,50 | 0 |
| 55 | MG | 1A | 3418 | 1/1 | 0.92 | 0.17 | 58,58,58,58 | 0 |
| 55 | MG | 2E | 307 | 1/1 | 0.92 | 0.11 | 56,56,56,56 | 0 |
| 55 | MG | 2E | 309 | 1/1 | 0.92 | 0.07 | 38,38,38,38 | 0 |
| 55 | MG | 2A | 3272 | 1/1 | 0.92 | 0.21 | 57,57,57,57 | 0 |
| 55 | MG | 2A | 3273 | 1/1 | 0.92 | 0.07 | 50,50,50,50 | 0 |
| 55 | MG | 1A | 3736 | 1/1 | 0.92 | 0.10 | 17,17,17,17 | 0 |
| 55 | MG | 1A | 3520 | 1/1 | 0.92 | 0.23 | 58,58,58,58 | 0 |
| 55 | MG | 1A | 3917 | 1/1 | 0.92 | 0.08 | 43,43,43,43 | 0 |
| 55 | MG | 2A | 3562 | 1/1 | 0.92 | 0.17 | 57,57,57,57 | 0 |
| 55 | MG | 2A | 3277 | 1/1 | 0.92 | 0.21 | 50,50,50,50 | 0 |
| 55 | MG | 1A | 3522 | 1/1 | 0.92 | 0.37 | 43,43,43,43 | 0 |
| 55 | MG | 1A | 3127 | 1/1 | 0.92 | 0.20 | 34,34,34,34 | 0 |
| 55 | MG | 1A | 3423 | 1/1 | 0.92 | 0.17 | 43,43,43,43 | 0 |
| 55 | MG | 1A | 3525 | 1/1 | 0.92 | 0.23 | 35,35,35,35 | 0 |
| 55 | MG | 1a | 1693 | 1/1 | 0.92 | 0.25 | 59,59,59,59 | 0 |
| 55 | MG | 2U | 202 | 1/1 | 0.92 | 0.22 | 30,30,30,30 | 0 |
| 55 | MG | 1A | 3426 | 1/1 | 0.92 | 0.09 | 50,50,50,50 | 0 |
| 55 | MG | 2V | 202 | 1/1 | 0.92 | 0.42 | 53,53,53,53 | 0 |
| 55 | MG | 2A | 3585 | 1/1 | 0.92 | 0.17 | 34,34,34,34 | 0 |
| 55 | MG | 1a | 1699 | 1/1 | 0.92 | 0.28 | 48,48,48,48 | 0 |
| 55 | MG | 2A | 3589 | 1/1 | 0.92 | 0.10 | 44,44,44,44 | 0 |
| 55 | MG | 2Z | 301 | 1/1 | 0.92 | 0.19 | 67,67,67,67 | 0 |
| 55 | MG | 2A | 3594 | 1/1 | 0.92 | 0.16 | 49,49,49,49 | 0 |
| 55 | MG | 1A | 3427 | 1/1 | 0.92 | 0.10 | 55,55,55,55 | 0 |
| 55 | MG | 25 | 102 | 1/1 | 0.92 | 0.08 | 43,43,43,43 | 0 |
| 55 | MG | 2A | 3050 | 1/1 | 0.92 | 0.15 | 56,56,56,56 | 0 |
| 55 | MG | 1A | 3936 | 1/1 | 0.92 | 0.09 | 39,39,39,39 | 0 |
| 55 | MG | 1A | 3240 | 1/1 | 0.92 | 0.10 | 61,61,61,61 | 0 |
| 55 | MG | 2A | 3295 | 1/1 | 0.92 | 0.08 | 52,52,52,52 | 0 |
| 55 | MG | 1B | 234 | 1/1 | 0.92 | 0.10 | 44,44,44,44 | 0 |
| 55 | MG | 2A | 3297 | 1/1 | 0.92 | 0.14 | 47,47,47,47 | 0 |
| 55 | MG | 1a | 1707 | 1/1 | 0.92 | 0.06 | 62,62,62,62 | 0 |
| 55 | MG | 1D | 309 | 1/1 | 0.92 | 0.11 | 53,53,53,53 | 0 |
| 55 | MG | 2a | 3010 | 1/1 | 0.92 | 0.09 | 55,55,55,55 | 0 |
| 55 | MG | 1a | 1709 | 1/1 | 0.92 | 0.27 | 59,59,59,59 | 0 |
| 55 | MG | 1A | 3171 | 1/1 | 0.92 | 0.11 | 31,31,31,31 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 55 | MG | 2a | 3014 | 1/1 | 0.92 | 0.11 | 71,71,71,71 | 0 |
| 55 | MG | 2A | 3308 | 1/1 | 0.92 | 0.10 | 54,54,54,54 | 0 |
| 55 | MG | 1D | 312 | 1/1 | 0.92 | 0.22 | 41,41,41,41 | 0 |
| 55 | MG | 1A | 3433 | 1/1 | 0.92 | 0.19 | 44,44,44,44 | 0 |
| 55 | MG | 2A | 3313 | 1/1 | 0.92 | 0.07 | 68,68,68,68 | 0 |
| 55 | MG | 2a | 3020 | 1/1 | 0.92 | 0.40 | 67,67,67,67 | 0 |
| 55 | MG | 1A | 3944 | 1/1 | 0.92 | 0.13 | 56,56,56,56 | 0 |
| 55 | MG | 2a | 3022 | 1/1 | 0.92 | 0.09 | 47,47,47,47 | 0 |
| 55 | MG | 1A | 3308 | 1/1 | 0.92 | 0.14 | 36,36,36,36 | 0 |
| 55 | MG | 1E | 310 | 1/1 | 0.92 | 0.26 | 43,43,43,43 | 0 |
| 55 | MG | 2A | 3621 | 1/1 | 0.92 | 0.12 | 46,46,46,46 | 0 |
| 55 | MG | 2a | 3026 | 1/1 | 0.92 | 0.23 | 49,49,49,49 | 0 |
| 55 | MG | 1F | 305 | 1/1 | 0.92 | 0.15 | 41,41,41,41 | 0 |
| 55 | MG | 1A | 3244 | 1/1 | 0.92 | 0.24 | 38,38,38,38 | 0 |
| 55 | MG | 1A | 3319 | 1/1 | 0.92 | 0.15 | 54,54,54,54 | 0 |
| 55 | MG | 1A | 3438 | 1/1 | 0.92 | 0.13 | 41,41,41,41 | 0 |
| 55 | MG | 1A | 3965 | 1/1 | 0.92 | 0.08 | 27,27,27,27 | 0 |
| 55 | MG | 2A | 3633 | 1/1 | 0.92 | 0.19 | 50,50,50,50 | 0 |
| 55 | MG | 1N | 201 | 1/1 | 0.92 | 0.23 | 43,43,43,43 | 0 |
| 55 | MG | 1N | 204 | 1/1 | 0.92 | 0.20 | 47,47,47,47 | 0 |
| 55 | MG | 1A | 3967 | 1/1 | 0.92 | 0.14 | 49,49,49,49 | 0 |
| 55 | MG | 1a | 1738 | 1/1 | 0.92 | 0.27 | 52,52,52,52 | 0 |
| 55 | MG | 1A | 3972 | 1/1 | 0.92 | 0.14 | 43,43,43,43 | 0 |
| 55 | MG | 2A | 3098 | 1/1 | 0.92 | 0.13 | 44,44,44,44 | 0 |
| 55 | MG | 2A | 3335 | 1/1 | 0.92 | 0.10 | 57,57,57,57 | 0 |
| 55 | MG | 2a | 3045 | 1/1 | 0.92 | 0.12 | 92,92,92,92 | 0 |
| 55 | MG | 2A | 3652 | 1/1 | 0.92 | 0.14 | 50,50,50,50 | 0 |
| 55 | MG | 1A | 3973 | 1/1 | 0.92 | 0.10 | 67,67,67,67 | 0 |
| 55 | MG | 1A | 3975 | 1/1 | 0.92 | 0.08 | 53,53,53,53 | 0 |
| 55 | MG | 1Q | 204 | 1/1 | 0.92 | 0.07 | 51,51,51,51 | 0 |
| 55 | MG | 1A | 3115 | 1/1 | 0.92 | 0.08 | 47,47,47,47 | 0 |
| 55 | MG | 2A | 3343 | 1/1 | 0.92 | 0.06 | 50,50,50,50 | 0 |
| 55 | MG | 2A | 3665 | 1/1 | 0.92 | 0.12 | 55,55,55,55 | 0 |
| 55 | MG | 1A | 3794 | 1/1 | 0.92 | 0.10 | 29,29,29,29 | 0 |
| 55 | MG | 1A | 3031 | 1/1 | 0.92 | 0.24 | 32,32,32,32 | 0 |
| 55 | MG | 1A | 3184 | 1/1 | 0.92 | 0.12 | 40,40,40,40 | 0 |
| 55 | MG | 2A | 3116 | 1/1 | 0.92 | 0.18 | 43,43,43,43 | 0 |
| 55 | MG | 2A | 3673 | 1/1 | 0.92 | 0.13 | 52,52,52,52 | 0 |
| 55 | MG | 1a | 1752 | 1/1 | 0.92 | 0.10 | 58,58,58,58 | 0 |
| 55 | MG | 2A | 3129 | 1/1 | 0.92 | 0.13 | 57,57,57,57 | 0 |
| 55 | MG | 1V | 202 | 1/1 | 0.92 | 0.18 | 45,45,45,45 | 0 |
| 55 | MG | 1a | 1755 | 1/1 | 0.92 | 0.08 | 60,60,60,60 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 55 | MG | 1A | 3333 | 1/1 | 0.92 | 0.07 | 41,41,41,41 | 0 |
| 55 | MG | 1A | 3805 | 1/1 | 0.92 | 0.18 | 33,33,33,33 | 0 |
| 55 | MG | 1A | 3995 | 1/1 | 0.92 | 0.16 | 53,53,53,53 | 0 |
| 55 | MG | 2a | 3074 | 1/1 | 0.92 | 0.20 | 47,47,47,47 | 0 |
| 55 | MG | 1A | 3998 | 1/1 | 0.92 | 0.14 | 57,57,57,57 | 0 |
| 55 | MG | 10 | 103 | 1/1 | 0.92 | 0.18 | 55,55,55,55 | 0 |
| 55 | MG | 1A | 3452 | 1/1 | 0.92 | 0.10 | 45,45,45,45 | 0 |
| 55 | MG | 1A | 3458 | 1/1 | 0.92 | 0.18 | 47,47,47,47 | 0 |
| 55 | MG | 1A | 3463 | 1/1 | 0.92 | 0.19 | 48,48,48,48 | 0 |
| 55 | MG | 2A | 3368 | 1/1 | 0.92 | 0.18 | 54,54,54,54 | 0 |
| 55 | MG | 1A | 3336 | 1/1 | 0.92 | 0.18 | 53,53,53,53 | 0 |
| 55 | MG | 1a | 1782 | 1/1 | 0.92 | 0.08 | 57,57,57,57 | 0 |
| 55 | MG | 1A | 3134 | 1/1 | 0.92 | 0.08 | 45,45,45,45 | 0 |
| 55 | MG | 1A | 3137 | 1/1 | 0.92 | 0.29 | 35,35,35,35 | 0 |
| 55 | MG | 1A | 3598 | 1/1 | 0.92 | 0.27 | 47,47,47,47 | 0 |
| 55 | MG | 1A | 3599 | 1/1 | 0.92 | 0.15 | 39,39,39,39 | 0 |
| 55 | MG | 1A | 3260 | 1/1 | 0.92 | 0.10 | 38,38,38,38 | 0 |
| 55 | MG | 1A | 3471 | 1/1 | 0.92 | 0.07 | 27,27,27,27 | 0 |
| 55 | MG | 1a | 1793 | 1/1 | 0.92 | 0.10 | 63,63,63,63 | 0 |
| 55 | MG | 1A | 4021 | 1/1 | 0.92 | 0.12 | 64,64,64,64 | 0 |
| 55 | MG | 1A | 4022 | 1/1 | 0.92 | 0.11 | 57,57,57,57 | 0 |
| 55 | MG | 2A | 3385 | 1/1 | 0.92 | 0.17 | 37,37,37,37 | 0 |
| 55 | MG | 2A | 3724 | 1/1 | 0.92 | 0.13 | 61,61,61,61 | 0 |
| 55 | MG | 1a | 1796 | 1/1 | 0.92 | 0.17 | 69,69,69,69 | 0 |
| 55 | MG | 2A | 3168 | 1/1 | 0.92 | 0.09 | 51,51,51,51 | 0 |
| 55 | MG | 1a | 1798 | 1/1 | 0.92 | 0.15 | 73,73,73,73 | 0 |
| 55 | MG | 1a | 1800 | 1/1 | 0.92 | 0.08 | 72,72,72,72 | 0 |
| 55 | MG | 1a | 1802 | 1/1 | 0.92 | 0.08 | 66,66,66,66 | 0 |
| 55 | MG | 1A | 3348 | 1/1 | 0.92 | 0.19 | 55,55,55,55 | 0 |
| 55 | MG | 2A | 3175 | 1/1 | 0.92 | 0.19 | 52,52,52,52 | 0 |
| 55 | MG | 2a | 3112 | 1/1 | 0.92 | 0.16 | 58,58,58,58 | 0 |
| 55 | MG | 1A | 4026 | 1/1 | 0.92 | 0.10 | 29,29,29,29 | 0 |
| 55 | MG | 1A | 3607 | 1/1 | 0.92 | 0.24 | 33,33,33,33 | 0 |
| 55 | MG | 2a | 3119 | 1/1 | 0.92 | 0.36 | 62,62,62,62 | 0 |
| 55 | MG | 2a | 3120 | 1/1 | 0.92 | 0.16 | 57,57,57,57 | 0 |
| 55 | MG | 2A | 3419 | 1/1 | 0.92 | 0.16 | 53,53,53,53 | 0 |
| 55 | MG | 2A | 3420 | 1/1 | 0.92 | 0.21 | 38,38,38,38 | 0 |
| 55 | MG | 1A | 3261 | 1/1 | 0.92 | 0.11 | 33,33,33,33 | 0 |
| 55 | MG | 2A | 3745 | 1/1 | 0.92 | 0.18 | 27,27,27,27 | 0 |
| 55 | MG | 1A | 3196 | 1/1 | 0.92 | 0.07 | 41,41,41,41 | 0 |
| 55 | MG | 2A | 3424 | 1/1 | 0.92 | 0.26 | 48,48,48,48 | 0 |
| 55 | MG | 2A | 3753 | 1/1 | 0.92 | 0.18 | 58,58,58,58 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 55 | MG | 1a | 1810 | 1/1 | 0.92 | 0.07 | 58,58,58,58 | 0 |
| 55 | MG | 2A | 3188 | 1/1 | 0.92 | 0.17 | 48,48,48,48 | 0 |
| 55 | MG | 1a | 1615 | 1/1 | 0.92 | 0.05 | 73,73,73,73 | 0 |
| 55 | MG | 2a | 3138 | 1/1 | 0.92 | 0.32 | 67,67,67,67 | 0 |
| 55 | MG | 2A | 3429 | 1/1 | 0.92 | 0.27 | 63,63,63,63 | 0 |
| 55 | MG | 2A | 3431 | 1/1 | 0.92 | 0.19 | 46,46,46,46 | 0 |
| 55 | MG | 1A | 4037 | 1/1 | 0.92 | 0.11 | 58,58,58,58 | 0 |
| 55 | MG | 1A | 3617 | 1/1 | 0.92 | 0.08 | 29,29,29,29 | 0 |
| 55 | MG | 2A | 3770 | 1/1 | 0.92 | 0.08 | 69,69,69,69 | 0 |
| 55 | MG | 1a | 1818 | 1/1 | 0.92 | 0.08 | 73,73,73,73 | 0 |
| 55 | MG | 2A | 3772 | 1/1 | 0.92 | 0.13 | 80,80,80,80 | 0 |
| 55 | MG | 2a | 3146 | 1/1 | 0.92 | 0.23 | 38,38,38,38 | 0 |
| 55 | MG | 1A | 3619 | 1/1 | 0.92 | 0.10 | 32,32,32,32 | 0 |
| 55 | MG | 2A | 3774 | 1/1 | 0.92 | 0.15 | 42,42,42,42 | 0 |
| 55 | MG | 2A | 3196 | 1/1 | 0.92 | 0.11 | 50,50,50,50 | 0 |
| 55 | MG | 1A | 3356 | 1/1 | 0.92 | 0.13 | 62,62,62,62 | 0 |
| 55 | MG | 2A | 3449 | 1/1 | 0.92 | 0.07 | 66,66,66,66 | 0 |
| 55 | MG | 1A | 3138 | 1/1 | 0.92 | 0.09 | 20,20,20,20 | 0 |
| 55 | MG | 1A | 3859 | 1/1 | 0.92 | 0.19 | 59,59,59,59 | 0 |
| 55 | MG | 1a | 1628 | 1/1 | 0.92 | 0.17 | 61,61,61,61 | 0 |
| 55 | MG | 1a | 1630 | 1/1 | 0.92 | 0.09 | 44,44,44,44 | 0 |
| 55 | MG | 2A | 3785 | 1/1 | 0.92 | 0.09 | 60,60,60,60 | 0 |
| 55 | MG | 2A | 3789 | 1/1 | 0.92 | 0.10 | 47,47,47,47 | 0 |
| 55 | MG | 1A | 4057 | 1/1 | 0.92 | 0.10 | 47,47,47,47 | 0 |
| 55 | MG | 2A | 3798 | 1/1 | 0.92 | 0.07 | 57,57,57,57 | 0 |
| 55 | MG | 2A | 3208 | 1/1 | 0.92 | 0.39 | 57,57,57,57 | 0 |
| 55 | MG | 1A | 3266 | 1/1 | 0.92 | 0.08 | 50,50,50,50 | 0 |
| 55 | MG | 1A | 3210 | 1/1 | 0.92 | 0.11 | 43,43,43,43 | 0 |
| 55 | MG | 1a | 1640 | 1/1 | 0.92 | 0.09 | 48,48,48,48 | 0 |
| 55 | MG | 2A | 3221 | 1/1 | 0.92 | 0.15 | 47,47,47,47 | 0 |
| 55 | MG | 1A | 3144 | 1/1 | 0.92 | 0.13 | 39,39,39,39 | 0 |
| 55 | MG | 2A | 3226 | 1/1 | 0.92 | 0.09 | 61,61,61,61 | 0 |
| 55 | MG | 1A | 4064 | 1/1 | 0.92 | 0.09 | 39,39,39,39 | 0 |
| 55 | MG | 2a | 3181 | 1/1 | 0.92 | 0.20 | 56,56,56,56 | 0 |
| 55 | MG | 2A | 3477 | 1/1 | 0.92 | 0.20 | 34,34,34,34 | 0 |
| 55 | MG | 2A | 3828 | 1/1 | 0.92 | 0.12 | 48,48,48,48 | 0 |
| 55 | MG | 2a | 3187 | 1/1 | 0.92 | 0.23 | 75,75,75,75 | 0 |
| 55 | MG | 1A | 3279 | 1/1 | 0.92 | 0.10 | 47,47,47,47 | 0 |
| 55 | MG | 2A | 3480 | 1/1 | 0.92 | 0.26 | 37,37,37,37 | 0 |
| 55 | MG | 1A | 3377 | 1/1 | 0.92 | 0.14 | 37,37,37,37 | 0 |
| 55 | MG | 1A | 3215 | 1/1 | 0.92 | 0.14 | 36,36,36,36 | 0 |
| 55 | MG | 1A | 3382 | 1/1 | 0.92 | 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 |
|---|---|---|---|---|---|---|---|---|
| 55 | MG | 1A | 4082 | 1/1 | 0.92 | 0.06 | 42,42,42,42 | 0 |
| 55 | MG | 1l | 204 | 1/1 | 0.92 | 0.07 | 64,64,64,64 | 0 |
| 55 | MG | 1A | 3145 | 1/1 | 0.92 | 0.14 | 25,25,25,25 | 0 |
| 55 | MG | 2A | 3846 | 1/1 | 0.92 | 0.10 | 51,51,51,51 | 0 |
| 55 | MG | 2a | 3203 | 1/1 | 0.92 | 0.14 | 72,72,72,72 | 0 |
| 55 | MG | 1A | 3881 | 1/1 | 0.92 | 0.09 | 34,34,34,34 | 0 |
| 55 | MG | 2A | 3848 | 1/1 | 0.92 | 0.21 | 55,55,55,55 | 0 |
| 55 | MG | 1A | 3069 | 1/1 | 0.92 | 0.14 | 36,36,36,36 | 0 |
| 55 | MG | 2A | 3241 | 1/1 | 0.92 | 0.30 | 58,58,58,58 | 0 |
| 55 | MG | 1A | 3678 | 1/1 | 0.92 | 0.12 | 20,20,20,20 | 0 |
| 55 | MG | 1a | 1659 | 1/1 | 0.92 | 0.07 | 67,67,67,67 | 0 |
| 55 | MG | 1A | 3124 | 1/1 | 0.92 | 0.13 | 47,47,47,47 | 0 |
| 55 | MG | 2A | 3506 | 1/1 | 0.92 | 0.16 | 60,60,60,60 | 0 |
| 55 | MG | 2A | 3509 | 1/1 | 0.92 | 0.16 | 57,57,57,57 | 0 |
| 55 | MG | 1A | 3508 | 1/1 | 0.92 | 0.17 | 35,35,35,35 | 0 |
| 55 | MG | 1A | 3161 | 1/1 | 0.92 | 0.11 | 37,37,37,37 | 0 |
| 55 | MG | 1A | 3395 | 1/1 | 0.92 | 0.06 | 58,58,58,58 | 0 |
| 55 | MG | 2A | 3519 | 1/1 | 0.92 | 0.12 | 39,39,39,39 | 0 |
| 55 | MG | 1A | 3291 | 1/1 | 0.92 | 0.23 | 43,43,43,43 | 0 |
| 55 | MG | 2A | 3257 | 1/1 | 0.92 | 0.12 | 52,52,52,52 | 0 |
| 55 | MG | 1A | 3410 | 1/1 | 0.92 | 0.10 | 40,40,40,40 | 0 |
| 55 | MG | 2B | 207 | 1/1 | 0.92 | 0.18 | 57,57,57,57 | 0 |
| 55 | MG | 2A | 3528 | 1/1 | 0.92 | 0.08 | 32,32,32,32 | 0 |
| 55 | MG | 2A | 3529 | 1/1 | 0.92 | 0.11 | 49,49,49,49 | 0 |
| 55 | MG | 1A | 3162 | 1/1 | 0.92 | 0.14 | 43,43,43,43 | 0 |
| 55 | MG | 2x | 103 | 1/1 | 0.92 | 0.18 | 63,63,63,63 | 0 |
| 55 | MG | 1A | 4110 | 1/1 | 0.92 | 0.16 | 53,53,53,53 | 0 |
| 55 | MG | 1A | 3125 | 1/1 | 0.92 | 0.58 | 30,30,30,30 | 0 |
| 55 | MG | 1A | 4117 | 1/1 | 0.92 | 0.22 | 49,49,49,49 | 0 |
| 55 | MG | 2B | 218 | 1/1 | 0.92 | 0.08 | 59,59,59,59 | 0 |
| 55 | MG | 2A | 3518 | 1/1 | 0.93 | 0.21 | 68,68,68,68 | 0 |
| 55 | MG | 1a | 1637 | 1/1 | 0.93 | 0.25 | 59,59,59,59 | 0 |
| 55 | MG | 1A | 3421 | 1/1 | 0.93 | 0.27 | 52,52,52,52 | 0 |
| 55 | MG | 1A | 3875 | 1/1 | 0.93 | 0.12 | 32,32,32,32 | 0 |
| 55 | MG | 2A | 3240 | 1/1 | 0.93 | 0.17 | 54,54,54,54 | 0 |
| 55 | MG | 1A | 3017 | 1/1 | 0.93 | 0.07 | 25,25,25,25 | 0 |
| 55 | MG | 1A | 3646 | 1/1 | 0.93 | 0.13 | 30,30,30,30 | 0 |
| 55 | MG | 2A | 3531 | 1/1 | 0.93 | 0.20 | 31,31,31,31 | 0 |
| 55 | MG | 1A | 3052 | 1/1 | 0.93 | 0.20 | 21,21,21,21 | 0 |
| 55 | MG | 1A | 3098 | 1/1 | 0.93 | 0.06 | 36,36,36,36 | 0 |
| 55 | MG | 2E | 302 | 1/1 | 0.93 | 0.10 | 47,47,47,47 | 0 |
| 55 | MG | 1l | 201 | 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 |
|---|---|---|---|---|---|---|---|---|
| 55 | MG | 1A | 3337 | 1/1 | 0.93 | 0.11 | 45,45,45,45 | 0 |
| 55 | MG | 1A | 3889 | 1/1 | 0.93 | 0.15 | 43,43,43,43 | 0 |
| 55 | MG | 1A | 3659 | 1/1 | 0.93 | 0.18 | 52,52,52,52 | 0 |
| 55 | MG | 1A | 3430 | 1/1 | 0.93 | 0.35 | 41,41,41,41 | 0 |
| 55 | MG | 1a | 1653 | 1/1 | 0.93 | 0.10 | 69,69,69,69 | 0 |
| 55 | MG | 2A | 3549 | 1/1 | 0.93 | 0.13 | 35,35,35,35 | 0 |
| 55 | MG | 1A | 3274 | 1/1 | 0.93 | 0.09 | 37,37,37,37 | 0 |
| 55 | MG | 1A | 3896 | 1/1 | 0.93 | 0.38 | 32,32,32,32 | 0 |
| 55 | MG | 1A | 3669 | 1/1 | 0.93 | 0.08 | 21,21,21,21 | 0 |
| 55 | MG | 1A | 4106 | 1/1 | 0.93 | 0.08 | 52,52,52,52 | 0 |
| 55 | MG | 1x | 106 | 1/1 | 0.93 | 0.13 | 55,55,55,55 | 0 |
| 55 | MG | 2Q | 203 | 1/1 | 0.93 | 0.09 | 43,43,43,43 | 0 |
| 55 | MG | 1A | 3675 | 1/1 | 0.93 | 0.10 | 14,14,14,14 | 0 |
| 55 | MG | 2R | 202 | 1/1 | 0.93 | 0.22 | 52,52,52,52 | 0 |
| 55 | MG | 1a | 1660 | 1/1 | 0.93 | 0.15 | 77,77,77,77 | 0 |
| 55 | MG | 1a | 1661 | 1/1 | 0.93 | 0.15 | 62,62,62,62 | 0 |
| 55 | MG | 1x | 112 | 1/1 | 0.93 | 0.13 | 64,64,64,64 | 0 |
| 55 | MG | 1A | 3054 | 1/1 | 0.93 | 0.11 | 37,37,37,37 | 0 |
| 55 | MG | 1A | 3186 | 1/1 | 0.93 | 0.13 | 37,37,37,37 | 0 |
| 55 | MG | 1A | 3128 | 1/1 | 0.93 | 0.41 | 37,37,37,37 | 0 |
| 55 | MG | 2A | 3573 | 1/1 | 0.93 | 0.13 | 34,34,34,34 | 0 |
| 55 | MG | 2A | 3576 | 1/1 | 0.93 | 0.10 | 50,50,50,50 | 0 |
| 55 | MG | 1a | 1665 | 1/1 | 0.93 | 0.15 | 49,49,49,49 | 0 |
| 55 | MG | 1A | 4112 | 1/1 | 0.93 | 0.10 | 56,56,56,56 | 0 |
| 55 | MG | 1A | 3159 | 1/1 | 0.93 | 0.21 | 47,47,47,47 | 0 |
| 55 | MG | 1A | 4114 | 1/1 | 0.93 | 0.17 | 53,53,53,53 | 0 |
| 55 | MG | 1A | 4116 | 1/1 | 0.93 | 0.13 | 61,61,61,61 | 0 |
| 55 | MG | 26 | 101 | 1/1 | 0.93 | 0.25 | 52,52,52,52 | 0 |
| 55 | MG | 2A | 3591 | 1/1 | 0.93 | 0.14 | 56,56,56,56 | 0 |
| 55 | MG | 2A | 3593 | 1/1 | 0.93 | 0.12 | 68,68,68,68 | 0 |
| 55 | MG | 1A | 3910 | 1/1 | 0.93 | 0.09 | 41,41,41,41 | 0 |
| 55 | MG | 2a | 3001 | 1/1 | 0.93 | 0.10 | 57,57,57,57 | 0 |
| 55 | MG | 2A | 3015 | 1/1 | 0.93 | 0.24 | 63,63,63,63 | 0 |
| 55 | MG | 2A | 3017 | 1/1 | 0.93 | 0.12 | 46,46,46,46 | 0 |
| 55 | MG | 2A | 3597 | 1/1 | 0.93 | 0.10 | 49,49,49,49 | 0 |
| 55 | MG | 1a | 1672 | 1/1 | 0.93 | 0.12 | 47,47,47,47 | 0 |
| 55 | MG | 1A | 3688 | 1/1 | 0.93 | 0.11 | 52,52,52,52 | 0 |
| 55 | MG | 1a | 1674 | 1/1 | 0.93 | 0.32 | 56,56,56,56 | 0 |
| 55 | MG | 1A | 3695 | 1/1 | 0.93 | 0.09 | 20,20,20,20 | 0 |
| 55 | MG | 2A | 3029 | 1/1 | 0.93 | 0.12 | 27,27,27,27 | 0 |
| 55 | MG | 2A | 3030 | 1/1 | 0.93 | 0.34 | 56,56,56,56 | 0 |
| 55 | MG | 2A | 3033 | 1/1 | 0.93 | 0.28 | 59,59,59,59 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 55 | MG | 2a | 3016 | 1/1 | 0.93 | 0.05 | 46,46,46,46 | 0 |
| 55 | MG | 1A | 3247 | 1/1 | 0.93 | 0.19 | 57,57,57,57 | 0 |
| 55 | MG | 1A | 3444 | 1/1 | 0.93 | 0.16 | 43,43,43,43 | 0 |
| 55 | MG | 2A | 3040 | 1/1 | 0.93 | 0.15 | 59,59,59,59 | 0 |
| 55 | MG | 1A | 3206 | 1/1 | 0.93 | 0.14 | 36,36,36,36 | 0 |
| 55 | MG | 2A | 3042 | 1/1 | 0.93 | 0.08 | 54,54,54,54 | 0 |
| 55 | MG | 1A | 3035 | 1/1 | 0.93 | 0.35 | 36,36,36,36 | 0 |
| 55 | MG | 1A | 3362 | 1/1 | 0.93 | 0.27 | 52,52,52,52 | 0 |
| 55 | MG | 2A | 3616 | 1/1 | 0.93 | 0.17 | 45,45,45,45 | 0 |
| 55 | MG | 1a | 1682 | 1/1 | 0.93 | 0.09 | 45,45,45,45 | 0 |
| 55 | MG | 1A | 3528 | 1/1 | 0.93 | 0.13 | 29,29,29,29 | 0 |
| 55 | MG | 1B | 225 | 1/1 | 0.93 | 0.11 | 46,46,46,46 | 0 |
| 55 | MG | 2A | 3624 | 1/1 | 0.93 | 0.13 | 47,47,47,47 | 0 |
| 55 | MG | 1A | 3251 | 1/1 | 0.93 | 0.08 | 28,28,28,28 | 0 |
| 55 | MG | 2A | 3060 | 1/1 | 0.93 | 0.21 | 38,38,38,38 | 0 |
| 55 | MG | 2A | 3061 | 1/1 | 0.93 | 0.17 | 51,51,51,51 | 0 |
| 55 | MG | 1a | 1688 | 1/1 | 0.93 | 0.09 | 53,53,53,53 | 0 |
| 55 | MG | 1a | 1689 | 1/1 | 0.93 | 0.18 | 42,42,42,42 | 0 |
| 55 | MG | 1A | 3451 | 1/1 | 0.93 | 0.09 | 36,36,36,36 | 0 |
| 55 | MG | 1A | 3296 | 1/1 | 0.93 | 0.13 | 27,27,27,27 | 0 |
| 55 | MG | 1A | 3455 | 1/1 | 0.93 | 0.09 | 48,48,48,48 | 0 |
| 55 | MG | 2A | 3641 | 1/1 | 0.93 | 0.15 | 55,55,55,55 | 0 |
| 55 | MG | 2A | 3643 | 1/1 | 0.93 | 0.08 | 64,64,64,64 | 0 |
| 55 | MG | 1A | 3004 | 1/1 | 0.93 | 0.07 | 23,23,23,23 | 0 |
| 55 | MG | 1B | 233 | 1/1 | 0.93 | 0.15 | 53,53,53,53 | 0 |
| 55 | MG | 1A | 3939 | 1/1 | 0.93 | 0.06 | 49,49,49,49 | 0 |
| 55 | MG | 1D | 301 | 1/1 | 0.93 | 0.46 | 36,36,36,36 | 0 |
| 55 | MG | 2A | 3079 | 1/1 | 0.93 | 0.11 | 35,35,35,35 | 0 |
| 55 | MG | 1A | 3546 | 1/1 | 0.93 | 0.09 | 31,31,31,31 | 0 |
| 55 | MG | 1A | 3460 | 1/1 | 0.93 | 0.14 | 38,38,38,38 | 0 |
| 55 | MG | 1A | 3551 | 1/1 | 0.93 | 0.16 | 31,31,31,31 | 0 |
| 55 | MG | 1A | 3750 | 1/1 | 0.93 | 0.08 | 41,41,41,41 | 0 |
| 55 | MG | 2a | 3055 | 1/1 | 0.93 | 0.15 | 59,59,59,59 | 0 |
| 55 | MG | 1A | 3752 | 1/1 | 0.93 | 0.13 | 23,23,23,23 | 0 |
| 55 | MG | 2A | 3661 | 1/1 | 0.93 | 0.18 | 52,52,52,52 | 0 |
| 55 | MG | 1a | 1713 | 1/1 | 0.93 | 0.17 | 49,49,49,49 | 0 |
| 55 | MG | 1E | 304 | 1/1 | 0.93 | 0.16 | 37,37,37,37 | 0 |
| 55 | MG | 1A | 3461 | 1/1 | 0.93 | 0.21 | 48,48,48,48 | 0 |
| 55 | MG | 2a | 3062 | 1/1 | 0.93 | 0.07 | 50,50,50,50 | 0 |
| 55 | MG | 1A | 3962 | 1/1 | 0.93 | 0.15 | 51,51,51,51 | 0 |
| 55 | MG | 1A | 3963 | 1/1 | 0.93 | 0.24 | 42,42,42,42 | 0 |
| 55 | MG | 1A | 3462 | 1/1 | 0.93 | 0.12 | 57,57,57,57 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 55 | MG | 1A | 3765 | 1/1 | 0.93 | 0.08 | 34,34,34,34 | 0 |
| 55 | MG | 1A | 3766 | 1/1 | 0.93 | 0.24 | 64,64,64,64 | 0 |
| 55 | MG | 1A | 3254 | 1/1 | 0.93 | 0.30 | 58,58,58,58 | 0 |
| 55 | MG | 2A | 3103 | 1/1 | 0.93 | 0.06 | 30,30,30,30 | 0 |
| 55 | MG | 2a | 3072 | 1/1 | 0.93 | 0.12 | 62,62,62,62 | 0 |
| 55 | MG | 2a | 3073 | 1/1 | 0.93 | 0.24 | 61,61,61,61 | 0 |
| 55 | MG | 1A | 3132 | 1/1 | 0.93 | 0.17 | 40,40,40,40 | 0 |
| 55 | MG | 2A | 3356 | 1/1 | 0.93 | 0.08 | 37,37,37,37 | 0 |
| 55 | MG | 1a | 1725 | 1/1 | 0.93 | 0.20 | 48,48,48,48 | 0 |
| 55 | MG | 2a | 3077 | 1/1 | 0.93 | 0.22 | 39,39,39,39 | 0 |
| 55 | MG | 1A | 3981 | 1/1 | 0.93 | 0.08 | 59,59,59,59 | 0 |
| 55 | MG | 1A | 3213 | 1/1 | 0.93 | 0.21 | 50,50,50,50 | 0 |
| 55 | MG | 2A | 3112 | 1/1 | 0.93 | 0.10 | 89,89,89,89 | 0 |
| 55 | MG | 1a | 1729 | 1/1 | 0.93 | 0.18 | 54,54,54,54 | 0 |
| 55 | MG | 2a | 3085 | 1/1 | 0.93 | 0.24 | 64,64,64,64 | 0 |
| 55 | MG | 2A | 3691 | 1/1 | 0.93 | 0.14 | 57,57,57,57 | 0 |
| 55 | MG | 1A | 3307 | 1/1 | 0.93 | 0.22 | 43,43,43,43 | 0 |
| 55 | MG | 1O | 204 | 1/1 | 0.93 | 0.17 | 60,60,60,60 | 0 |
| 55 | MG | 2A | 3701 | 1/1 | 0.93 | 0.14 | 49,49,49,49 | 0 |
| 55 | MG | 2A | 3366 | 1/1 | 0.93 | 0.19 | 49,49,49,49 | 0 |
| 55 | MG | 1A | 3987 | 1/1 | 0.93 | 0.13 | 32,32,32,32 | 0 |
| 55 | MG | 2A | 3123 | 1/1 | 0.93 | 0.15 | 39,39,39,39 | 0 |
| 55 | MG | 2A | 3127 | 1/1 | 0.93 | 0.18 | 44,44,44,44 | 0 |
| 55 | MG | 1Q | 202 | 1/1 | 0.93 | 0.07 | 35,35,35,35 | 0 |
| 55 | MG | 2a | 3095 | 1/1 | 0.93 | 0.20 | 46,46,46,46 | 0 |
| 55 | MG | 2A | 3373 | 1/1 | 0.93 | 0.22 | 64,64,64,64 | 0 |
| 55 | MG | 1A | 3777 | 1/1 | 0.93 | 0.07 | 51,51,51,51 | 0 |
| 55 | MG | 1A | 3469 | 1/1 | 0.93 | 0.29 | 49,49,49,49 | 0 |
| 55 | MG | 2A | 3132 | 1/1 | 0.93 | 0.18 | 52,52,52,52 | 0 |
| 55 | MG | 1a | 1743 | 1/1 | 0.93 | 0.25 | 62,62,62,62 | 0 |
| 55 | MG | 1R | 201 | 1/1 | 0.93 | 0.35 | 44,44,44,44 | 0 |
| 55 | MG | 2A | 3379 | 1/1 | 0.93 | 0.06 | 45,45,45,45 | 0 |
| 55 | MG | 1A | 3089 | 1/1 | 0.93 | 0.11 | 42,42,42,42 | 0 |
| 55 | MG | 1a | 1746 | 1/1 | 0.93 | 0.28 | 52,52,52,52 | 0 |
| 55 | MG | 2a | 3109 | 1/1 | 0.93 | 0.07 | 75,75,75,75 | 0 |
| 55 | MG | 1a | 1747 | 1/1 | 0.93 | 0.30 | 50,50,50,50 | 0 |
| 55 | MG | 2A | 3726 | 1/1 | 0.93 | 0.12 | 51,51,51,51 | 0 |
| 55 | MG | 1A | 3586 | 1/1 | 0.93 | 0.11 | 44,44,44,44 | 0 |
| 55 | MG | 2a | 3113 | 1/1 | 0.93 | 0.13 | 50,50,50,50 | 0 |
| 55 | MG | 2A | 3386 | 1/1 | 0.93 | 0.15 | 53,53,53,53 | 0 |
| 55 | MG | 2A | 3389 | 1/1 | 0.93 | 0.23 | 47,47,47,47 | 0 |
| 55 | MG | 1A | 3309 | 1/1 | 0.93 | 0.16 | 40,40,40,40 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 55 | MG | 1A | 3997 | 1/1 | 0.93 | 0.08 | 56,56,56,56 | 0 |
| 55 | MG | 2A | 3396 | 1/1 | 0.93 | 0.25 | 47,47,47,47 | 0 |
| 55 | MG | 2A | 3398 | 1/1 | 0.93 | 0.22 | 33,33,33,33 | 0 |
| 55 | MG | 2a | 3126 | 1/1 | 0.93 | 0.27 | 62,62,62,62 | 0 |
| 55 | MG | 2A | 3739 | 1/1 | 0.93 | 0.18 | 43,43,43,43 | 0 |
| 55 | MG | 1A | 3472 | 1/1 | 0.93 | 0.26 | 54,54,54,54 | 0 |
| 55 | MG | 1A | 3092 | 1/1 | 0.93 | 0.20 | 32,32,32,32 | 0 |
| 55 | MG | 1A | 4000 | 1/1 | 0.93 | 0.13 | 60,60,60,60 | 0 |
| 55 | MG | 1W | 202 | 1/1 | 0.93 | 0.10 | 44,44,44,44 | 0 |
| 55 | MG | 2A | 3410 | 1/1 | 0.93 | 0.18 | 35,35,35,35 | 0 |
| 55 | MG | 2A | 3747 | 1/1 | 0.93 | 0.10 | 56,56,56,56 | 0 |
| 55 | MG | 2A | 3411 | 1/1 | 0.93 | 0.25 | 51,51,51,51 | 0 |
| 55 | MG | 2A | 3154 | 1/1 | 0.93 | 0.11 | 38,38,38,38 | 0 |
| 55 | MG | 2A | 3413 | 1/1 | 0.93 | 0.36 | 42,42,42,42 | 0 |
| 55 | MG | 2A | 3155 | 1/1 | 0.93 | 0.10 | 47,47,47,47 | 0 |
| 55 | MG | 2A | 3417 | 1/1 | 0.93 | 0.10 | 50,50,50,50 | 0 |
| 55 | MG | 1a | 1762 | 1/1 | 0.93 | 0.20 | 54,54,54,54 | 0 |
| 55 | MG | 1X | 103 | 1/1 | 0.93 | 0.13 | 37,37,37,37 | 0 |
| 55 | MG | 1A | 3479 | 1/1 | 0.93 | 0.12 | 33,33,33,33 | 0 |
| 55 | MG | 2A | 3160 | 1/1 | 0.93 | 0.13 | 30,30,30,30 | 0 |
| 55 | MG | 1A | 4007 | 1/1 | 0.93 | 0.12 | 25,25,25,25 | 0 |
| 55 | MG | 1Y | 204 | 1/1 | 0.93 | 0.24 | 49,49,49,49 | 0 |
| 55 | MG | 1A | 3480 | 1/1 | 0.93 | 0.12 | 42,42,42,42 | 0 |
| 55 | MG | 11 | 103 | 1/1 | 0.93 | 0.08 | 35,35,35,35 | 0 |
| 55 | MG | 1a | 1772 | 1/1 | 0.93 | 0.08 | 64,64,64,64 | 0 |
| 55 | MG | 2a | 3151 | 1/1 | 0.93 | 0.13 | 69,69,69,69 | 0 |
| 55 | MG | 1A | 3313 | 1/1 | 0.93 | 0.14 | 44,44,44,44 | 0 |
| 55 | MG | 1a | 1774 | 1/1 | 0.93 | 0.16 | 34,34,34,34 | 0 |
| 55 | MG | 12 | 102 | 1/1 | 0.93 | 0.15 | 43,43,43,43 | 0 |
| 55 | MG | 1A | 3814 | 1/1 | 0.93 | 0.09 | 41,41,41,41 | 0 |
| 55 | MG | 1A | 3600 | 1/1 | 0.93 | 0.15 | 40,40,40,40 | 0 |
| 55 | MG | 1A | 3314 | 1/1 | 0.93 | 0.06 | 27,27,27,27 | 0 |
| 55 | MG | 2A | 3782 | 1/1 | 0.93 | 0.20 | 77,77,77,77 | 0 |
| 55 | MG | 1A | 3399 | 1/1 | 0.93 | 0.17 | 32,32,32,32 | 0 |
| 55 | MG | 17 | 102 | 1/1 | 0.93 | 0.14 | 39,39,39,39 | 0 |
| 55 | MG | 1a | 1788 | 1/1 | 0.93 | 0.20 | 66,66,66,66 | 0 |
| 55 | MG | 2a | 3172 | 1/1 | 0.93 | 0.16 | 56,56,56,56 | 0 |
| 55 | MG | 2A | 3452 | 1/1 | 0.93 | 0.50 | 46,46,46,46 | 0 |
| 55 | MG | 2A | 3791 | 1/1 | 0.93 | 0.20 | 46,46,46,46 | 0 |
| 55 | MG | 1A | 3827 | 1/1 | 0.93 | 0.13 | 42,42,42,42 | 0 |
| 55 | MG | 2A | 3795 | 1/1 | 0.93 | 0.08 | 42,42,42,42 | 0 |
| 55 | MG | 2A | 3796 | 1/1 | 0.93 | 0.13 | 61,61,61,61 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 55 | MG | 18 | 104 | 1/1 | 0.93 | 0.11 | 40,40,40,40 | 0 |
| 55 | MG | 2A | 3800 | 1/1 | 0.93 | 0.10 | 52,52,52,52 | 0 |
| 55 | MG | 2A | 3456 | 1/1 | 0.93 | 0.07 | 54,54,54,54 | 0 |
| 55 | MG | 1A | 3400 | 1/1 | 0.93 | 0.09 | 40,40,40,40 | 0 |
| 55 | MG | 1A | 3318 | 1/1 | 0.93 | 0.26 | 51,51,51,51 | 0 |
| 55 | MG | 1A | 3409 | 1/1 | 0.93 | 0.08 | 54,54,54,54 | 0 |
| 55 | MG | 1A | 3177 | 1/1 | 0.93 | 0.13 | 41,41,41,41 | 0 |
| 55 | MG | 2a | 3189 | 1/1 | 0.93 | 0.21 | 62,62,62,62 | 0 |
| 55 | MG | 1A | 3612 | 1/1 | 0.93 | 0.28 | 61,61,61,61 | 0 |
| 55 | MG | 2A | 3819 | 1/1 | 0.93 | 0.15 | 33,33,33,33 | 0 |
| 55 | MG | 1a | 1605 | 1/1 | 0.93 | 0.19 | 60,60,60,60 | 0 |
| 55 | MG | 1A | 3320 | 1/1 | 0.93 | 0.21 | 45,45,45,45 | 0 |
| 55 | MG | 2a | 3194 | 1/1 | 0.93 | 0.18 | 61,61,61,61 | 0 |
| 55 | MG | 1A | 3321 | 1/1 | 0.93 | 0.17 | 47,47,47,47 | 0 |
| 55 | MG | 1A | 3416 | 1/1 | 0.93 | 0.30 | 49,49,49,49 | 0 |
| 55 | MG | 2A | 3469 | 1/1 | 0.93 | 0.16 | 48,48,48,48 | 0 |
| 55 | MG | 1A | 3621 | 1/1 | 0.93 | 0.12 | 26,26,26,26 | 0 |
| 55 | MG | 2A | 3473 | 1/1 | 0.93 | 0.23 | 23,23,23,23 | 0 |
| 55 | MG | 1A | 3263 | 1/1 | 0.93 | 0.16 | 38,38,38,38 | 0 |
| 55 | MG | 1A | 3625 | 1/1 | 0.93 | 0.23 | 50,50,50,50 | 0 |
| 55 | MG | 2A | 3203 | 1/1 | 0.93 | 0.34 | 45,45,45,45 | 0 |
| 55 | MG | 2A | 3204 | 1/1 | 0.93 | 0.21 | 49,49,49,49 | 0 |
| 55 | MG | 2A | 3483 | 1/1 | 0.93 | 0.18 | 34,34,34,34 | 0 |
| 55 | MG | 1A | 3626 | 1/1 | 0.93 | 0.12 | 53,53,53,53 | 0 |
| 55 | MG | 1a | 1616 | 1/1 | 0.93 | 0.13 | 51,51,51,51 | 0 |
| 55 | MG | 1A | 3179 | 1/1 | 0.93 | 0.17 | 42,42,42,42 | 0 |
| 55 | MG | 1A | 3630 | 1/1 | 0.93 | 0.22 | 30,30,30,30 | 0 |
| 55 | MG | 1a | 1816 | 1/1 | 0.93 | 0.16 | 48,48,48,48 | 0 |
| 55 | MG | 1a | 1620 | 1/1 | 0.93 | 0.13 | 46,46,46,46 | 0 |
| 55 | MG | 1A | 3631 | 1/1 | 0.93 | 0.21 | 16,16,16,16 | 0 |
| 55 | MG | 2A | 3223 | 1/1 | 0.93 | 0.10 | 52,52,52,52 | 0 |
| 55 | MG | 2A | 3224 | 1/1 | 0.93 | 0.13 | 45,45,45,45 | 0 |
| 55 | MG | 1A | 3632 | 1/1 | 0.93 | 0.14 | 35,35,35,35 | 0 |
| 55 | MG | 1A | 3869 | 1/1 | 0.93 | 0.10 | 60,60,60,60 | 0 |
| 55 | MG | 2A | 3501 | 1/1 | 0.93 | 0.17 | 58,58,58,58 | 0 |
| 55 | MG | 1A | 3633 | 1/1 | 0.93 | 0.09 | 54,54,54,54 | 0 |
| 55 | MG | 1A | 3501 | 1/1 | 0.93 | 0.11 | 46,46,46,46 | 0 |
| 55 | MG | 2B | 203 | 1/1 | 0.93 | 0.10 | 40,40,40,40 | 0 |
| 55 | MG | 1A | 4069 | 1/1 | 0.93 | 0.10 | 34,34,34,34 | 0 |
| 55 | MG | 2A | 3512 | 1/1 | 0.93 | 0.19 | 53,53,53,53 | 0 |
| 55 | MG | 1a | 1632 | 1/1 | 0.93 | 0.17 | 50,50,50,50 | 0 |
| 55 | MG | 1a | 1633 | 1/1 | 0.93 | 0.26 | 48,48,48,48 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 55 | MG | 1A | 4071 | 1/1 | 0.93 | 0.08 | 20,20,20,20 | 0 |
| 55 | MG | 2A | 3842 | 1/1 | 0.94 | 0.13 | 48,48,48,48 | 0 |
| 55 | MG | 1A | 3608 | 1/1 | 0.94 | 0.19 | 23,23,23,23 | 0 |
| 55 | MG | 1A | 3823 | 1/1 | 0.94 | 0.12 | 17,17,17,17 | 0 |
| 55 | MG | 1a | 1811 | 1/1 | 0.94 | 0.14 | 73,73,73,73 | 0 |
| 55 | MG | 1A | 3072 | 1/1 | 0.94 | 0.10 | 17,17,17,17 | 0 |
| 55 | MG | 2A | 3850 | 1/1 | 0.94 | 0.09 | 51,51,51,51 | 0 |
| 55 | MG | 2A | 3851 | 1/1 | 0.94 | 0.17 | 49,49,49,49 | 0 |
| 55 | MG | 1A | 3390 | 1/1 | 0.94 | 0.29 | 34,34,34,34 | 0 |
| 55 | MG | 1A | 4030 | 1/1 | 0.94 | 0.05 | 21,21,21,21 | 0 |
| 55 | MG | 1A | 4032 | 1/1 | 0.94 | 0.07 | 39,39,39,39 | 0 |
| 55 | MG | 2A | 3482 | 1/1 | 0.94 | 0.25 | 51,51,51,51 | 0 |
| 55 | MG | 1A | 3831 | 1/1 | 0.94 | 0.12 | 31,31,31,31 | 0 |
| 55 | MG | 1A | 3832 | 1/1 | 0.94 | 0.30 | 32,32,32,32 | 0 |
| 55 | MG | 2A | 3209 | 1/1 | 0.94 | 0.09 | 45,45,45,45 | 0 |
| 55 | MG | 2A | 3212 | 1/1 | 0.94 | 0.08 | 42,42,42,42 | 0 |
| 55 | MG | 2A | 3487 | 1/1 | 0.94 | 0.36 | 49,49,49,49 | 0 |
| 55 | MG | 1a | 1622 | 1/1 | 0.94 | 0.15 | 44,44,44,44 | 0 |
| 55 | MG | 2A | 3217 | 1/1 | 0.94 | 0.07 | 35,35,35,35 | 0 |
| 55 | MG | 1a | 1623 | 1/1 | 0.94 | 0.08 | 50,50,50,50 | 0 |
| 55 | MG | 1A | 3393 | 1/1 | 0.94 | 0.06 | 43,43,43,43 | 0 |
| 55 | MG | 1A | 3613 | 1/1 | 0.94 | 0.08 | 32,32,32,32 | 0 |
| 55 | MG | 2A | 3495 | 1/1 | 0.94 | 0.16 | 43,43,43,43 | 0 |
| 55 | MG | 1A | 3838 | 1/1 | 0.94 | 0.12 | 40,40,40,40 | 0 |
| 55 | MG | 1A | 3104 | 1/1 | 0.94 | 0.12 | 31,31,31,31 | 0 |
| 55 | MG | 1a | 1629 | 1/1 | 0.94 | 0.17 | 51,51,51,51 | 0 |
| 55 | MG | 1A | 4047 | 1/1 | 0.94 | 0.10 | 56,56,56,56 | 0 |
| 55 | MG | 2A | 3503 | 1/1 | 0.94 | 0.12 | 39,39,39,39 | 0 |
| 55 | MG | 1A | 3136 | 1/1 | 0.94 | 0.08 | 44,44,44,44 | 0 |
| 55 | MG | 1A | 3843 | 1/1 | 0.94 | 0.07 | 44,44,44,44 | 0 |
| 55 | MG | 1A | 3077 | 1/1 | 0.94 | 0.09 | 30,30,30,30 | 0 |
| 55 | MG | 1A | 3845 | 1/1 | 0.94 | 0.11 | 29,29,29,29 | 0 |
| 55 | MG | 1A | 3311 | 1/1 | 0.94 | 0.07 | 28,28,28,28 | 0 |
| 55 | MG | 2A | 3515 | 1/1 | 0.94 | 0.15 | 57,57,57,57 | 0 |
| 55 | MG | 1A | 3848 | 1/1 | 0.94 | 0.09 | 37,37,37,37 | 0 |
| 55 | MG | 2A | 3233 | 1/1 | 0.94 | 0.08 | 54,54,54,54 | 0 |
| 55 | MG | 1A | 4065 | 1/1 | 0.94 | 0.14 | 26,26,26,26 | 0 |
| 55 | MG | 1f | 202 | 1/1 | 0.94 | 0.07 | 48,48,48,48 | 0 |
| 55 | MG | 1A | 4066 | 1/1 | 0.94 | 0.11 | 29,29,29,29 | 0 |
| 55 | MG | 1A | 3622 | 1/1 | 0.94 | 0.13 | 37,37,37,37 | 0 |
| 55 | MG | 2A | 3525 | 1/1 | 0.94 | 0.10 | 42,42,42,42 | 0 |
| 55 | MG | 2A | 3526 | 1/1 | 0.94 | 0.12 | 60,60,60,60 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 55 | MG | 2A | 3239 | 1/1 | 0.94 | 0.13 | 49,49,49,49 | 0 |
| 55 | MG | 1A | 3623 | 1/1 | 0.94 | 0.11 | 38,38,38,38 | 0 |
| 55 | MG | 1A | 3312 | 1/1 | 0.94 | 0.12 | 38,38,38,38 | 0 |
| 55 | MG | 1A | 3188 | 1/1 | 0.94 | 0.17 | 46,46,46,46 | 0 |
| 55 | MG | 2A | 3245 | 1/1 | 0.94 | 0.09 | 64,64,64,64 | 0 |
| 55 | MG | 1a | 1646 | 1/1 | 0.94 | 0.12 | 37,37,37,37 | 0 |
| 55 | MG | 1A | 3011 | 1/1 | 0.94 | 0.15 | 39,39,39,39 | 0 |
| 55 | MG | 1A | 4080 | 1/1 | 0.94 | 0.17 | 40,40,40,40 | 0 |
| 55 | MG | 2A | 3542 | 1/1 | 0.94 | 0.23 | 45,45,45,45 | 0 |
| 55 | MG | 1a | 1652 | 1/1 | 0.94 | 0.19 | 51,51,51,51 | 0 |
| 55 | MG | 2A | 3544 | 1/1 | 0.94 | 0.10 | 41,41,41,41 | 0 |
| 55 | MG | 1x | 103 | 1/1 | 0.94 | 0.25 | 67,67,67,67 | 0 |
| 55 | MG | 1A | 3316 | 1/1 | 0.94 | 0.18 | 42,42,42,42 | 0 |
| 55 | MG | 1A | 3140 | 1/1 | 0.94 | 0.16 | 36,36,36,36 | 0 |
| 55 | MG | 1A | 4083 | 1/1 | 0.94 | 0.06 | 26,26,26,26 | 0 |
| 55 | MG | 1x | 108 | 1/1 | 0.94 | 0.06 | 55,55,55,55 | 0 |
| 55 | MG | 1A | 3198 | 1/1 | 0.94 | 0.09 | 38,38,38,38 | 0 |
| 55 | MG | 2A | 3262 | 1/1 | 0.94 | 0.21 | 41,41,41,41 | 0 |
| 55 | MG | 1A | 3202 | 1/1 | 0.94 | 0.08 | 38,38,38,38 | 0 |
| 55 | MG | 1A | 3112 | 1/1 | 0.94 | 0.10 | 38,38,38,38 | 0 |
| 55 | MG | 1A | 3865 | 1/1 | 0.94 | 0.05 | 45,45,45,45 | 0 |
| 55 | MG | 1A | 3083 | 1/1 | 0.94 | 0.14 | 41,41,41,41 | 0 |
| 55 | MG | 1A | 3422 | 1/1 | 0.94 | 0.16 | 41,41,41,41 | 0 |
| 55 | MG | 2A | 3565 | 1/1 | 0.94 | 0.13 | 44,44,44,44 | 0 |
| 55 | MG | 2A | 3566 | 1/1 | 0.94 | 0.17 | 48,48,48,48 | 0 |
| 55 | MG | 1A | 3871 | 1/1 | 0.94 | 0.06 | 32,32,32,32 | 0 |
| 55 | MG | 1A | 3515 | 1/1 | 0.94 | 0.13 | 55,55,55,55 | 0 |
| 55 | MG | 2a | 3002 | 1/1 | 0.94 | 0.14 | 60,60,60,60 | 0 |
| 55 | MG | 1A | 3645 | 1/1 | 0.94 | 0.08 | 50,50,50,50 | 0 |
| 55 | MG | 1A | 3874 | 1/1 | 0.94 | 0.10 | 50,50,50,50 | 0 |
| 55 | MG | 2A | 3011 | 1/1 | 0.94 | 0.10 | 50,50,50,50 | 0 |
| 55 | MG | 2A | 3574 | 1/1 | 0.94 | 0.17 | 48,48,48,48 | 0 |
| 55 | MG | 1A | 3324 | 1/1 | 0.94 | 0.24 | 43,43,43,43 | 0 |
| 55 | MG | 1A | 3650 | 1/1 | 0.94 | 0.11 | 12,12,12,12 | 0 |
| 55 | MG | 1a | 1669 | 1/1 | 0.94 | 0.12 | 54,54,54,54 | 0 |
| 55 | MG | 2A | 3278 | 1/1 | 0.94 | 0.16 | 76,76,76,76 | 0 |
| 55 | MG | 1A | 3147 | 1/1 | 0.94 | 0.07 | 32,32,32,32 | 0 |
| 55 | MG | 2A | 3587 | 1/1 | 0.94 | 0.10 | 39,39,39,39 | 0 |
| 55 | MG | 2A | 3281 | 1/1 | 0.94 | 0.05 | 42,42,42,42 | 0 |
| 55 | MG | 2A | 3590 | 1/1 | 0.94 | 0.08 | 53,53,53,53 | 0 |
| 55 | MG | 2A | 3019 | 1/1 | 0.94 | 0.13 | 53,53,53,53 | 0 |
| 55 | MG | 1A | 3053 | 1/1 | 0.94 | 0.24 | 33,33,33,33 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 55 | MG | 2A | 3284 | 1/1 | 0.94 | 0.23 | 50,50,50,50 | 0 |
| 55 | MG | 1A | 3331 | 1/1 | 0.94 | 0.08 | 41,41,41,41 | 0 |
| 55 | MG | 2A | 3286 | 1/1 | 0.94 | 0.19 | 60,60,60,60 | 0 |
| 55 | MG | 2A | 3022 | 1/1 | 0.94 | 0.10 | 54,54,54,54 | 0 |
| 55 | MG | 1A | 3040 | 1/1 | 0.94 | 0.24 | 35,35,35,35 | 0 |
| 55 | MG | 1A | 4115 | 1/1 | 0.94 | 0.13 | 59,59,59,59 | 0 |
| 55 | MG | 2A | 3600 | 1/1 | 0.94 | 0.12 | 50,50,50,50 | 0 |
| 55 | MG | 1A | 3521 | 1/1 | 0.94 | 0.11 | 40,40,40,40 | 0 |
| 55 | MG | 1A | 3267 | 1/1 | 0.94 | 0.09 | 33,33,33,33 | 0 |
| 55 | MG | 2A | 3604 | 1/1 | 0.94 | 0.09 | 31,31,31,31 | 0 |
| 55 | MG | 2A | 3031 | 1/1 | 0.94 | 0.25 | 45,45,45,45 | 0 |
| 55 | MG | 1A | 3157 | 1/1 | 0.94 | 0.14 | 26,26,26,26 | 0 |
| 55 | MG | 1A | 3672 | 1/1 | 0.94 | 0.11 | 37,37,37,37 | 0 |
| 55 | MG | 2a | 3033 | 1/1 | 0.94 | 0.31 | 60,60,60,60 | 0 |
| 55 | MG | 2A | 3037 | 1/1 | 0.94 | 0.15 | 35,35,35,35 | 0 |
| 55 | MG | 2A | 3038 | 1/1 | 0.94 | 0.18 | 44,44,44,44 | 0 |
| 55 | MG | 1A | 3674 | 1/1 | 0.94 | 0.11 | 14,14,14,14 | 0 |
| 55 | MG | 2a | 3038 | 1/1 | 0.94 | 0.12 | 45,45,45,45 | 0 |
| 55 | MG | 1A | 3216 | 1/1 | 0.94 | 0.08 | 37,37,37,37 | 0 |
| 55 | MG | 1A | 3676 | 1/1 | 0.94 | 0.12 | 55,55,55,55 | 0 |
| 55 | MG | 2a | 3042 | 1/1 | 0.94 | 0.20 | 54,54,54,54 | 0 |
| 55 | MG | 1A | 3677 | 1/1 | 0.94 | 0.11 | 57,57,57,57 | 0 |
| 55 | MG | 2A | 3304 | 1/1 | 0.94 | 0.21 | 51,51,51,51 | 0 |
| 55 | MG | 2A | 3305 | 1/1 | 0.94 | 0.12 | 53,53,53,53 | 0 |
| 55 | MG | 2A | 3307 | 1/1 | 0.94 | 0.08 | 47,47,47,47 | 0 |
| 55 | MG | 1A | 3340 | 1/1 | 0.94 | 0.10 | 35,35,35,35 | 0 |
| 55 | MG | 1A | 3526 | 1/1 | 0.94 | 0.12 | 43,43,43,43 | 0 |
| 55 | MG | 2A | 3622 | 1/1 | 0.94 | 0.15 | 61,61,61,61 | 0 |
| 55 | MG | 1A | 3341 | 1/1 | 0.94 | 0.10 | 33,33,33,33 | 0 |
| 55 | MG | 1A | 3908 | 1/1 | 0.94 | 0.12 | 40,40,40,40 | 0 |
| 55 | MG | 2A | 3314 | 1/1 | 0.94 | 0.08 | 50,50,50,50 | 0 |
| 55 | MG | 1a | 1691 | 1/1 | 0.94 | 0.17 | 46,46,46,46 | 0 |
| 55 | MG | 2A | 3629 | 1/1 | 0.94 | 0.18 | 36,36,36,36 | 0 |
| 55 | MG | 2A | 3316 | 1/1 | 0.94 | 0.26 | 48,48,48,48 | 0 |
| 55 | MG | 1B | 228 | 1/1 | 0.94 | 0.14 | 37,37,37,37 | 0 |
| 55 | MG | 1A | 3681 | 1/1 | 0.94 | 0.07 | 34,34,34,34 | 0 |
| 55 | MG | 2A | 3635 | 1/1 | 0.94 | 0.08 | 42,42,42,42 | 0 |
| 55 | MG | 1a | 1694 | 1/1 | 0.94 | 0.05 | 53,53,53,53 | 0 |
| 55 | MG | 1a | 1695 | 1/1 | 0.94 | 0.13 | 39,39,39,39 | 0 |
| 55 | MG | 1A | 3911 | 1/1 | 0.94 | 0.11 | 17,17,17,17 | 0 |
| 55 | MG | 2a | 3065 | 1/1 | 0.94 | 0.22 | 60,60,60,60 | 0 |
| 55 | MG | 1A | 3217 | 1/1 | 0.94 | 0.13 | 40,40,40,40 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 55 | MG | 2A | 3644 | 1/1 | 0.94 | 0.17 | 68,68,68,68 | 0 |
| 55 | MG | 1A | 3686 | 1/1 | 0.94 | 0.07 | 33,33,33,33 | 0 |
| 55 | MG | 1A | 3687 | 1/1 | 0.94 | 0.07 | 35,35,35,35 | 0 |
| 55 | MG | 1A | 3439 | 1/1 | 0.94 | 0.09 | 37,37,37,37 | 0 |
| 55 | MG | 1A | 3918 | 1/1 | 0.94 | 0.09 | 38,38,38,38 | 0 |
| 55 | MG | 2A | 3074 | 1/1 | 0.94 | 0.19 | 43,43,43,43 | 0 |
| 55 | MG | 1a | 1705 | 1/1 | 0.94 | 0.11 | 57,57,57,57 | 0 |
| 55 | MG | 1a | 1706 | 1/1 | 0.94 | 0.24 | 54,54,54,54 | 0 |
| 55 | MG | 1A | 3531 | 1/1 | 0.94 | 0.24 | 49,49,49,49 | 0 |
| 55 | MG | 1A | 3920 | 1/1 | 0.94 | 0.07 | 56,56,56,56 | 0 |
| 55 | MG | 2a | 3078 | 1/1 | 0.94 | 0.28 | 53,53,53,53 | 0 |
| 55 | MG | 1D | 311 | 1/1 | 0.94 | 0.28 | 30,30,30,30 | 0 |
| 55 | MG | 2a | 3080 | 1/1 | 0.94 | 0.18 | 51,51,51,51 | 0 |
| 55 | MG | 2A | 3340 | 1/1 | 0.94 | 0.10 | 61,61,61,61 | 0 |
| 55 | MG | 1A | 3921 | 1/1 | 0.94 | 0.07 | 45,45,45,45 | 0 |
| 55 | MG | 1A | 3121 | 1/1 | 0.94 | 0.15 | 29,29,29,29 | 0 |
| 55 | MG | 1A | 3925 | 1/1 | 0.94 | 0.18 | 49,49,49,49 | 0 |
| 55 | MG | 1A | 3122 | 1/1 | 0.94 | 0.19 | 34,34,34,34 | 0 |
| 55 | MG | 2A | 3345 | 1/1 | 0.94 | 0.12 | 49,49,49,49 | 0 |
| 55 | MG | 1A | 3714 | 1/1 | 0.94 | 0.08 | 30,30,30,30 | 0 |
| 55 | MG | 1A | 3538 | 1/1 | 0.94 | 0.07 | 44,44,44,44 | 0 |
| 55 | MG | 1A | 3716 | 1/1 | 0.94 | 0.13 | 30,30,30,30 | 0 |
| 55 | MG | 1A | 3123 | 1/1 | 0.94 | 0.09 | 35,35,35,35 | 0 |
| 55 | MG | 1F | 311 | 1/1 | 0.94 | 0.15 | 27,27,27,27 | 0 |
| 55 | MG | 1A | 3041 | 1/1 | 0.94 | 0.14 | 45,45,45,45 | 0 |
| 55 | MG | 2A | 3096 | 1/1 | 0.94 | 0.20 | 47,47,47,47 | 0 |
| 55 | MG | 1A | 3725 | 1/1 | 0.94 | 0.07 | 25,25,25,25 | 0 |
| 55 | MG | 1A | 3731 | 1/1 | 0.94 | 0.08 | 31,31,31,31 | 0 |
| 55 | MG | 1A | 3733 | 1/1 | 0.94 | 0.16 | 20,20,20,20 | 0 |
| 55 | MG | 2A | 3358 | 1/1 | 0.94 | 0.15 | 37,37,37,37 | 0 |
| 55 | MG | 1A | 3542 | 1/1 | 0.94 | 0.36 | 35,35,35,35 | 0 |
| 55 | MG | 1a | 1728 | 1/1 | 0.94 | 0.13 | 50,50,50,50 | 0 |
| 55 | MG | 2A | 3693 | 1/1 | 0.94 | 0.08 | 44,44,44,44 | 0 |
| 55 | MG | 2A | 3696 | 1/1 | 0.94 | 0.10 | 36,36,36,36 | 0 |
| 55 | MG | 1A | 3354 | 1/1 | 0.94 | 0.12 | 48,48,48,48 | 0 |
| 55 | MG | 1A | 3548 | 1/1 | 0.94 | 0.28 | 42,42,42,42 | 0 |
| 55 | MG | 1A | 3355 | 1/1 | 0.94 | 0.10 | 45,45,45,45 | 0 |
| 55 | MG | 2A | 3703 | 1/1 | 0.94 | 0.11 | 55,55,55,55 | 0 |
| 55 | MG | 1a | 1734 | 1/1 | 0.94 | 0.22 | 43,43,43,43 | 0 |
| 55 | MG | 1A | 3550 | 1/1 | 0.94 | 0.21 | 41,41,41,41 | 0 |
| 55 | MG | 2A | 3367 | 1/1 | 0.94 | 0.20 | 41,41,41,41 | 0 |
| 55 | MG | 2a | 3114 | 1/1 | 0.94 | 0.26 | 56,56,56,56 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 55 | MG | 2a | 3115 | 1/1 | 0.94 | 0.38 | 57,57,57,57 | 0 |
| 55 | MG | 1A | 3952 | 1/1 | 0.94 | 0.10 | 45,45,45,45 | 0 |
| 55 | MG | 2A | 3117 | 1/1 | 0.94 | 0.19 | 38,38,38,38 | 0 |
| 55 | MG | 2a | 3118 | 1/1 | 0.94 | 0.17 | 45,45,45,45 | 0 |
| 55 | MG | 2A | 3712 | 1/1 | 0.94 | 0.12 | 61,61,61,61 | 0 |
| 55 | MG | 1A | 3287 | 1/1 | 0.94 | 0.13 | 51,51,51,51 | 0 |
| 55 | MG | 2A | 3120 | 1/1 | 0.94 | 0.16 | 55,55,55,55 | 0 |
| 55 | MG | 1A | 3360 | 1/1 | 0.94 | 0.11 | 41,41,41,41 | 0 |
| 55 | MG | 2A | 3124 | 1/1 | 0.94 | 0.20 | 55,55,55,55 | 0 |
| 55 | MG | 1A | 3560 | 1/1 | 0.94 | 0.07 | 41,41,41,41 | 0 |
| 55 | MG | 1A | 3456 | 1/1 | 0.94 | 0.15 | 32,32,32,32 | 0 |
| 55 | MG | 1A | 3969 | 1/1 | 0.94 | 0.10 | 45,45,45,45 | 0 |
| 55 | MG | 1A | 3042 | 1/1 | 0.94 | 0.10 | 25,25,25,25 | 0 |
| 55 | MG | 1A | 3232 | 1/1 | 0.94 | 0.15 | 23,23,23,23 | 0 |
| 55 | MG | 1A | 3755 | 1/1 | 0.94 | 0.15 | 55,55,55,55 | 0 |
| 55 | MG | 1A | 3979 | 1/1 | 0.94 | 0.07 | 52,52,52,52 | 0 |
| 55 | MG | 2A | 3727 | 1/1 | 0.94 | 0.07 | 66,66,66,66 | 0 |
| 55 | MG | 2A | 3138 | 1/1 | 0.94 | 0.21 | 52,52,52,52 | 0 |
| 55 | MG | 2A | 3139 | 1/1 | 0.94 | 0.16 | 59,59,59,59 | 0 |
| 55 | MG | 1A | 3756 | 1/1 | 0.94 | 0.07 | 49,49,49,49 | 0 |
| 55 | MG | 2A | 3388 | 1/1 | 0.94 | 0.14 | 42,42,42,42 | 0 |
| 55 | MG | 1A | 3364 | 1/1 | 0.94 | 0.07 | 29,29,29,29 | 0 |
| 55 | MG | 2A | 3143 | 1/1 | 0.94 | 0.20 | 44,44,44,44 | 0 |
| 55 | MG | 1X | 101 | 1/1 | 0.94 | 0.12 | 35,35,35,35 | 0 |
| 55 | MG | 2A | 3394 | 1/1 | 0.94 | 0.27 | 37,37,37,37 | 0 |
| 55 | MG | 2A | 3395 | 1/1 | 0.94 | 0.23 | 35,35,35,35 | 0 |
| 55 | MG | 1a | 1754 | 1/1 | 0.94 | 0.24 | 61,61,61,61 | 0 |
| 55 | MG | 1A | 3983 | 1/1 | 0.94 | 0.10 | 56,56,56,56 | 0 |
| 55 | MG | 2A | 3399 | 1/1 | 0.94 | 0.06 | 47,47,47,47 | 0 |
| 55 | MG | 2A | 3744 | 1/1 | 0.94 | 0.17 | 61,61,61,61 | 0 |
| 55 | MG | 2A | 3400 | 1/1 | 0.94 | 0.36 | 48,48,48,48 | 0 |
| 55 | MG | 1A | 3763 | 1/1 | 0.94 | 0.07 | 46,46,46,46 | 0 |
| 55 | MG | 1A | 3046 | 1/1 | 0.94 | 0.07 | 33,33,33,33 | 0 |
| 55 | MG | 2A | 3749 | 1/1 | 0.94 | 0.18 | 45,45,45,45 | 0 |
| 55 | MG | 2A | 3750 | 1/1 | 0.94 | 0.11 | 40,40,40,40 | 0 |
| 55 | MG | 1A | 3368 | 1/1 | 0.94 | 0.10 | 40,40,40,40 | 0 |
| 55 | MG | 1Z | 301 | 1/1 | 0.94 | 0.09 | 36,36,36,36 | 0 |
| 55 | MG | 2A | 3407 | 1/1 | 0.94 | 0.21 | 53,53,53,53 | 0 |
| 55 | MG | 2a | 3163 | 1/1 | 0.94 | 0.09 | 60,60,60,60 | 0 |
| 55 | MG | 2A | 3755 | 1/1 | 0.94 | 0.06 | 52,52,52,52 | 0 |
| 55 | MG | 2A | 3757 | 1/1 | 0.94 | 0.12 | 50,50,50,50 | 0 |
| 55 | MG | 2a | 3166 | 1/1 | 0.94 | 0.21 | 54,54,54,54 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 55 | MG | 10 | 102 | 1/1 | 0.94 | 0.07 | 37,37,37,37 | 0 |
| 55 | MG | 2a | 3168 | 1/1 | 0.94 | 0.17 | 40,40,40,40 | 0 |
| 55 | MG | 1A | 3237 | 1/1 | 0.94 | 0.20 | 33,33,33,33 | 0 |
| 55 | MG | 1A | 3370 | 1/1 | 0.94 | 0.13 | 42,42,42,42 | 0 |
| 55 | MG | 1A | 3588 | 1/1 | 0.94 | 0.33 | 58,58,58,58 | 0 |
| 55 | MG | 1A | 3993 | 1/1 | 0.94 | 0.07 | 54,54,54,54 | 0 |
| 55 | MG | 2A | 3415 | 1/1 | 0.94 | 0.10 | 57,57,57,57 | 0 |
| 55 | MG | 2A | 3416 | 1/1 | 0.94 | 0.23 | 44,44,44,44 | 0 |
| 55 | MG | 13 | 101 | 1/1 | 0.94 | 0.11 | 50,50,50,50 | 0 |
| 55 | MG | 2A | 3159 | 1/1 | 0.94 | 0.16 | 48,48,48,48 | 0 |
| 55 | MG | 1A | 3770 | 1/1 | 0.94 | 0.08 | 37,37,37,37 | 0 |
| 55 | MG | 1A | 3293 | 1/1 | 0.94 | 0.23 | 31,31,31,31 | 0 |
| 55 | MG | 2A | 3421 | 1/1 | 0.94 | 0.27 | 48,48,48,48 | 0 |
| 55 | MG | 15 | 102 | 1/1 | 0.94 | 0.07 | 47,47,47,47 | 0 |
| 55 | MG | 2A | 3777 | 1/1 | 0.94 | 0.08 | 52,52,52,52 | 0 |
| 55 | MG | 15 | 103 | 1/1 | 0.94 | 0.11 | 41,41,41,41 | 0 |
| 55 | MG | 1A | 3372 | 1/1 | 0.94 | 0.22 | 38,38,38,38 | 0 |
| 55 | MG | 1A | 3591 | 1/1 | 0.94 | 0.14 | 48,48,48,48 | 0 |
| 55 | MG | 2A | 3167 | 1/1 | 0.94 | 0.18 | 68,68,68,68 | 0 |
| 55 | MG | 1A | 3172 | 1/1 | 0.94 | 0.23 | 28,28,28,28 | 0 |
| 55 | MG | 1A | 3063 | 1/1 | 0.94 | 0.14 | 44,44,44,44 | 0 |
| 55 | MG | 18 | 101 | 1/1 | 0.94 | 0.12 | 44,44,44,44 | 0 |
| 55 | MG | 2A | 3787 | 1/1 | 0.94 | 0.26 | 66,66,66,66 | 0 |
| 55 | MG | 1a | 1790 | 1/1 | 0.94 | 0.09 | 48,48,48,48 | 0 |
| 55 | MG | 2A | 3436 | 1/1 | 0.94 | 0.07 | 55,55,55,55 | 0 |
| 55 | MG | 2A | 3437 | 1/1 | 0.94 | 0.18 | 36,36,36,36 | 0 |
| 55 | MG | 1a | 1791 | 1/1 | 0.94 | 0.09 | 54,54,54,54 | 0 |
| 55 | MG | 18 | 102 | 1/1 | 0.94 | 0.39 | 46,46,46,46 | 0 |
| 55 | MG | 2A | 3443 | 1/1 | 0.94 | 0.13 | 41,41,41,41 | 0 |
| 55 | MG | 2A | 3176 | 1/1 | 0.94 | 0.24 | 56,56,56,56 | 0 |
| 55 | MG | 1A | 3025 | 1/1 | 0.94 | 0.09 | 44,44,44,44 | 0 |
| 55 | MG | 2A | 3178 | 1/1 | 0.94 | 0.09 | 37,37,37,37 | 0 |
| 55 | MG | 2d | 301 | 1/1 | 0.94 | 0.18 | 50,50,50,50 | 0 |
| 55 | MG | 1A | 3381 | 1/1 | 0.94 | 0.05 | 38,38,38,38 | 0 |
| 55 | MG | 2A | 3450 | 1/1 | 0.94 | 0.28 | 61,61,61,61 | 0 |
| 55 | MG | 2A | 3451 | 1/1 | 0.94 | 0.48 | 51,51,51,51 | 0 |
| 55 | MG | 2A | 3181 | 1/1 | 0.94 | 0.08 | 59,59,59,59 | 0 |
| 55 | MG | 1A | 3243 | 1/1 | 0.94 | 0.06 | 41,41,41,41 | 0 |
| 55 | MG | 2A | 3821 | 1/1 | 0.94 | 0.21 | 54,54,54,54 | 0 |
| 55 | MG | 2A | 3823 | 1/1 | 0.94 | 0.23 | 60,60,60,60 | 0 |
| 55 | MG | 1A | 3803 | 1/1 | 0.94 | 0.06 | 45,45,45,45 | 0 |
| 55 | MG | 2l | 203 | 1/1 | 0.94 | 0.07 | 47,47,47,47 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 55 | MG | 2A | 3184 | 1/1 | 0.94 | 0.06 | 39,39,39,39 | 0 |
| 55 | MG | 1A | 3102 | 1/1 | 0.94 | 0.09 | 47,47,47,47 | 0 |
| 55 | MG | 1A | 3306 | 1/1 | 0.94 | 0.08 | 47,47,47,47 | 0 |
| 55 | MG | 1A | 3806 | 1/1 | 0.94 | 0.09 | 28,28,28,28 | 0 |
| 55 | MG | 1A | 3387 | 1/1 | 0.94 | 0.27 | 34,34,34,34 | 0 |
| 55 | MG | 1A | 3605 | 1/1 | 0.94 | 0.12 | 33,33,33,33 | 0 |
| 55 | MG | 1a | 1805 | 1/1 | 0.94 | 0.12 | 74,74,74,74 | 0 |
| 55 | MG | 1A | 3606 | 1/1 | 0.94 | 0.18 | 37,37,37,37 | 0 |
| 55 | MG | 2A | 3194 | 1/1 | 0.94 | 0.09 | 28,28,28,28 | 0 |
| 55 | MG | 2A | 3837 | 1/1 | 0.94 | 0.11 | 48,48,48,48 | 0 |
| 55 | MG | 1A | 3485 | 1/1 | 0.94 | 0.09 | 50,50,50,50 | 0 |
| 55 | MG | 2A | 3474 | 1/1 | 0.95 | 0.17 | 38,38,38,38 | 0 |
| 55 | MG | 1A | 3322 | 1/1 | 0.95 | 0.18 | 43,43,43,43 | 0 |
| 55 | MG | 2A | 3476 | 1/1 | 0.95 | 0.26 | 37,37,37,37 | 0 |
| 55 | MG | 1A | 3797 | 1/1 | 0.95 | 0.13 | 26,26,26,26 | 0 |
| 55 | MG | 2A | 3829 | 1/1 | 0.95 | 0.10 | 40,40,40,40 | 0 |
| 55 | MG | 1A | 3798 | 1/1 | 0.95 | 0.15 | 29,29,29,29 | 0 |
| 55 | MG | 2A | 3479 | 1/1 | 0.95 | 0.41 | 51,51,51,51 | 0 |
| 55 | MG | 2A | 3207 | 1/1 | 0.95 | 0.10 | 50,50,50,50 | 0 |
| 55 | MG | 1A | 3038 | 1/1 | 0.95 | 0.14 | 18,18,18,18 | 0 |
| 55 | MG | 15 | 104 | 1/1 | 0.95 | 0.09 | 36,36,36,36 | 0 |
| 55 | MG | 2A | 3835 | 1/1 | 0.95 | 0.05 | 59,59,59,59 | 0 |
| 55 | MG | 2A | 3211 | 1/1 | 0.95 | 0.07 | 38,38,38,38 | 0 |
| 55 | MG | 1A | 3126 | 1/1 | 0.95 | 0.27 | 37,37,37,37 | 0 |
| 55 | MG | 2A | 3839 | 1/1 | 0.95 | 0.13 | 40,40,40,40 | 0 |
| 55 | MG | 2A | 3840 | 1/1 | 0.95 | 0.17 | 43,43,43,43 | 0 |
| 55 | MG | 1A | 4001 | 1/1 | 0.95 | 0.07 | 43,43,43,43 | 0 |
| 55 | MG | 1A | 3325 | 1/1 | 0.95 | 0.18 | 48,48,48,48 | 0 |
| 55 | MG | 1A | 3500 | 1/1 | 0.95 | 0.07 | 37,37,37,37 | 0 |
| 55 | MG | 1A | 3265 | 1/1 | 0.95 | 0.06 | 37,37,37,37 | 0 |
| 55 | MG | 2A | 3491 | 1/1 | 0.95 | 0.26 | 49,49,49,49 | 0 |
| 55 | MG | 1A | 3414 | 1/1 | 0.95 | 0.04 | 47,47,47,47 | 0 |
| 55 | MG | 2A | 3849 | 1/1 | 0.95 | 0.07 | 48,48,48,48 | 0 |
| 55 | MG | 1a | 1819 | 1/1 | 0.95 | 0.05 | 71,71,71,71 | 0 |
| 55 | MG | 1A | 4010 | 1/1 | 0.95 | 0.09 | 54,54,54,54 | 0 |
| 55 | MG | 1A | 3503 | 1/1 | 0.95 | 0.27 | 49,49,49,49 | 0 |
| 55 | MG | 1A | 3812 | 1/1 | 0.95 | 0.09 | 24,24,24,24 | 0 |
| 55 | MG | 1A | 4013 | 1/1 | 0.95 | 0.24 | 35,35,35,35 | 0 |
| 55 | MG | 1A | 3415 | 1/1 | 0.95 | 0.08 | 44,44,44,44 | 0 |
| 55 | MG | 2A | 3500 | 1/1 | 0.95 | 0.17 | 38,38,38,38 | 0 |
| 55 | MG | 1A | 3506 | 1/1 | 0.95 | 0.18 | 21,21,21,21 | 0 |
| 55 | MG | 1A | 3327 | 1/1 | 0.95 | 0.11 | 41,41,41,41 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 55 | MG | 1A | 3417 | 1/1 | 0.95 | 0.08 | 44,44,44,44 | 0 |
| 55 | MG | 1A | 3510 | 1/1 | 0.95 | 0.14 | 33,33,33,33 | 0 |
| 55 | MG | 2A | 3507 | 1/1 | 0.95 | 0.13 | 30,30,30,30 | 0 |
| 55 | MG | 1A | 3826 | 1/1 | 0.95 | 0.08 | 35,35,35,35 | 0 |
| 55 | MG | 1a | 1610 | 1/1 | 0.95 | 0.08 | 63,63,63,63 | 0 |
| 55 | MG | 1A | 3628 | 1/1 | 0.95 | 0.11 | 54,54,54,54 | 0 |
| 55 | MG | 1A | 4024 | 1/1 | 0.95 | 0.15 | 39,39,39,39 | 0 |
| 55 | MG | 1A | 3100 | 1/1 | 0.95 | 0.17 | 40,40,40,40 | 0 |
| 55 | MG | 1A | 3330 | 1/1 | 0.95 | 0.09 | 34,34,34,34 | 0 |
| 55 | MG | 2B | 209 | 1/1 | 0.95 | 0.10 | 57,57,57,57 | 0 |
| 55 | MG | 1A | 3513 | 1/1 | 0.95 | 0.15 | 39,39,39,39 | 0 |
| 55 | MG | 1A | 3073 | 1/1 | 0.95 | 0.16 | 37,37,37,37 | 0 |
| 55 | MG | 1A | 3835 | 1/1 | 0.95 | 0.09 | 39,39,39,39 | 0 |
| 55 | MG | 1A | 3836 | 1/1 | 0.95 | 0.11 | 40,40,40,40 | 0 |
| 55 | MG | 2A | 3522 | 1/1 | 0.95 | 0.15 | 31,31,31,31 | 0 |
| 55 | MG | 2A | 3523 | 1/1 | 0.95 | 0.12 | 42,42,42,42 | 0 |
| 55 | MG | 2A | 3524 | 1/1 | 0.95 | 0.10 | 37,37,37,37 | 0 |
| 55 | MG | 2A | 3247 | 1/1 | 0.95 | 0.08 | 54,54,54,54 | 0 |
| 55 | MG | 1l | 203 | 1/1 | 0.95 | 0.07 | 54,54,54,54 | 0 |
| 55 | MG | 1A | 4035 | 1/1 | 0.95 | 0.10 | 57,57,57,57 | 0 |
| 55 | MG | 1A | 3837 | 1/1 | 0.95 | 0.10 | 51,51,51,51 | 0 |
| 55 | MG | 1A | 3163 | 1/1 | 0.95 | 0.21 | 23,23,23,23 | 0 |
| 55 | MG | 1A | 3334 | 1/1 | 0.95 | 0.14 | 33,33,33,33 | 0 |
| 55 | MG | 2A | 3533 | 1/1 | 0.95 | 0.25 | 50,50,50,50 | 0 |
| 55 | MG | 1A | 3642 | 1/1 | 0.95 | 0.14 | 26,26,26,26 | 0 |
| 55 | MG | 2A | 3256 | 1/1 | 0.95 | 0.17 | 47,47,47,47 | 0 |
| 55 | MG | 1A | 3425 | 1/1 | 0.95 | 0.07 | 53,53,53,53 | 0 |
| 55 | MG | 1a | 1627 | 1/1 | 0.95 | 0.13 | 52,52,52,52 | 0 |
| 55 | MG | 2F | 304 | 1/1 | 0.95 | 0.19 | 51,51,51,51 | 0 |
| 55 | MG | 1A | 3335 | 1/1 | 0.95 | 0.14 | 36,36,36,36 | 0 |
| 55 | MG | 1A | 3164 | 1/1 | 0.95 | 0.17 | 42,42,42,42 | 0 |
| 55 | MG | 1A | 4054 | 1/1 | 0.95 | 0.09 | 37,37,37,37 | 0 |
| 55 | MG | 2N | 202 | 1/1 | 0.95 | 0.06 | 48,48,48,48 | 0 |
| 55 | MG | 1a | 1631 | 1/1 | 0.95 | 0.13 | 57,57,57,57 | 0 |
| 55 | MG | 2P | 201 | 1/1 | 0.95 | 0.07 | 40,40,40,40 | 0 |
| 55 | MG | 2A | 3546 | 1/1 | 0.95 | 0.21 | 33,33,33,33 | 0 |
| 55 | MG | 1A | 4056 | 1/1 | 0.95 | 0.14 | 56,56,56,56 | 0 |
| 55 | MG | 1A | 3074 | 1/1 | 0.95 | 0.14 | 24,24,24,24 | 0 |
| 55 | MG | 1x | 110 | 1/1 | 0.95 | 0.14 | 63,63,63,63 | 0 |
| 55 | MG | 1A | 3277 | 1/1 | 0.95 | 0.07 | 38,38,38,38 | 0 |
| 55 | MG | 1A | 4059 | 1/1 | 0.95 | 0.06 | 34,34,34,34 | 0 |
| 55 | MG | 1A | 3849 | 1/1 | 0.95 | 0.07 | 39,39,39,39 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 55 | MG | 2T | 203 | 1/1 | 0.95 | 0.09 | 35,35,35,35 | 0 |
| 55 | MG | 2A | 3271 | 1/1 | 0.95 | 0.23 | 61,61,61,61 | 0 |
| 55 | MG | 1A | 3278 | 1/1 | 0.95 | 0.07 | 40,40,40,40 | 0 |
| 55 | MG | 2A | 3555 | 1/1 | 0.95 | 0.17 | 44,44,44,44 | 0 |
| 55 | MG | 2A | 3556 | 1/1 | 0.95 | 0.08 | 35,35,35,35 | 0 |
| 55 | MG | 2V | 203 | 1/1 | 0.95 | 0.08 | 47,47,47,47 | 0 |
| 55 | MG | 1A | 4063 | 1/1 | 0.95 | 0.12 | 36,36,36,36 | 0 |
| 55 | MG | 1A | 3166 | 1/1 | 0.95 | 0.15 | 28,28,28,28 | 0 |
| 55 | MG | 1A | 3658 | 1/1 | 0.95 | 0.10 | 43,43,43,43 | 0 |
| 55 | MG | 1A | 3167 | 1/1 | 0.95 | 0.11 | 37,37,37,37 | 0 |
| 55 | MG | 1A | 3168 | 1/1 | 0.95 | 0.08 | 38,38,38,38 | 0 |
| 55 | MG | 2A | 3009 | 1/1 | 0.95 | 0.11 | 40,40,40,40 | 0 |
| 55 | MG | 2A | 3010 | 1/1 | 0.95 | 0.06 | 30,30,30,30 | 0 |
| 55 | MG | 2A | 3569 | 1/1 | 0.95 | 0.14 | 38,38,38,38 | 0 |
| 55 | MG | 1A | 3667 | 1/1 | 0.95 | 0.20 | 49,49,49,49 | 0 |
| 55 | MG | 1A | 3225 | 1/1 | 0.95 | 0.12 | 26,26,26,26 | 0 |
| 55 | MG | 1a | 1647 | 1/1 | 0.95 | 0.13 | 53,53,53,53 | 0 |
| 55 | MG | 1A | 4074 | 1/1 | 0.95 | 0.09 | 14,14,14,14 | 0 |
| 55 | MG | 1A | 3169 | 1/1 | 0.95 | 0.10 | 26,26,26,26 | 0 |
| 55 | MG | 2A | 3577 | 1/1 | 0.95 | 0.09 | 44,44,44,44 | 0 |
| 55 | MG | 2A | 3578 | 1/1 | 0.95 | 0.21 | 28,28,28,28 | 0 |
| 55 | MG | 2A | 3579 | 1/1 | 0.95 | 0.08 | 55,55,55,55 | 0 |
| 55 | MG | 1A | 4077 | 1/1 | 0.95 | 0.10 | 34,34,34,34 | 0 |
| 55 | MG | 1A | 3670 | 1/1 | 0.95 | 0.08 | 46,46,46,46 | 0 |
| 55 | MG | 2A | 3583 | 1/1 | 0.95 | 0.16 | 53,53,53,53 | 0 |
| 55 | MG | 2a | 3011 | 1/1 | 0.95 | 0.32 | 55,55,55,55 | 0 |
| 55 | MG | 2A | 3584 | 1/1 | 0.95 | 0.10 | 35,35,35,35 | 0 |
| 55 | MG | 1A | 3671 | 1/1 | 0.95 | 0.05 | 36,36,36,36 | 0 |
| 55 | MG | 1a | 1655 | 1/1 | 0.95 | 0.20 | 39,39,39,39 | 0 |
| 55 | MG | 1A | 3130 | 1/1 | 0.95 | 0.11 | 27,27,27,27 | 0 |
| 55 | MG | 2A | 3588 | 1/1 | 0.95 | 0.12 | 49,49,49,49 | 0 |
| 55 | MG | 2A | 3024 | 1/1 | 0.95 | 0.16 | 40,40,40,40 | 0 |
| 55 | MG | 1A | 3057 | 1/1 | 0.95 | 0.07 | 21,21,21,21 | 0 |
| 55 | MG | 2A | 3026 | 1/1 | 0.95 | 0.13 | 42,42,42,42 | 0 |
| 55 | MG | 1A | 3233 | 1/1 | 0.95 | 0.21 | 38,38,38,38 | 0 |
| 55 | MG | 1A | 3446 | 1/1 | 0.95 | 0.07 | 31,31,31,31 | 0 |
| 55 | MG | 1A | 3447 | 1/1 | 0.95 | 0.09 | 42,42,42,42 | 0 |
| 55 | MG | 1A | 3079 | 1/1 | 0.95 | 0.15 | 34,34,34,34 | 0 |
| 55 | MG | 1A | 4090 | 1/1 | 0.95 | 0.06 | 42,42,42,42 | 0 |
| 55 | MG | 1A | 4094 | 1/1 | 0.95 | 0.10 | 14,14,14,14 | 0 |
| 55 | MG | 1A | 4096 | 1/1 | 0.95 | 0.08 | 47,47,47,47 | 0 |
| 55 | MG | 1A | 4097 | 1/1 | 0.95 | 0.12 | 35,35,35,35 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 55 | MG | 1A | 3359 | 1/1 | 0.95 | 0.07 | 44,44,44,44 | 0 |
| 55 | MG | 2A | 3306 | 1/1 | 0.95 | 0.14 | 55,55,55,55 | 0 |
| 55 | MG | 1A | 4100 | 1/1 | 0.95 | 0.09 | 37,37,37,37 | 0 |
| 55 | MG | 1A | 3235 | 1/1 | 0.95 | 0.18 | 35,35,35,35 | 0 |
| 55 | MG | 1A | 3876 | 1/1 | 0.95 | 0.11 | 19,19,19,19 | 0 |
| 55 | MG | 2A | 3311 | 1/1 | 0.95 | 0.12 | 41,41,41,41 | 0 |
| 55 | MG | 1A | 4103 | 1/1 | 0.95 | 0.10 | 57,57,57,57 | 0 |
| 55 | MG | 1A | 3295 | 1/1 | 0.95 | 0.08 | 31,31,31,31 | 0 |
| 55 | MG | 2A | 3046 | 1/1 | 0.95 | 0.17 | 55,55,55,55 | 0 |
| 55 | MG | 2A | 3047 | 1/1 | 0.95 | 0.12 | 53,53,53,53 | 0 |
| 55 | MG | 1A | 3058 | 1/1 | 0.95 | 0.17 | 35,35,35,35 | 0 |
| 55 | MG | 1A | 3685 | 1/1 | 0.95 | 0.08 | 34,34,34,34 | 0 |
| 55 | MG | 2A | 3053 | 1/1 | 0.95 | 0.06 | 41,41,41,41 | 0 |
| 55 | MG | 2A | 3319 | 1/1 | 0.95 | 0.22 | 62,62,62,62 | 0 |
| 55 | MG | 2A | 3056 | 1/1 | 0.95 | 0.06 | 42,42,42,42 | 0 |
| 55 | MG | 1A | 3297 | 1/1 | 0.95 | 0.12 | 36,36,36,36 | 0 |
| 55 | MG | 2A | 3620 | 1/1 | 0.95 | 0.15 | 38,38,38,38 | 0 |
| 55 | MG | 1A | 3365 | 1/1 | 0.95 | 0.10 | 48,48,48,48 | 0 |
| 55 | MG | 1A | 3885 | 1/1 | 0.95 | 0.10 | 50,50,50,50 | 0 |
| 55 | MG | 2A | 3623 | 1/1 | 0.95 | 0.15 | 26,26,26,26 | 0 |
| 55 | MG | 2A | 3062 | 1/1 | 0.95 | 0.20 | 45,45,45,45 | 0 |
| 55 | MG | 1A | 3238 | 1/1 | 0.95 | 0.10 | 31,31,31,31 | 0 |
| 55 | MG | 2A | 3626 | 1/1 | 0.95 | 0.19 | 44,44,44,44 | 0 |
| 55 | MG | 2a | 3053 | 1/1 | 0.95 | 0.10 | 42,42,42,42 | 0 |
| 55 | MG | 2A | 3328 | 1/1 | 0.95 | 0.06 | 43,43,43,43 | 0 |
| 55 | MG | 1A | 3553 | 1/1 | 0.95 | 0.06 | 33,33,33,33 | 0 |
| 55 | MG | 1A | 3699 | 1/1 | 0.95 | 0.09 | 21,21,21,21 | 0 |
| 55 | MG | 1A | 3299 | 1/1 | 0.95 | 0.15 | 42,42,42,42 | 0 |
| 55 | MG | 1A | 3704 | 1/1 | 0.95 | 0.11 | 42,42,42,42 | 0 |
| 55 | MG | 1A | 3705 | 1/1 | 0.95 | 0.09 | 23,23,23,23 | 0 |
| 55 | MG | 1A | 3556 | 1/1 | 0.95 | 0.20 | 31,31,31,31 | 0 |
| 55 | MG | 2A | 3636 | 1/1 | 0.95 | 0.13 | 57,57,57,57 | 0 |
| 55 | MG | 2A | 3637 | 1/1 | 0.95 | 0.28 | 38,38,38,38 | 0 |
| 55 | MG | 2A | 3337 | 1/1 | 0.95 | 0.12 | 51,51,51,51 | 0 |
| 55 | MG | 1A | 3710 | 1/1 | 0.95 | 0.07 | 21,21,21,21 | 0 |
| 55 | MG | 2A | 3640 | 1/1 | 0.95 | 0.10 | 55,55,55,55 | 0 |
| 55 | MG | 1B | 203 | 1/1 | 0.95 | 0.13 | 39,39,39,39 | 0 |
| 55 | MG | 2A | 3642 | 1/1 | 0.95 | 0.07 | 69,69,69,69 | 0 |
| 55 | MG | 1B | 204 | 1/1 | 0.95 | 0.13 | 52,52,52,52 | 0 |
| 55 | MG | 2A | 3078 | 1/1 | 0.95 | 0.09 | 43,43,43,43 | 0 |
| 55 | MG | 1B | 205 | 1/1 | 0.95 | 0.07 | 39,39,39,39 | 0 |
| 55 | MG | 1A | 3902 | 1/1 | 0.95 | 0.07 | 58,58,58,58 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 55 | MG | 1A | 3712 | 1/1 | 0.95 | 0.10 | 41,41,41,41 | 0 |
| 55 | MG | 1A | 3713 | 1/1 | 0.95 | 0.14 | 42,42,42,42 | 0 |
| 55 | MG | 2A | 3649 | 1/1 | 0.95 | 0.07 | 40,40,40,40 | 0 |
| 55 | MG | 1B | 211 | 1/1 | 0.95 | 0.05 | 33,33,33,33 | 0 |
| 55 | MG | 1a | 1696 | 1/1 | 0.95 | 0.27 | 55,55,55,55 | 0 |
| 55 | MG | 1A | 3558 | 1/1 | 0.95 | 0.36 | 30,30,30,30 | 0 |
| 55 | MG | 1B | 217 | 1/1 | 0.95 | 0.06 | 38,38,38,38 | 0 |
| 55 | MG | 2A | 3656 | 1/1 | 0.95 | 0.09 | 53,53,53,53 | 0 |
| 55 | MG | 1A | 3300 | 1/1 | 0.95 | 0.05 | 28,28,28,28 | 0 |
| 55 | MG | 2a | 3084 | 1/1 | 0.95 | 0.06 | 69,69,69,69 | 0 |
| 55 | MG | 1A | 3111 | 1/1 | 0.95 | 0.18 | 30,30,30,30 | 0 |
| 55 | MG | 1A | 3565 | 1/1 | 0.95 | 0.12 | 40,40,40,40 | 0 |
| 55 | MG | 2A | 3093 | 1/1 | 0.95 | 0.21 | 48,48,48,48 | 0 |
| 55 | MG | 2A | 3663 | 1/1 | 0.95 | 0.10 | 52,52,52,52 | 0 |
| 55 | MG | 1A | 3719 | 1/1 | 0.95 | 0.06 | 60,60,60,60 | 0 |
| 55 | MG | 1A | 3913 | 1/1 | 0.95 | 0.08 | 22,22,22,22 | 0 |
| 55 | MG | 1B | 227 | 1/1 | 0.95 | 0.11 | 57,57,57,57 | 0 |
| 55 | MG | 1A | 3721 | 1/1 | 0.95 | 0.09 | 27,27,27,27 | 0 |
| 55 | MG | 1A | 3566 | 1/1 | 0.95 | 0.09 | 32,32,32,32 | 0 |
| 55 | MG | 2A | 3672 | 1/1 | 0.95 | 0.14 | 59,59,59,59 | 0 |
| 55 | MG | 2A | 3102 | 1/1 | 0.95 | 0.07 | 63,63,63,63 | 0 |
| 55 | MG | 1A | 3916 | 1/1 | 0.95 | 0.18 | 68,68,68,68 | 0 |
| 55 | MG | 1A | 3051 | 1/1 | 0.95 | 0.15 | 23,23,23,23 | 0 |
| 55 | MG | 1a | 1711 | 1/1 | 0.95 | 0.06 | 57,57,57,57 | 0 |
| 55 | MG | 2A | 3677 | 1/1 | 0.95 | 0.08 | 37,37,37,37 | 0 |
| 55 | MG | 1a | 1712 | 1/1 | 0.95 | 0.16 | 65,65,65,65 | 0 |
| 55 | MG | 2A | 3680 | 1/1 | 0.95 | 0.12 | 47,47,47,47 | 0 |
| 55 | MG | 2a | 3104 | 1/1 | 0.95 | 0.10 | 64,64,64,64 | 0 |
| 55 | MG | 2A | 3109 | 1/1 | 0.95 | 0.15 | 52,52,52,52 | 0 |
| 55 | MG | 2a | 3106 | 1/1 | 0.95 | 0.10 | 46,46,46,46 | 0 |
| 55 | MG | 1A | 3726 | 1/1 | 0.95 | 0.08 | 64,64,64,64 | 0 |
| 55 | MG | 1A | 3304 | 1/1 | 0.95 | 0.22 | 34,34,34,34 | 0 |
| 55 | MG | 2A | 3370 | 1/1 | 0.95 | 0.08 | 63,63,63,63 | 0 |
| 55 | MG | 2A | 3688 | 1/1 | 0.95 | 0.16 | 32,32,32,32 | 0 |
| 55 | MG | 2A | 3113 | 1/1 | 0.95 | 0.08 | 40,40,40,40 | 0 |
| 55 | MG | 1A | 3572 | 1/1 | 0.95 | 0.06 | 32,32,32,32 | 0 |
| 55 | MG | 1A | 3574 | 1/1 | 0.95 | 0.12 | 41,41,41,41 | 0 |
| 55 | MG | 1D | 304 | 1/1 | 0.95 | 0.13 | 32,32,32,32 | 0 |
| 55 | MG | 1D | 307 | 1/1 | 0.95 | 0.29 | 38,38,38,38 | 0 |
| 55 | MG | 1D | 308 | 1/1 | 0.95 | 0.37 | 35,35,35,35 | 0 |
| 55 | MG | 1a | 1720 | 1/1 | 0.95 | 0.10 | 41,41,41,41 | 0 |
| 55 | MG | 1A | 3373 | 1/1 | 0.95 | 0.20 | 47,47,47,47 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 55 | MG | 1A | 3181 | 1/1 | 0.95 | 0.17 | 58,58,58,58 | 0 |
| 55 | MG | 2A | 3125 | 1/1 | 0.95 | 0.23 | 58,58,58,58 | 0 |
| 55 | MG | 2A | 3705 | 1/1 | 0.95 | 0.06 | 55,55,55,55 | 0 |
| 55 | MG | 1A | 3242 | 1/1 | 0.95 | 0.17 | 36,36,36,36 | 0 |
| 55 | MG | 2A | 3128 | 1/1 | 0.95 | 0.13 | 35,35,35,35 | 0 |
| 55 | MG | 1A | 3018 | 1/1 | 0.95 | 0.20 | 43,43,43,43 | 0 |
| 55 | MG | 1A | 3929 | 1/1 | 0.95 | 0.08 | 37,37,37,37 | 0 |
| 55 | MG | 1A | 3086 | 1/1 | 0.95 | 0.12 | 39,39,39,39 | 0 |
| 55 | MG | 1A | 3744 | 1/1 | 0.95 | 0.05 | 53,53,53,53 | 0 |
| 55 | MG | 2A | 3390 | 1/1 | 0.95 | 0.12 | 53,53,53,53 | 0 |
| 55 | MG | 1E | 305 | 1/1 | 0.95 | 0.21 | 30,30,30,30 | 0 |
| 55 | MG | 2A | 3134 | 1/1 | 0.95 | 0.08 | 45,45,45,45 | 0 |
| 55 | MG | 1A | 3935 | 1/1 | 0.95 | 0.09 | 21,21,21,21 | 0 |
| 55 | MG | 1E | 307 | 1/1 | 0.95 | 0.11 | 44,44,44,44 | 0 |
| 55 | MG | 1a | 1732 | 1/1 | 0.95 | 0.12 | 42,42,42,42 | 0 |
| 55 | MG | 2A | 3140 | 1/1 | 0.95 | 0.08 | 40,40,40,40 | 0 |
| 55 | MG | 1a | 1733 | 1/1 | 0.95 | 0.20 | 50,50,50,50 | 0 |
| 55 | MG | 1A | 3587 | 1/1 | 0.95 | 0.07 | 57,57,57,57 | 0 |
| 55 | MG | 2A | 3401 | 1/1 | 0.95 | 0.24 | 43,43,43,43 | 0 |
| 55 | MG | 1a | 1737 | 1/1 | 0.95 | 0.14 | 42,42,42,42 | 0 |
| 55 | MG | 2A | 3728 | 1/1 | 0.95 | 0.07 | 53,53,53,53 | 0 |
| 55 | MG | 1F | 304 | 1/1 | 0.95 | 0.19 | 46,46,46,46 | 0 |
| 55 | MG | 2A | 3404 | 1/1 | 0.95 | 0.12 | 61,61,61,61 | 0 |
| 55 | MG | 1A | 3746 | 1/1 | 0.95 | 0.24 | 39,39,39,39 | 0 |
| 55 | MG | 2A | 3733 | 1/1 | 0.95 | 0.13 | 49,49,49,49 | 0 |
| 55 | MG | 1F | 308 | 1/1 | 0.95 | 0.11 | 34,34,34,34 | 0 |
| 55 | MG | 1A | 3044 | 1/1 | 0.95 | 0.17 | 27,27,27,27 | 0 |
| 55 | MG | 2A | 3408 | 1/1 | 0.95 | 0.30 | 60,60,60,60 | 0 |
| 55 | MG | 2A | 3409 | 1/1 | 0.95 | 0.22 | 45,45,45,45 | 0 |
| 55 | MG | 1A | 3474 | 1/1 | 0.95 | 0.19 | 39,39,39,39 | 0 |
| 55 | MG | 1A | 3067 | 1/1 | 0.95 | 0.10 | 49,49,49,49 | 0 |
| 55 | MG | 1A | 3751 | 1/1 | 0.95 | 0.17 | 50,50,50,50 | 0 |
| 55 | MG | 1A | 3477 | 1/1 | 0.95 | 0.08 | 49,49,49,49 | 0 |
| 55 | MG | 2a | 3161 | 1/1 | 0.95 | 0.13 | 51,51,51,51 | 0 |
| 55 | MG | 2A | 3153 | 1/1 | 0.95 | 0.19 | 47,47,47,47 | 0 |
| 55 | MG | 1A | 3478 | 1/1 | 0.95 | 0.08 | 44,44,44,44 | 0 |
| 55 | MG | 1N | 203 | 1/1 | 0.95 | 0.06 | 47,47,47,47 | 0 |
| 55 | MG | 1A | 3594 | 1/1 | 0.95 | 0.15 | 23,23,23,23 | 0 |
| 55 | MG | 1A | 3757 | 1/1 | 0.95 | 0.10 | 55,55,55,55 | 0 |
| 55 | MG | 1A | 3951 | 1/1 | 0.95 | 0.09 | 34,34,34,34 | 0 |
| 55 | MG | 1A | 3036 | 1/1 | 0.95 | 0.07 | 34,34,34,34 | 0 |
| 55 | MG | 2a | 3171 | 1/1 | 0.95 | 0.15 | 53,53,53,53 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 55 | MG | 1P | 201 | 1/1 | 0.95 | 0.20 | 27,27,27,27 | 0 |
| 55 | MG | 2A | 3752 | 1/1 | 0.95 | 0.18 | 51,51,51,51 | 0 |
| 55 | MG | 1A | 3958 | 1/1 | 0.95 | 0.11 | 31,31,31,31 | 0 |
| 55 | MG | 1A | 3961 | 1/1 | 0.95 | 0.08 | 41,41,41,41 | 0 |
| 55 | MG | 1A | 3597 | 1/1 | 0.95 | 0.21 | 45,45,45,45 | 0 |
| 55 | MG | 1A | 3149 | 1/1 | 0.95 | 0.31 | 30,30,30,30 | 0 |
| 55 | MG | 1A | 3964 | 1/1 | 0.95 | 0.13 | 18,18,18,18 | 0 |
| 55 | MG | 1R | 202 | 1/1 | 0.95 | 0.11 | 35,35,35,35 | 0 |
| 55 | MG | 1S | 201 | 1/1 | 0.95 | 0.09 | 47,47,47,47 | 0 |
| 55 | MG | 2A | 3430 | 1/1 | 0.95 | 0.22 | 31,31,31,31 | 0 |
| 55 | MG | 1A | 3195 | 1/1 | 0.95 | 0.06 | 40,40,40,40 | 0 |
| 55 | MG | 2A | 3767 | 1/1 | 0.95 | 0.19 | 51,51,51,51 | 0 |
| 55 | MG | 1A | 3152 | 1/1 | 0.95 | 0.10 | 26,26,26,26 | 0 |
| 55 | MG | 2A | 3769 | 1/1 | 0.95 | 0.11 | 48,48,48,48 | 0 |
| 55 | MG | 2A | 3435 | 1/1 | 0.95 | 0.16 | 41,41,41,41 | 0 |
| 55 | MG | 1A | 3483 | 1/1 | 0.95 | 0.31 | 53,53,53,53 | 0 |
| 55 | MG | 1U | 206 | 1/1 | 0.95 | 0.18 | 28,28,28,28 | 0 |
| 55 | MG | 2A | 3438 | 1/1 | 0.95 | 0.17 | 51,51,51,51 | 0 |
| 55 | MG | 2A | 3440 | 1/1 | 0.95 | 0.19 | 50,50,50,50 | 0 |
| 55 | MG | 2a | 3195 | 1/1 | 0.95 | 0.04 | 62,62,62,62 | 0 |
| 55 | MG | 1A | 3971 | 1/1 | 0.95 | 0.14 | 42,42,42,42 | 0 |
| 55 | MG | 1A | 3391 | 1/1 | 0.95 | 0.18 | 52,52,52,52 | 0 |
| 55 | MG | 1a | 1778 | 1/1 | 0.95 | 0.12 | 43,43,43,43 | 0 |
| 55 | MG | 2a | 3200 | 1/1 | 0.95 | 0.13 | 47,47,47,47 | 0 |
| 55 | MG | 1a | 1780 | 1/1 | 0.95 | 0.17 | 42,42,42,42 | 0 |
| 55 | MG | 1A | 3070 | 1/1 | 0.95 | 0.16 | 49,49,49,49 | 0 |
| 55 | MG | 1A | 3772 | 1/1 | 0.95 | 0.09 | 16,16,16,16 | 0 |
| 55 | MG | 1A | 3976 | 1/1 | 0.95 | 0.07 | 46,46,46,46 | 0 |
| 55 | MG | 1W | 205 | 1/1 | 0.95 | 0.10 | 35,35,35,35 | 0 |
| 55 | MG | 1A | 3977 | 1/1 | 0.95 | 0.05 | 40,40,40,40 | 0 |
| 55 | MG | 1A | 3604 | 1/1 | 0.95 | 0.15 | 31,31,31,31 | 0 |
| 55 | MG | 1A | 3155 | 1/1 | 0.95 | 0.10 | 32,32,32,32 | 0 |
| 55 | MG | 1A | 3205 | 1/1 | 0.95 | 0.07 | 39,39,39,39 | 0 |
| 55 | MG | 1A | 3778 | 1/1 | 0.95 | 0.09 | 29,29,29,29 | 0 |
| 55 | MG | 1A | 3784 | 1/1 | 0.95 | 0.09 | 49,49,49,49 | 0 |
| 55 | MG | 2A | 3794 | 1/1 | 0.95 | 0.06 | 57,57,57,57 | 0 |
| 55 | MG | 10 | 101 | 1/1 | 0.95 | 0.06 | 31,31,31,31 | 0 |
| 55 | MG | 1A | 3071 | 1/1 | 0.95 | 0.09 | 28,28,28,28 | 0 |
| 55 | MG | 2A | 3797 | 1/1 | 0.95 | 0.07 | 35,35,35,35 | 0 |
| 55 | MG | 1A | 3207 | 1/1 | 0.95 | 0.12 | 41,41,41,41 | 0 |
| 55 | MG | 2A | 3799 | 1/1 | 0.95 | 0.15 | 56,56,56,56 | 0 |
| 55 | MG | 2A | 3195 | 1/1 | 0.95 | 0.09 | 39,39,39,39 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 55 | MG | 10 | 105 | 1/1 | 0.95 | 0.05 | 44,44,44,44 | 0 |
| 55 | MG | 2A | 3802 | 1/1 | 0.95 | 0.08 | 40,40,40,40 | 0 |
| 55 | MG | 11 | 102 | 1/1 | 0.95 | 0.08 | 28,28,28,28 | 0 |
| 55 | MG | 2A | 3198 | 1/1 | 0.95 | 0.26 | 47,47,47,47 | 0 |
| 55 | MG | 2A | 3812 | 1/1 | 0.95 | 0.07 | 55,55,55,55 | 0 |
| 55 | MG | 1A | 3789 | 1/1 | 0.95 | 0.12 | 37,37,37,37 | 0 |
| 55 | MG | 1A | 3790 | 1/1 | 0.95 | 0.12 | 16,16,16,16 | 0 |
| 55 | MG | 2A | 3470 | 1/1 | 0.95 | 0.13 | 49,49,49,49 | 0 |
| 55 | MG | 2A | 3471 | 1/1 | 0.95 | 0.12 | 21,21,21,21 | 0 |
| 56 | ZN | 24 | 501 | 1/1 | 0.95 | 0.09 | 132,132,132,132 | 0 |
| 55 | MG | 1A | 3791 | 1/1 | 0.95 | 0.09 | 24,24,24,24 | 0 |
| 55 | MG | 1A | 3404 | 1/1 | 0.95 | 0.13 | 55,55,55,55 | 0 |
| 55 | MG | 1A | 3825 | 1/1 | 0.96 | 0.04 | 27,27,27,27 | 0 |
| 55 | MG | 2A | 3336 | 1/1 | 0.96 | 0.20 | 48,48,48,48 | 0 |
| 55 | MG | 1P | 203 | 1/1 | 0.96 | 0.15 | 49,49,49,49 | 0 |
| 55 | MG | 2A | 3104 | 1/1 | 0.96 | 0.18 | 51,51,51,51 | 0 |
| 55 | MG | 2B | 217 | 1/1 | 0.96 | 0.07 | 57,57,57,57 | 0 |
| 55 | MG | 1Q | 201 | 1/1 | 0.96 | 0.17 | 28,28,28,28 | 0 |
| 55 | MG | 2A | 3592 | 1/1 | 0.96 | 0.12 | 36,36,36,36 | 0 |
| 55 | MG | 1A | 3994 | 1/1 | 0.96 | 0.12 | 36,36,36,36 | 0 |
| 55 | MG | 1a | 1735 | 1/1 | 0.96 | 0.20 | 50,50,50,50 | 0 |
| 55 | MG | 1A | 3091 | 1/1 | 0.96 | 0.11 | 49,49,49,49 | 0 |
| 55 | MG | 1A | 3996 | 1/1 | 0.96 | 0.06 | 50,50,50,50 | 0 |
| 55 | MG | 1a | 1739 | 1/1 | 0.96 | 0.18 | 47,47,47,47 | 0 |
| 55 | MG | 1A | 3150 | 1/1 | 0.96 | 0.08 | 25,25,25,25 | 0 |
| 55 | MG | 1A | 3828 | 1/1 | 0.96 | 0.10 | 25,25,25,25 | 0 |
| 55 | MG | 2E | 308 | 1/1 | 0.96 | 0.06 | 26,26,26,26 | 0 |
| 55 | MG | 1A | 3829 | 1/1 | 0.96 | 0.08 | 24,24,24,24 | 0 |
| 55 | MG | 1A | 3543 | 1/1 | 0.96 | 0.10 | 48,48,48,48 | 0 |
| 55 | MG | 1A | 3545 | 1/1 | 0.96 | 0.17 | 31,31,31,31 | 0 |
| 55 | MG | 2F | 303 | 1/1 | 0.96 | 0.15 | 45,45,45,45 | 0 |
| 55 | MG | 2A | 3603 | 1/1 | 0.96 | 0.12 | 34,34,34,34 | 0 |
| 55 | MG | 2F | 305 | 1/1 | 0.96 | 0.14 | 49,49,49,49 | 0 |
| 55 | MG | 1A | 4002 | 1/1 | 0.96 | 0.07 | 60,60,60,60 | 0 |
| 55 | MG | 2A | 3351 | 1/1 | 0.96 | 0.19 | 38,38,38,38 | 0 |
| 55 | MG | 2A | 3119 | 1/1 | 0.96 | 0.20 | 32,32,32,32 | 0 |
| 55 | MG | 1A | 4004 | 1/1 | 0.96 | 0.11 | 14,14,14,14 | 0 |
| 55 | MG | 2A | 3608 | 1/1 | 0.96 | 0.22 | 38,38,38,38 | 0 |
| 55 | MG | 2O | 202 | 1/1 | 0.96 | 0.16 | 46,46,46,46 | 0 |
| 55 | MG | 2A | 3122 | 1/1 | 0.96 | 0.13 | 32,32,32,32 | 0 |
| 55 | MG | 1A | 3383 | 1/1 | 0.96 | 0.12 | 35,35,35,35 | 0 |
| 55 | MG | 1A | 4006 | 1/1 | 0.96 | 0.08 | 30,30,30,30 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 55 | MG | 1A | 3547 | 1/1 | 0.96 | 0.23 | 30,30,30,30 | 0 |
| 55 | MG | 1A | 3007 | 1/1 | 0.96 | 0.08 | 39,39,39,39 | 0 |
| 55 | MG | 1a | 1751 | 1/1 | 0.96 | 0.10 | 54,54,54,54 | 0 |
| 55 | MG | 1A | 3226 | 1/1 | 0.96 | 0.18 | 32,32,32,32 | 0 |
| 55 | MG | 1A | 3227 | 1/1 | 0.96 | 0.06 | 41,41,41,41 | 0 |
| 55 | MG | 1A | 3228 | 1/1 | 0.96 | 0.17 | 44,44,44,44 | 0 |
| 55 | MG | 1A | 3673 | 1/1 | 0.96 | 0.17 | 40,40,40,40 | 0 |
| 55 | MG | 2A | 3619 | 1/1 | 0.96 | 0.18 | 48,48,48,48 | 0 |
| 55 | MG | 1X | 104 | 1/1 | 0.96 | 0.07 | 40,40,40,40 | 0 |
| 55 | MG | 1X | 105 | 1/1 | 0.96 | 0.05 | 34,34,34,34 | 0 |
| 55 | MG | 2A | 3135 | 1/1 | 0.96 | 0.05 | 36,36,36,36 | 0 |
| 55 | MG | 1A | 3840 | 1/1 | 0.96 | 0.10 | 28,28,28,28 | 0 |
| 55 | MG | 2A | 3137 | 1/1 | 0.96 | 0.20 | 51,51,51,51 | 0 |
| 55 | MG | 1A | 4014 | 1/1 | 0.96 | 0.09 | 39,39,39,39 | 0 |
| 55 | MG | 1A | 3841 | 1/1 | 0.96 | 0.13 | 38,38,38,38 | 0 |
| 55 | MG | 1A | 3552 | 1/1 | 0.96 | 0.04 | 33,33,33,33 | 0 |
| 55 | MG | 1Z | 302 | 1/1 | 0.96 | 0.12 | 43,43,43,43 | 0 |
| 55 | MG | 25 | 101 | 1/1 | 0.96 | 0.11 | 44,44,44,44 | 0 |
| 55 | MG | 1A | 4017 | 1/1 | 0.96 | 0.10 | 20,20,20,20 | 0 |
| 55 | MG | 1A | 3389 | 1/1 | 0.96 | 0.14 | 48,48,48,48 | 0 |
| 55 | MG | 27 | 101 | 1/1 | 0.96 | 0.08 | 44,44,44,44 | 0 |
| 55 | MG | 2A | 3631 | 1/1 | 0.96 | 0.11 | 35,35,35,35 | 0 |
| 55 | MG | 2A | 3144 | 1/1 | 0.96 | 0.22 | 45,45,45,45 | 0 |
| 55 | MG | 1A | 3093 | 1/1 | 0.96 | 0.10 | 41,41,41,41 | 0 |
| 55 | MG | 10 | 104 | 1/1 | 0.96 | 0.09 | 51,51,51,51 | 0 |
| 55 | MG | 1A | 3555 | 1/1 | 0.96 | 0.21 | 32,32,32,32 | 0 |
| 55 | MG | 2A | 3381 | 1/1 | 0.96 | 0.04 | 49,49,49,49 | 0 |
| 55 | MG | 1A | 3001 | 1/1 | 0.96 | 0.05 | 33,33,33,33 | 0 |
| 55 | MG | 2A | 3383 | 1/1 | 0.96 | 0.14 | 52,52,52,52 | 0 |
| 55 | MG | 1A | 3557 | 1/1 | 0.96 | 0.12 | 21,21,21,21 | 0 |
| 55 | MG | 1a | 1781 | 1/1 | 0.96 | 0.15 | 56,56,56,56 | 0 |
| 55 | MG | 2a | 3009 | 1/1 | 0.96 | 0.12 | 59,59,59,59 | 0 |
| 55 | MG | 1A | 3392 | 1/1 | 0.96 | 0.07 | 53,53,53,53 | 0 |
| 55 | MG | 12 | 101 | 1/1 | 0.96 | 0.08 | 42,42,42,42 | 0 |
| 55 | MG | 1A | 3020 | 1/1 | 0.96 | 0.07 | 22,22,22,22 | 0 |
| 55 | MG | 1A | 3561 | 1/1 | 0.96 | 0.19 | 38,38,38,38 | 0 |
| 55 | MG | 1A | 3473 | 1/1 | 0.96 | 0.15 | 36,36,36,36 | 0 |
| 55 | MG | 1A | 3283 | 1/1 | 0.96 | 0.18 | 26,26,26,26 | 0 |
| 55 | MG | 2A | 3393 | 1/1 | 0.96 | 0.10 | 40,40,40,40 | 0 |
| 55 | MG | 1A | 4031 | 1/1 | 0.96 | 0.09 | 33,33,33,33 | 0 |
| 55 | MG | 1A | 3475 | 1/1 | 0.96 | 0.15 | 40,40,40,40 | 0 |
| 55 | MG | 2A | 3651 | 1/1 | 0.96 | 0.06 | 50,50,50,50 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 55 | MG | 1A | 3855 | 1/1 | 0.96 | 0.18 | 50,50,50,50 | 0 |
| 55 | MG | 1A | 3032 | 1/1 | 0.96 | 0.08 | 20,20,20,20 | 0 |
| 55 | MG | 1A | 3692 | 1/1 | 0.96 | 0.08 | 36,36,36,36 | 0 |
| 55 | MG | 2A | 3655 | 1/1 | 0.96 | 0.05 | 39,39,39,39 | 0 |
| 55 | MG | 1A | 3397 | 1/1 | 0.96 | 0.14 | 38,38,38,38 | 0 |
| 55 | MG | 17 | 103 | 1/1 | 0.96 | 0.09 | 32,32,32,32 | 0 |
| 55 | MG | 2A | 3164 | 1/1 | 0.96 | 0.09 | 57,57,57,57 | 0 |
| 55 | MG | 1A | 3860 | 1/1 | 0.96 | 0.07 | 38,38,38,38 | 0 |
| 55 | MG | 1A | 3697 | 1/1 | 0.96 | 0.08 | 48,48,48,48 | 0 |
| 55 | MG | 1A | 4042 | 1/1 | 0.96 | 0.06 | 57,57,57,57 | 0 |
| 55 | MG | 2A | 3664 | 1/1 | 0.96 | 0.10 | 58,58,58,58 | 0 |
| 55 | MG | 1a | 1801 | 1/1 | 0.96 | 0.15 | 62,62,62,62 | 0 |
| 55 | MG | 2A | 3169 | 1/1 | 0.96 | 0.24 | 48,48,48,48 | 0 |
| 55 | MG | 18 | 103 | 1/1 | 0.96 | 0.16 | 38,38,38,38 | 0 |
| 55 | MG | 1A | 4043 | 1/1 | 0.96 | 0.05 | 49,49,49,49 | 0 |
| 55 | MG | 1A | 3570 | 1/1 | 0.96 | 0.17 | 31,31,31,31 | 0 |
| 55 | MG | 2a | 3036 | 1/1 | 0.96 | 0.06 | 43,43,43,43 | 0 |
| 55 | MG | 1A | 3863 | 1/1 | 0.96 | 0.07 | 45,45,45,45 | 0 |
| 55 | MG | 1A | 3398 | 1/1 | 0.96 | 0.22 | 29,29,29,29 | 0 |
| 55 | MG | 2a | 3039 | 1/1 | 0.96 | 0.11 | 43,43,43,43 | 0 |
| 55 | MG | 1A | 3868 | 1/1 | 0.96 | 0.05 | 57,57,57,57 | 0 |
| 55 | MG | 1a | 1603 | 1/1 | 0.96 | 0.08 | 55,55,55,55 | 0 |
| 55 | MG | 1A | 3332 | 1/1 | 0.96 | 0.12 | 44,44,44,44 | 0 |
| 55 | MG | 1A | 3285 | 1/1 | 0.96 | 0.13 | 38,38,38,38 | 0 |
| 55 | MG | 2A | 3180 | 1/1 | 0.96 | 0.11 | 44,44,44,44 | 0 |
| 55 | MG | 2A | 3679 | 1/1 | 0.96 | 0.05 | 43,43,43,43 | 0 |
| 55 | MG | 1A | 3577 | 1/1 | 0.96 | 0.24 | 37,37,37,37 | 0 |
| 55 | MG | 1a | 1813 | 1/1 | 0.96 | 0.13 | 40,40,40,40 | 0 |
| 55 | MG | 1A | 3709 | 1/1 | 0.96 | 0.08 | 23,23,23,23 | 0 |
| 55 | MG | 1A | 4060 | 1/1 | 0.96 | 0.08 | 37,37,37,37 | 0 |
| 55 | MG | 2A | 3684 | 1/1 | 0.96 | 0.04 | 54,54,54,54 | 0 |
| 55 | MG | 1a | 1609 | 1/1 | 0.96 | 0.29 | 62,62,62,62 | 0 |
| 55 | MG | 1A | 3578 | 1/1 | 0.96 | 0.08 | 33,33,33,33 | 0 |
| 55 | MG | 1A | 3401 | 1/1 | 0.96 | 0.07 | 37,37,37,37 | 0 |
| 55 | MG | 2a | 3054 | 1/1 | 0.96 | 0.21 | 46,46,46,46 | 0 |
| 55 | MG | 1A | 3580 | 1/1 | 0.96 | 0.08 | 35,35,35,35 | 0 |
| 55 | MG | 1a | 1613 | 1/1 | 0.96 | 0.11 | 37,37,37,37 | 0 |
| 55 | MG | 1a | 1822 | 1/1 | 0.96 | 0.16 | 54,54,54,54 | 0 |
| 55 | MG | 2A | 3695 | 1/1 | 0.96 | 0.17 | 29,29,29,29 | 0 |
| 55 | MG | 2a | 3059 | 1/1 | 0.96 | 0.10 | 50,50,50,50 | 0 |
| 55 | MG | 1a | 1823 | 1/1 | 0.96 | 0.25 | 51,51,51,51 | 0 |
| 55 | MG | 1A | 3581 | 1/1 | 0.96 | 0.14 | 41,41,41,41 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 55 | MG | 1A | 3187 | 1/1 | 0.96 | 0.08 | 29,29,29,29 | 0 |
| 55 | MG | 2A | 3699 | 1/1 | 0.96 | 0.06 | 43,43,43,43 | 0 |
| 55 | MG | 1A | 3584 | 1/1 | 0.96 | 0.28 | 33,33,33,33 | 0 |
| 55 | MG | 2A | 3434 | 1/1 | 0.96 | 0.05 | 69,69,69,69 | 0 |
| 55 | MG | 1A | 3406 | 1/1 | 0.96 | 0.14 | 37,37,37,37 | 0 |
| 55 | MG | 1A | 3880 | 1/1 | 0.96 | 0.10 | 21,21,21,21 | 0 |
| 55 | MG | 1A | 3407 | 1/1 | 0.96 | 0.10 | 49,49,49,49 | 0 |
| 55 | MG | 1A | 3158 | 1/1 | 0.96 | 0.11 | 34,34,34,34 | 0 |
| 55 | MG | 1A | 4075 | 1/1 | 0.96 | 0.10 | 58,58,58,58 | 0 |
| 55 | MG | 1A | 3884 | 1/1 | 0.96 | 0.12 | 28,28,28,28 | 0 |
| 55 | MG | 1A | 3722 | 1/1 | 0.96 | 0.07 | 33,33,33,33 | 0 |
| 55 | MG | 2A | 3713 | 1/1 | 0.96 | 0.06 | 52,52,52,52 | 0 |
| 55 | MG | 2A | 3714 | 1/1 | 0.96 | 0.11 | 55,55,55,55 | 0 |
| 55 | MG | 1A | 4078 | 1/1 | 0.96 | 0.08 | 61,61,61,61 | 0 |
| 55 | MG | 1A | 3888 | 1/1 | 0.96 | 0.04 | 29,29,29,29 | 0 |
| 55 | MG | 2A | 3446 | 1/1 | 0.96 | 0.08 | 48,48,48,48 | 0 |
| 55 | MG | 1A | 3236 | 1/1 | 0.96 | 0.16 | 23,23,23,23 | 0 |
| 55 | MG | 1A | 3056 | 1/1 | 0.96 | 0.10 | 39,39,39,39 | 0 |
| 55 | MG | 1A | 3891 | 1/1 | 0.96 | 0.08 | 39,39,39,39 | 0 |
| 55 | MG | 1A | 3191 | 1/1 | 0.96 | 0.17 | 29,29,29,29 | 0 |
| 55 | MG | 1A | 3893 | 1/1 | 0.96 | 0.08 | 35,35,35,35 | 0 |
| 55 | MG | 2A | 3723 | 1/1 | 0.96 | 0.07 | 29,29,29,29 | 0 |
| 55 | MG | 2A | 3213 | 1/1 | 0.96 | 0.13 | 57,57,57,57 | 0 |
| 55 | MG | 2A | 3214 | 1/1 | 0.96 | 0.28 | 43,43,43,43 | 0 |
| 55 | MG | 1A | 3727 | 1/1 | 0.96 | 0.12 | 31,31,31,31 | 0 |
| 55 | MG | 1A | 3730 | 1/1 | 0.96 | 0.07 | 16,16,16,16 | 0 |
| 55 | MG | 1A | 3339 | 1/1 | 0.96 | 0.25 | 42,42,42,42 | 0 |
| 55 | MG | 2A | 3458 | 1/1 | 0.96 | 0.13 | 52,52,52,52 | 0 |
| 55 | MG | 1A | 3898 | 1/1 | 0.96 | 0.16 | 22,22,22,22 | 0 |
| 55 | MG | 2A | 3220 | 1/1 | 0.96 | 0.14 | 62,62,62,62 | 0 |
| 55 | MG | 1A | 3899 | 1/1 | 0.96 | 0.11 | 41,41,41,41 | 0 |
| 55 | MG | 1A | 3193 | 1/1 | 0.96 | 0.47 | 33,33,33,33 | 0 |
| 55 | MG | 1A | 3494 | 1/1 | 0.96 | 0.15 | 35,35,35,35 | 0 |
| 55 | MG | 2A | 3736 | 1/1 | 0.96 | 0.05 | 58,58,58,58 | 0 |
| 55 | MG | 2a | 3097 | 1/1 | 0.96 | 0.07 | 75,75,75,75 | 0 |
| 55 | MG | 1A | 4099 | 1/1 | 0.96 | 0.08 | 37,37,37,37 | 0 |
| 55 | MG | 1x | 102 | 1/1 | 0.96 | 0.06 | 59,59,59,59 | 0 |
| 55 | MG | 1A | 3595 | 1/1 | 0.96 | 0.15 | 36,36,36,36 | 0 |
| 55 | MG | 1A | 3160 | 1/1 | 0.96 | 0.11 | 29,29,29,29 | 0 |
| 55 | MG | 1A | 3739 | 1/1 | 0.96 | 0.15 | 27,27,27,27 | 0 |
| 55 | MG | 1A | 3905 | 1/1 | 0.96 | 0.07 | 23,23,23,23 | 0 |
| 55 | MG | 1A | 3342 | 1/1 | 0.96 | 0.21 | 28,28,28,28 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 55 | MG | 1A | 3345 | 1/1 | 0.96 | 0.26 | 25,25,25,25 | 0 |
| 55 | MG | 1A | 3498 | 1/1 | 0.96 | 0.09 | 24,24,24,24 | 0 |
| 55 | MG | 1A | 3743 | 1/1 | 0.96 | 0.18 | 49,49,49,49 | 0 |
| 55 | MG | 2A | 3235 | 1/1 | 0.96 | 0.07 | 53,53,53,53 | 0 |
| 55 | MG | 1A | 3101 | 1/1 | 0.96 | 0.14 | 39,39,39,39 | 0 |
| 55 | MG | 1A | 3197 | 1/1 | 0.96 | 0.14 | 42,42,42,42 | 0 |
| 55 | MG | 1A | 3420 | 1/1 | 0.96 | 0.06 | 45,45,45,45 | 0 |
| 55 | MG | 1A | 3033 | 1/1 | 0.96 | 0.07 | 24,24,24,24 | 0 |
| 55 | MG | 2A | 3481 | 1/1 | 0.96 | 0.17 | 38,38,38,38 | 0 |
| 55 | MG | 1A | 3199 | 1/1 | 0.96 | 0.16 | 18,18,18,18 | 0 |
| 55 | MG | 1A | 3245 | 1/1 | 0.96 | 0.13 | 57,57,57,57 | 0 |
| 55 | MG | 2A | 3242 | 1/1 | 0.96 | 0.20 | 49,49,49,49 | 0 |
| 55 | MG | 1A | 3352 | 1/1 | 0.96 | 0.07 | 40,40,40,40 | 0 |
| 55 | MG | 2A | 3759 | 1/1 | 0.96 | 0.09 | 46,46,46,46 | 0 |
| 55 | MG | 1A | 3353 | 1/1 | 0.96 | 0.07 | 50,50,50,50 | 0 |
| 55 | MG | 2a | 3121 | 1/1 | 0.96 | 0.38 | 51,51,51,51 | 0 |
| 55 | MG | 2a | 3122 | 1/1 | 0.96 | 0.25 | 34,34,34,34 | 0 |
| 55 | MG | 1A | 3246 | 1/1 | 0.96 | 0.15 | 43,43,43,43 | 0 |
| 55 | MG | 1A | 3021 | 1/1 | 0.96 | 0.06 | 24,24,24,24 | 0 |
| 55 | MG | 1A | 3429 | 1/1 | 0.96 | 0.09 | 48,48,48,48 | 0 |
| 55 | MG | 2A | 3490 | 1/1 | 0.96 | 0.19 | 46,46,46,46 | 0 |
| 55 | MG | 1A | 3759 | 1/1 | 0.96 | 0.06 | 39,39,39,39 | 0 |
| 55 | MG | 1A | 3203 | 1/1 | 0.96 | 0.17 | 29,29,29,29 | 0 |
| 55 | MG | 1A | 3357 | 1/1 | 0.96 | 0.05 | 36,36,36,36 | 0 |
| 55 | MG | 2a | 3131 | 1/1 | 0.96 | 0.21 | 37,37,37,37 | 0 |
| 55 | MG | 2a | 3133 | 1/1 | 0.96 | 0.41 | 46,46,46,46 | 0 |
| 55 | MG | 1A | 3614 | 1/1 | 0.96 | 0.14 | 15,15,15,15 | 0 |
| 55 | MG | 1A | 3615 | 1/1 | 0.96 | 0.20 | 48,48,48,48 | 0 |
| 55 | MG | 1A | 3931 | 1/1 | 0.96 | 0.17 | 35,35,35,35 | 0 |
| 55 | MG | 1B | 212 | 1/1 | 0.96 | 0.14 | 52,52,52,52 | 0 |
| 55 | MG | 1A | 3616 | 1/1 | 0.96 | 0.21 | 38,38,38,38 | 0 |
| 55 | MG | 1B | 215 | 1/1 | 0.96 | 0.06 | 43,43,43,43 | 0 |
| 55 | MG | 1B | 216 | 1/1 | 0.96 | 0.11 | 48,48,48,48 | 0 |
| 55 | MG | 1A | 3934 | 1/1 | 0.96 | 0.06 | 28,28,28,28 | 0 |
| 55 | MG | 1A | 3514 | 1/1 | 0.96 | 0.09 | 59,59,59,59 | 0 |
| 55 | MG | 1B | 221 | 1/1 | 0.96 | 0.06 | 34,34,34,34 | 0 |
| 55 | MG | 1A | 3358 | 1/1 | 0.96 | 0.10 | 56,56,56,56 | 0 |
| 55 | MG | 2A | 3508 | 1/1 | 0.96 | 0.14 | 50,50,50,50 | 0 |
| 55 | MG | 1A | 3249 | 1/1 | 0.96 | 0.15 | 37,37,37,37 | 0 |
| 55 | MG | 1A | 3771 | 1/1 | 0.96 | 0.13 | 33,33,33,33 | 0 |
| 55 | MG | 2A | 3035 | 1/1 | 0.96 | 0.17 | 58,58,58,58 | 0 |
| 55 | MG | 1A | 3204 | 1/1 | 0.96 | 0.06 | 24,24,24,24 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 55 | MG | 1a | 1680 | 1/1 | 0.96 | 0.08 | 61,61,61,61 | 0 |
| 55 | MG | 2A | 3792 | 1/1 | 0.96 | 0.08 | 60,60,60,60 | 0 |
| 55 | MG | 1A | 3013 | 1/1 | 0.96 | 0.18 | 27,27,27,27 | 0 |
| 55 | MG | 1A | 3252 | 1/1 | 0.96 | 0.15 | 33,33,33,33 | 0 |
| 55 | MG | 2a | 3156 | 1/1 | 0.96 | 0.15 | 48,48,48,48 | 0 |
| 55 | MG | 1A | 3945 | 1/1 | 0.96 | 0.10 | 56,56,56,56 | 0 |
| 55 | MG | 1A | 3108 | 1/1 | 0.96 | 0.04 | 29,29,29,29 | 0 |
| 55 | MG | 1a | 1685 | 1/1 | 0.96 | 0.13 | 58,58,58,58 | 0 |
| 55 | MG | 1A | 3440 | 1/1 | 0.96 | 0.17 | 39,39,39,39 | 0 |
| 55 | MG | 1A | 3948 | 1/1 | 0.96 | 0.07 | 30,30,30,30 | 0 |
| 55 | MG | 1A | 3780 | 1/1 | 0.96 | 0.08 | 57,57,57,57 | 0 |
| 55 | MG | 1A | 3443 | 1/1 | 0.96 | 0.09 | 33,33,33,33 | 0 |
| 55 | MG | 1A | 3049 | 1/1 | 0.96 | 0.11 | 27,27,27,27 | 0 |
| 55 | MG | 1A | 3050 | 1/1 | 0.96 | 0.18 | 36,36,36,36 | 0 |
| 55 | MG | 1A | 3954 | 1/1 | 0.96 | 0.06 | 52,52,52,52 | 0 |
| 55 | MG | 2A | 3051 | 1/1 | 0.96 | 0.22 | 53,53,53,53 | 0 |
| 55 | MG | 2A | 3287 | 1/1 | 0.96 | 0.10 | 46,46,46,46 | 0 |
| 55 | MG | 2a | 3169 | 1/1 | 0.96 | 0.14 | 59,59,59,59 | 0 |
| 55 | MG | 2A | 3815 | 1/1 | 0.96 | 0.10 | 40,40,40,40 | 0 |
| 55 | MG | 1A | 3957 | 1/1 | 0.96 | 0.13 | 28,28,28,28 | 0 |
| 55 | MG | 2A | 3535 | 1/1 | 0.96 | 0.11 | 39,39,39,39 | 0 |
| 55 | MG | 2A | 3054 | 1/1 | 0.96 | 0.23 | 47,47,47,47 | 0 |
| 55 | MG | 2A | 3820 | 1/1 | 0.96 | 0.12 | 33,33,33,33 | 0 |
| 55 | MG | 1A | 3064 | 1/1 | 0.96 | 0.17 | 40,40,40,40 | 0 |
| 55 | MG | 2A | 3538 | 1/1 | 0.96 | 0.16 | 32,32,32,32 | 0 |
| 55 | MG | 2A | 3539 | 1/1 | 0.96 | 0.09 | 57,57,57,57 | 0 |
| 55 | MG | 1A | 3065 | 1/1 | 0.96 | 0.20 | 50,50,50,50 | 0 |
| 55 | MG | 2A | 3059 | 1/1 | 0.96 | 0.05 | 42,42,42,42 | 0 |
| 55 | MG | 2a | 3182 | 1/1 | 0.96 | 0.09 | 51,51,51,51 | 0 |
| 55 | MG | 1A | 3114 | 1/1 | 0.96 | 0.15 | 38,38,38,38 | 0 |
| 55 | MG | 2a | 3184 | 1/1 | 0.96 | 0.10 | 72,72,72,72 | 0 |
| 55 | MG | 1A | 3793 | 1/1 | 0.96 | 0.06 | 42,42,42,42 | 0 |
| 55 | MG | 1A | 3087 | 1/1 | 0.96 | 0.17 | 29,29,29,29 | 0 |
| 55 | MG | 1A | 3315 | 1/1 | 0.96 | 0.16 | 51,51,51,51 | 0 |
| 55 | MG | 1A | 3966 | 1/1 | 0.96 | 0.11 | 57,57,57,57 | 0 |
| 55 | MG | 1A | 3635 | 1/1 | 0.96 | 0.12 | 49,49,49,49 | 0 |
| 55 | MG | 1A | 3637 | 1/1 | 0.96 | 0.07 | 39,39,39,39 | 0 |
| 55 | MG | 1A | 3638 | 1/1 | 0.96 | 0.13 | 43,43,43,43 | 0 |
| 55 | MG | 2A | 3302 | 1/1 | 0.96 | 0.06 | 42,42,42,42 | 0 |
| 55 | MG | 1E | 309 | 1/1 | 0.96 | 0.07 | 43,43,43,43 | 0 |
| 55 | MG | 2A | 3838 | 1/1 | 0.96 | 0.10 | 46,46,46,46 | 0 |
| 55 | MG | 2a | 3196 | 1/1 | 0.96 | 0.11 | 52,52,52,52 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 55 | MG | 1A | 3005 | 1/1 | 0.96 | 0.04 | 34,34,34,34 | 0 |
| 55 | MG | 2A | 3072 | 1/1 | 0.96 | 0.18 | 29,29,29,29 | 0 |
| 55 | MG | 1F | 301 | 1/1 | 0.96 | 0.08 | 49,49,49,49 | 0 |
| 55 | MG | 1A | 3317 | 1/1 | 0.96 | 0.21 | 36,36,36,36 | 0 |
| 55 | MG | 1A | 3533 | 1/1 | 0.96 | 0.09 | 24,24,24,24 | 0 |
| 55 | MG | 2A | 3845 | 1/1 | 0.96 | 0.17 | 42,42,42,42 | 0 |
| 55 | MG | 2A | 3557 | 1/1 | 0.96 | 0.11 | 40,40,40,40 | 0 |
| 55 | MG | 1A | 3534 | 1/1 | 0.96 | 0.19 | 31,31,31,31 | 0 |
| 55 | MG | 2A | 3559 | 1/1 | 0.96 | 0.11 | 50,50,50,50 | 0 |
| 55 | MG | 1F | 309 | 1/1 | 0.96 | 0.11 | 41,41,41,41 | 0 |
| 55 | MG | 1A | 3454 | 1/1 | 0.96 | 0.26 | 46,46,46,46 | 0 |
| 55 | MG | 1A | 3809 | 1/1 | 0.96 | 0.10 | 28,28,28,28 | 0 |
| 55 | MG | 1A | 3980 | 1/1 | 0.96 | 0.06 | 34,34,34,34 | 0 |
| 55 | MG | 1G | 202 | 1/1 | 0.96 | 0.11 | 57,57,57,57 | 0 |
| 55 | MG | 2A | 3084 | 1/1 | 0.96 | 0.25 | 48,48,48,48 | 0 |
| 55 | MG | 1A | 3647 | 1/1 | 0.96 | 0.06 | 42,42,42,42 | 0 |
| 55 | MG | 2f | 202 | 1/1 | 0.96 | 0.15 | 56,56,56,56 | 0 |
| 55 | MG | 1A | 3648 | 1/1 | 0.96 | 0.15 | 41,41,41,41 | 0 |
| 55 | MG | 1a | 1721 | 1/1 | 0.96 | 0.14 | 28,28,28,28 | 0 |
| 55 | MG | 2A | 3088 | 1/1 | 0.96 | 0.07 | 32,32,32,32 | 0 |
| 55 | MG | 1A | 3649 | 1/1 | 0.96 | 0.10 | 21,21,21,21 | 0 |
| 55 | MG | 2A | 3575 | 1/1 | 0.96 | 0.18 | 49,49,49,49 | 0 |
| 55 | MG | 2l | 202 | 1/1 | 0.96 | 0.07 | 67,67,67,67 | 0 |
| 55 | MG | 2A | 3862 | 1/1 | 0.96 | 0.08 | 56,56,56,56 | 0 |
| 55 | MG | 1N | 202 | 1/1 | 0.96 | 0.10 | 33,33,33,33 | 0 |
| 55 | MG | 1A | 3174 | 1/1 | 0.96 | 0.16 | 25,25,25,25 | 0 |
| 55 | MG | 1A | 3652 | 1/1 | 0.96 | 0.16 | 26,26,26,26 | 0 |
| 55 | MG | 1A | 3820 | 1/1 | 0.96 | 0.09 | 22,22,22,22 | 0 |
| 55 | MG | 1A | 3822 | 1/1 | 0.96 | 0.14 | 21,21,21,21 | 0 |
| 55 | MG | 1O | 203 | 1/1 | 0.96 | 0.05 | 35,35,35,35 | 0 |
| 55 | MG | 1A | 3068 | 1/1 | 0.96 | 0.12 | 34,34,34,34 | 0 |
| 55 | MG | 2B | 208 | 1/1 | 0.96 | 0.27 | 57,57,57,57 | 0 |
| 55 | MG | 1A | 3540 | 1/1 | 0.96 | 0.20 | 41,41,41,41 | 0 |
| 55 | MG | 2A | 3100 | 1/1 | 0.96 | 0.12 | 27,27,27,27 | 0 |
| 55 | MG | 2A | 3101 | 1/1 | 0.96 | 0.08 | 44,44,44,44 | 0 |
| 55 | MG | 2B | 212 | 1/1 | 0.96 | 0.26 | 52,52,52,52 | 0 |
| 55 | MG | 1A | 3432 | 1/1 | 0.97 | 0.12 | 32,32,32,32 | 0 |
| 55 | MG | 2A | 3324 | 1/1 | 0.97 | 0.14 | 45,45,45,45 | 0 |
| 55 | MG | 1A | 3294 | 1/1 | 0.97 | 0.14 | 40,40,40,40 | 0 |
| 55 | MG | 2A | 3326 | 1/1 | 0.97 | 0.13 | 46,46,46,46 | 0 |
| 55 | MG | 1A | 3618 | 1/1 | 0.97 | 0.12 | 23,23,23,23 | 0 |
| 55 | MG | 1A | 3008 | 1/1 | 0.97 | 0.05 | 25,25,25,25 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 55 | MG | 2A | 3329 | 1/1 | 0.97 | 0.23 | 45,45,45,45 | 0 |
| 55 | MG | 1A | 3218 | 1/1 | 0.97 | 0.18 | 39,39,39,39 | 0 |
| 55 | MG | 1A | 3094 | 1/1 | 0.97 | 0.09 | 16,16,16,16 | 0 |
| 55 | MG | 2A | 3731 | 1/1 | 0.97 | 0.04 | 59,59,59,59 | 0 |
| 55 | MG | 1A | 3220 | 1/1 | 0.97 | 0.11 | 44,44,44,44 | 0 |
| 55 | MG | 1A | 3133 | 1/1 | 0.97 | 0.23 | 31,31,31,31 | 0 |
| 55 | MG | 1A | 3043 | 1/1 | 0.97 | 0.12 | 25,25,25,25 | 0 |
| 55 | MG | 1A | 3441 | 1/1 | 0.97 | 0.14 | 32,32,32,32 | 0 |
| 55 | MG | 1Q | 205 | 1/1 | 0.97 | 0.15 | 36,36,36,36 | 0 |
| 55 | MG | 1A | 4067 | 1/1 | 0.97 | 0.07 | 26,26,26,26 | 0 |
| 55 | MG | 1A | 3442 | 1/1 | 0.97 | 0.10 | 51,51,51,51 | 0 |
| 55 | MG | 1A | 3559 | 1/1 | 0.97 | 0.20 | 31,31,31,31 | 0 |
| 55 | MG | 2A | 3534 | 1/1 | 0.97 | 0.09 | 40,40,40,40 | 0 |
| 55 | MG | 1T | 201 | 1/1 | 0.97 | 0.05 | 50,50,50,50 | 0 |
| 55 | MG | 1A | 3942 | 1/1 | 0.97 | 0.08 | 34,34,34,34 | 0 |
| 55 | MG | 1A | 4073 | 1/1 | 0.97 | 0.06 | 61,61,61,61 | 0 |
| 55 | MG | 1A | 3257 | 1/1 | 0.97 | 0.06 | 40,40,40,40 | 0 |
| 55 | MG | 1U | 204 | 1/1 | 0.97 | 0.09 | 25,25,25,25 | 0 |
| 55 | MG | 2A | 3746 | 1/1 | 0.97 | 0.22 | 37,37,37,37 | 0 |
| 55 | MG | 1a | 1690 | 1/1 | 0.97 | 0.11 | 28,28,28,28 | 0 |
| 55 | MG | 1x | 104 | 1/1 | 0.97 | 0.16 | 41,41,41,41 | 0 |
| 55 | MG | 1U | 205 | 1/1 | 0.97 | 0.21 | 32,32,32,32 | 0 |
| 55 | MG | 1A | 3258 | 1/1 | 0.97 | 0.08 | 47,47,47,47 | 0 |
| 55 | MG | 1A | 3729 | 1/1 | 0.97 | 0.06 | 23,23,23,23 | 0 |
| 55 | MG | 1V | 201 | 1/1 | 0.97 | 0.23 | 26,26,26,26 | 0 |
| 55 | MG | 1A | 3563 | 1/1 | 0.97 | 0.10 | 36,36,36,36 | 0 |
| 55 | MG | 1A | 3343 | 1/1 | 0.97 | 0.11 | 33,33,33,33 | 0 |
| 55 | MG | 2A | 3171 | 1/1 | 0.97 | 0.09 | 45,45,45,45 | 0 |
| 55 | MG | 2A | 3354 | 1/1 | 0.97 | 0.10 | 28,28,28,28 | 0 |
| 55 | MG | 1a | 1697 | 1/1 | 0.97 | 0.19 | 35,35,35,35 | 0 |
| 55 | MG | 1A | 3732 | 1/1 | 0.97 | 0.15 | 27,27,27,27 | 0 |
| 55 | MG | 1W | 201 | 1/1 | 0.97 | 0.17 | 34,34,34,34 | 0 |
| 55 | MG | 1A | 3344 | 1/1 | 0.97 | 0.07 | 37,37,37,37 | 0 |
| 55 | MG | 2A | 3762 | 1/1 | 0.97 | 0.10 | 74,74,74,74 | 0 |
| 55 | MG | 2A | 3764 | 1/1 | 0.97 | 0.06 | 65,65,65,65 | 0 |
| 55 | MG | 1W | 203 | 1/1 | 0.97 | 0.09 | 29,29,29,29 | 0 |
| 55 | MG | 1W | 204 | 1/1 | 0.97 | 0.08 | 38,38,38,38 | 0 |
| 55 | MG | 1A | 3734 | 1/1 | 0.97 | 0.10 | 16,16,16,16 | 0 |
| 55 | MG | 1A | 3504 | 1/1 | 0.97 | 0.07 | 41,41,41,41 | 0 |
| 55 | MG | 2A | 3363 | 1/1 | 0.97 | 0.06 | 44,44,44,44 | 0 |
| 55 | MG | 2A | 3007 | 1/1 | 0.97 | 0.07 | 43,43,43,43 | 0 |
| 55 | MG | 2A | 3560 | 1/1 | 0.97 | 0.13 | 30,30,30,30 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 55 | MG | 1X | 102 | 1/1 | 0.97 | 0.05 | 31,31,31,31 | 0 |
| 55 | MG | 1A | 3259 | 1/1 | 0.97 | 0.29 | 36,36,36,36 | 0 |
| 55 | MG | 2A | 3564 | 1/1 | 0.97 | 0.09 | 40,40,40,40 | 0 |
| 55 | MG | 1A | 3955 | 1/1 | 0.97 | 0.14 | 50,50,50,50 | 0 |
| 55 | MG | 1A | 4086 | 1/1 | 0.97 | 0.06 | 27,27,27,27 | 0 |
| 55 | MG | 1X | 106 | 1/1 | 0.97 | 0.08 | 47,47,47,47 | 0 |
| 55 | MG | 1A | 3636 | 1/1 | 0.97 | 0.13 | 15,15,15,15 | 0 |
| 55 | MG | 2A | 3014 | 1/1 | 0.97 | 0.09 | 38,38,38,38 | 0 |
| 55 | MG | 2A | 3780 | 1/1 | 0.97 | 0.05 | 53,53,53,53 | 0 |
| 55 | MG | 2a | 3071 | 1/1 | 0.97 | 0.14 | 51,51,51,51 | 0 |
| 55 | MG | 1Y | 202 | 1/1 | 0.97 | 0.19 | 45,45,45,45 | 0 |
| 55 | MG | 1A | 3568 | 1/1 | 0.97 | 0.05 | 25,25,25,25 | 0 |
| 55 | MG | 2A | 3572 | 1/1 | 0.97 | 0.15 | 27,27,27,27 | 0 |
| 55 | MG | 1A | 3960 | 1/1 | 0.97 | 0.07 | 36,36,36,36 | 0 |
| 55 | MG | 1A | 4091 | 1/1 | 0.97 | 0.12 | 24,24,24,24 | 0 |
| 55 | MG | 1A | 4092 | 1/1 | 0.97 | 0.06 | 41,41,41,41 | 0 |
| 55 | MG | 2A | 3788 | 1/1 | 0.97 | 0.05 | 73,73,73,73 | 0 |
| 55 | MG | 1A | 4093 | 1/1 | 0.97 | 0.07 | 41,41,41,41 | 0 |
| 55 | MG | 1A | 3189 | 1/1 | 0.97 | 0.06 | 43,43,43,43 | 0 |
| 55 | MG | 1A | 3507 | 1/1 | 0.97 | 0.13 | 27,27,27,27 | 0 |
| 55 | MG | 1A | 3029 | 1/1 | 0.97 | 0.25 | 30,30,30,30 | 0 |
| 55 | MG | 1A | 3643 | 1/1 | 0.97 | 0.09 | 43,43,43,43 | 0 |
| 55 | MG | 2A | 3027 | 1/1 | 0.97 | 0.13 | 31,31,31,31 | 0 |
| 55 | MG | 2A | 3028 | 1/1 | 0.97 | 0.07 | 41,41,41,41 | 0 |
| 55 | MG | 11 | 101 | 1/1 | 0.97 | 0.11 | 34,34,34,34 | 0 |
| 55 | MG | 1A | 3573 | 1/1 | 0.97 | 0.08 | 28,28,28,28 | 0 |
| 55 | MG | 1A | 3082 | 1/1 | 0.97 | 0.09 | 29,29,29,29 | 0 |
| 55 | MG | 2A | 3387 | 1/1 | 0.97 | 0.18 | 29,29,29,29 | 0 |
| 55 | MG | 2A | 3032 | 1/1 | 0.97 | 0.10 | 42,42,42,42 | 0 |
| 55 | MG | 2A | 3206 | 1/1 | 0.97 | 0.05 | 38,38,38,38 | 0 |
| 55 | MG | 2A | 3804 | 1/1 | 0.97 | 0.09 | 46,46,46,46 | 0 |
| 55 | MG | 2A | 3805 | 1/1 | 0.97 | 0.06 | 54,54,54,54 | 0 |
| 55 | MG | 1A | 3575 | 1/1 | 0.97 | 0.12 | 32,32,32,32 | 0 |
| 55 | MG | 1A | 3192 | 1/1 | 0.97 | 0.09 | 32,32,32,32 | 0 |
| 55 | MG | 2A | 3809 | 1/1 | 0.97 | 0.07 | 43,43,43,43 | 0 |
| 55 | MG | 2A | 3810 | 1/1 | 0.97 | 0.13 | 38,38,38,38 | 0 |
| 55 | MG | 1A | 3856 | 1/1 | 0.97 | 0.18 | 40,40,40,40 | 0 |
| 55 | MG | 1A | 3119 | 1/1 | 0.97 | 0.10 | 30,30,30,30 | 0 |
| 55 | MG | 2a | 3100 | 1/1 | 0.97 | 0.11 | 57,57,57,57 | 0 |
| 55 | MG | 1A | 3749 | 1/1 | 0.97 | 0.12 | 37,37,37,37 | 0 |
| 55 | MG | 13 | 103 | 1/1 | 0.97 | 0.07 | 41,41,41,41 | 0 |
| 55 | MG | 1A | 3974 | 1/1 | 0.97 | 0.09 | 44,44,44,44 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 55 | MG | 2A | 3818 | 1/1 | 0.97 | 0.12 | 41,41,41,41 | 0 |
| 55 | MG | 2A | 3397 | 1/1 | 0.97 | 0.10 | 25,25,25,25 | 0 |
| 55 | MG | 1A | 3453 | 1/1 | 0.97 | 0.35 | 46,46,46,46 | 0 |
| 55 | MG | 2A | 3216 | 1/1 | 0.97 | 0.06 | 50,50,50,50 | 0 |
| 55 | MG | 1A | 3351 | 1/1 | 0.97 | 0.04 | 38,38,38,38 | 0 |
| 55 | MG | 1A | 3651 | 1/1 | 0.97 | 0.09 | 29,29,29,29 | 0 |
| 55 | MG | 1A | 3753 | 1/1 | 0.97 | 0.07 | 48,48,48,48 | 0 |
| 55 | MG | 1a | 1736 | 1/1 | 0.97 | 0.27 | 39,39,39,39 | 0 |
| 55 | MG | 16 | 101 | 1/1 | 0.97 | 0.04 | 42,42,42,42 | 0 |
| 55 | MG | 1A | 3194 | 1/1 | 0.97 | 0.18 | 35,35,35,35 | 0 |
| 55 | MG | 1A | 3139 | 1/1 | 0.97 | 0.06 | 37,37,37,37 | 0 |
| 55 | MG | 1A | 3866 | 1/1 | 0.97 | 0.17 | 45,45,45,45 | 0 |
| 55 | MG | 2A | 3225 | 1/1 | 0.97 | 0.09 | 54,54,54,54 | 0 |
| 55 | MG | 1A | 3867 | 1/1 | 0.97 | 0.10 | 37,37,37,37 | 0 |
| 55 | MG | 2A | 3052 | 1/1 | 0.97 | 0.06 | 30,30,30,30 | 0 |
| 55 | MG | 1A | 3582 | 1/1 | 0.97 | 0.04 | 32,32,32,32 | 0 |
| 55 | MG | 1A | 3758 | 1/1 | 0.97 | 0.09 | 34,34,34,34 | 0 |
| 55 | MG | 2A | 3055 | 1/1 | 0.97 | 0.07 | 34,34,34,34 | 0 |
| 55 | MG | 1A | 3045 | 1/1 | 0.97 | 0.08 | 37,37,37,37 | 0 |
| 55 | MG | 2a | 3123 | 1/1 | 0.97 | 0.22 | 46,46,46,46 | 0 |
| 55 | MG | 2A | 3057 | 1/1 | 0.97 | 0.07 | 40,40,40,40 | 0 |
| 55 | MG | 1A | 3459 | 1/1 | 0.97 | 0.40 | 37,37,37,37 | 0 |
| 55 | MG | 1A | 3141 | 1/1 | 0.97 | 0.07 | 32,32,32,32 | 0 |
| 55 | MG | 18 | 106 | 1/1 | 0.97 | 0.10 | 55,55,55,55 | 0 |
| 55 | MG | 1A | 3661 | 1/1 | 0.97 | 0.09 | 46,46,46,46 | 0 |
| 55 | MG | 1A | 3269 | 1/1 | 0.97 | 0.12 | 52,52,52,52 | 0 |
| 55 | MG | 1B | 208 | 1/1 | 0.97 | 0.06 | 54,54,54,54 | 0 |
| 55 | MG | 2A | 3064 | 1/1 | 0.97 | 0.16 | 47,47,47,47 | 0 |
| 55 | MG | 2a | 3132 | 1/1 | 0.97 | 0.32 | 45,45,45,45 | 0 |
| 55 | MG | 2A | 3065 | 1/1 | 0.97 | 0.11 | 48,48,48,48 | 0 |
| 55 | MG | 1A | 3142 | 1/1 | 0.97 | 0.12 | 15,15,15,15 | 0 |
| 55 | MG | 1A | 3273 | 1/1 | 0.97 | 0.08 | 36,36,36,36 | 0 |
| 55 | MG | 2A | 3243 | 1/1 | 0.97 | 0.14 | 39,39,39,39 | 0 |
| 55 | MG | 1A | 3037 | 1/1 | 0.97 | 0.06 | 28,28,28,28 | 0 |
| 55 | MG | 1A | 3769 | 1/1 | 0.97 | 0.04 | 42,42,42,42 | 0 |
| 55 | MG | 2A | 3246 | 1/1 | 0.97 | 0.09 | 51,51,51,51 | 0 |
| 55 | MG | 1B | 213 | 1/1 | 0.97 | 0.20 | 44,44,44,44 | 0 |
| 55 | MG | 1A | 3412 | 1/1 | 0.97 | 0.10 | 33,33,33,33 | 0 |
| 55 | MG | 2A | 3857 | 1/1 | 0.97 | 0.18 | 36,36,36,36 | 0 |
| 55 | MG | 2A | 3433 | 1/1 | 0.97 | 0.23 | 47,47,47,47 | 0 |
| 55 | MG | 1a | 1761 | 1/1 | 0.97 | 0.04 | 49,49,49,49 | 0 |
| 55 | MG | 2A | 3251 | 1/1 | 0.97 | 0.06 | 50,50,50,50 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 55 | MG | 1A | 3030 | 1/1 | 0.97 | 0.09 | 39,39,39,39 | 0 |
| 55 | MG | 1A | 3467 | 1/1 | 0.97 | 0.29 | 46,46,46,46 | 0 |
| 55 | MG | 1A | 3882 | 1/1 | 0.97 | 0.08 | 47,47,47,47 | 0 |
| 55 | MG | 2A | 3439 | 1/1 | 0.97 | 0.08 | 64,64,64,64 | 0 |
| 55 | MG | 1B | 219 | 1/1 | 0.97 | 0.10 | 38,38,38,38 | 0 |
| 55 | MG | 1A | 3773 | 1/1 | 0.97 | 0.19 | 29,29,29,29 | 0 |
| 55 | MG | 1a | 1767 | 1/1 | 0.97 | 0.05 | 32,32,32,32 | 0 |
| 55 | MG | 2a | 3153 | 1/1 | 0.97 | 0.11 | 36,36,36,36 | 0 |
| 55 | MG | 1A | 3593 | 1/1 | 0.97 | 0.23 | 53,53,53,53 | 0 |
| 55 | MG | 2a | 3155 | 1/1 | 0.97 | 0.13 | 58,58,58,58 | 0 |
| 55 | MG | 2A | 3444 | 1/1 | 0.97 | 0.09 | 18,18,18,18 | 0 |
| 55 | MG | 1A | 3048 | 1/1 | 0.97 | 0.05 | 32,32,32,32 | 0 |
| 55 | MG | 1a | 1771 | 1/1 | 0.97 | 0.08 | 64,64,64,64 | 0 |
| 55 | MG | 1A | 3009 | 1/1 | 0.97 | 0.06 | 28,28,28,28 | 0 |
| 55 | MG | 1A | 3363 | 1/1 | 0.97 | 0.18 | 36,36,36,36 | 0 |
| 55 | MG | 1A | 3779 | 1/1 | 0.97 | 0.11 | 28,28,28,28 | 0 |
| 55 | MG | 1A | 3280 | 1/1 | 0.97 | 0.24 | 45,45,45,45 | 0 |
| 55 | MG | 1a | 1777 | 1/1 | 0.97 | 0.06 | 45,45,45,45 | 0 |
| 55 | MG | 1A | 3105 | 1/1 | 0.97 | 0.18 | 31,31,31,31 | 0 |
| 55 | MG | 1a | 1779 | 1/1 | 0.97 | 0.09 | 49,49,49,49 | 0 |
| 55 | MG | 1A | 3151 | 1/1 | 0.97 | 0.14 | 38,38,38,38 | 0 |
| 55 | MG | 2A | 3455 | 1/1 | 0.97 | 0.05 | 56,56,56,56 | 0 |
| 55 | MG | 1A | 3894 | 1/1 | 0.97 | 0.08 | 26,26,26,26 | 0 |
| 55 | MG | 2D | 301 | 1/1 | 0.97 | 0.05 | 31,31,31,31 | 0 |
| 55 | MG | 2a | 3170 | 1/1 | 0.97 | 0.13 | 36,36,36,36 | 0 |
| 55 | MG | 2A | 3657 | 1/1 | 0.97 | 0.09 | 44,44,44,44 | 0 |
| 55 | MG | 2A | 3658 | 1/1 | 0.97 | 0.05 | 58,58,58,58 | 0 |
| 55 | MG | 1A | 3178 | 1/1 | 0.97 | 0.10 | 31,31,31,31 | 0 |
| 55 | MG | 1A | 3106 | 1/1 | 0.97 | 0.10 | 35,35,35,35 | 0 |
| 55 | MG | 1A | 3535 | 1/1 | 0.97 | 0.09 | 41,41,41,41 | 0 |
| 55 | MG | 2A | 3097 | 1/1 | 0.97 | 0.07 | 43,43,43,43 | 0 |
| 55 | MG | 2E | 306 | 1/1 | 0.97 | 0.14 | 42,42,42,42 | 0 |
| 55 | MG | 2a | 3178 | 1/1 | 0.97 | 0.15 | 43,43,43,43 | 0 |
| 55 | MG | 1A | 3536 | 1/1 | 0.97 | 0.17 | 56,56,56,56 | 0 |
| 55 | MG | 1A | 3209 | 1/1 | 0.97 | 0.08 | 27,27,27,27 | 0 |
| 55 | MG | 1D | 302 | 1/1 | 0.97 | 0.07 | 23,23,23,23 | 0 |
| 55 | MG | 2A | 3279 | 1/1 | 0.97 | 0.10 | 40,40,40,40 | 0 |
| 55 | MG | 2A | 3667 | 1/1 | 0.97 | 0.07 | 46,46,46,46 | 0 |
| 55 | MG | 1A | 3107 | 1/1 | 0.97 | 0.13 | 31,31,31,31 | 0 |
| 55 | MG | 1D | 305 | 1/1 | 0.97 | 0.07 | 33,33,33,33 | 0 |
| 55 | MG | 2a | 3186 | 1/1 | 0.97 | 0.16 | 50,50,50,50 | 0 |
| 55 | MG | 1A | 3424 | 1/1 | 0.97 | 0.14 | 29,29,29,29 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 55 | MG | 1A | 3691 | 1/1 | 0.97 | 0.07 | 24,24,24,24 | 0 |
| 55 | MG | 1a | 1634 | 1/1 | 0.97 | 0.14 | 58,58,58,58 | 0 |
| 55 | MG | 1A | 3211 | 1/1 | 0.97 | 0.33 | 33,33,33,33 | 0 |
| 55 | MG | 1A | 3693 | 1/1 | 0.97 | 0.06 | 26,26,26,26 | 0 |
| 55 | MG | 1A | 3801 | 1/1 | 0.97 | 0.11 | 18,18,18,18 | 0 |
| 55 | MG | 2A | 3110 | 1/1 | 0.97 | 0.09 | 56,56,56,56 | 0 |
| 55 | MG | 1A | 3694 | 1/1 | 0.97 | 0.09 | 19,19,19,19 | 0 |
| 55 | MG | 1A | 3026 | 1/1 | 0.97 | 0.11 | 32,32,32,32 | 0 |
| 55 | MG | 1A | 3696 | 1/1 | 0.97 | 0.07 | 39,39,39,39 | 0 |
| 55 | MG | 1A | 3374 | 1/1 | 0.97 | 0.05 | 31,31,31,31 | 0 |
| 55 | MG | 1A | 3006 | 1/1 | 0.97 | 0.07 | 50,50,50,50 | 0 |
| 55 | MG | 1A | 3700 | 1/1 | 0.97 | 0.05 | 23,23,23,23 | 0 |
| 55 | MG | 1A | 3611 | 1/1 | 0.97 | 0.11 | 12,12,12,12 | 0 |
| 55 | MG | 2a | 3201 | 1/1 | 0.97 | 0.06 | 55,55,55,55 | 0 |
| 55 | MG | 1E | 308 | 1/1 | 0.97 | 0.13 | 16,16,16,16 | 0 |
| 55 | MG | 2A | 3686 | 1/1 | 0.97 | 0.05 | 49,49,49,49 | 0 |
| 55 | MG | 1A | 3811 | 1/1 | 0.97 | 0.07 | 43,43,43,43 | 0 |
| 55 | MG | 2A | 3298 | 1/1 | 0.97 | 0.07 | 43,43,43,43 | 0 |
| 55 | MG | 1A | 4036 | 1/1 | 0.97 | 0.07 | 45,45,45,45 | 0 |
| 55 | MG | 2A | 3121 | 1/1 | 0.97 | 0.14 | 39,39,39,39 | 0 |
| 55 | MG | 1a | 1809 | 1/1 | 0.97 | 0.14 | 49,49,49,49 | 0 |
| 55 | MG | 1E | 311 | 1/1 | 0.97 | 0.05 | 43,43,43,43 | 0 |
| 55 | MG | 1a | 1651 | 1/1 | 0.97 | 0.13 | 41,41,41,41 | 0 |
| 55 | MG | 1A | 3484 | 1/1 | 0.97 | 0.04 | 35,35,35,35 | 0 |
| 55 | MG | 1A | 3813 | 1/1 | 0.97 | 0.06 | 41,41,41,41 | 0 |
| 55 | MG | 1A | 4039 | 1/1 | 0.97 | 0.07 | 38,38,38,38 | 0 |
| 55 | MG | 1F | 306 | 1/1 | 0.97 | 0.28 | 20,20,20,20 | 0 |
| 55 | MG | 2A | 3702 | 1/1 | 0.97 | 0.05 | 45,45,45,45 | 0 |
| 55 | MG | 1F | 307 | 1/1 | 0.97 | 0.08 | 33,33,33,33 | 0 |
| 55 | MG | 1A | 3183 | 1/1 | 0.97 | 0.09 | 46,46,46,46 | 0 |
| 55 | MG | 1A | 3815 | 1/1 | 0.97 | 0.08 | 16,16,16,16 | 0 |
| 55 | MG | 1A | 3816 | 1/1 | 0.97 | 0.13 | 42,42,42,42 | 0 |
| 55 | MG | 1A | 3817 | 1/1 | 0.97 | 0.08 | 50,50,50,50 | 0 |
| 55 | MG | 2A | 3709 | 1/1 | 0.97 | 0.07 | 39,39,39,39 | 0 |
| 55 | MG | 1A | 3706 | 1/1 | 0.97 | 0.08 | 15,15,15,15 | 0 |
| 55 | MG | 2A | 3502 | 1/1 | 0.97 | 0.06 | 48,48,48,48 | 0 |
| 55 | MG | 1A | 4046 | 1/1 | 0.97 | 0.04 | 66,66,66,66 | 0 |
| 55 | MG | 2A | 3504 | 1/1 | 0.97 | 0.11 | 35,35,35,35 | 0 |
| 55 | MG | 1A | 3924 | 1/1 | 0.97 | 0.09 | 38,38,38,38 | 0 |
| 55 | MG | 1A | 4048 | 1/1 | 0.97 | 0.06 | 40,40,40,40 | 0 |
| 55 | MG | 1A | 4049 | 1/1 | 0.97 | 0.11 | 53,53,53,53 | 0 |
| 55 | MG | 1A | 3378 | 1/1 | 0.97 | 0.16 | 41,41,41,41 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 55 | MG | 1A | 3076 | 1/1 | 0.97 | 0.14 | 40,40,40,40 | 0 |
| 55 | MG | 2A | 3510 | 1/1 | 0.97 | 0.08 | 36,36,36,36 | 0 |
| 56 | ZN | 2n | 501 | 1/1 | 0.97 | 0.05 | 100,100,100,100 | 0 |
| 55 | MG | 1A | 4055 | 1/1 | 0.97 | 0.13 | 38,38,38,38 | 0 |
| 55 | MG | 1A | 3927 | 1/1 | 0.97 | 0.12 | 34,34,34,34 | 0 |
| 55 | MG | 1A | 3328 | 1/1 | 0.98 | 0.20 | 40,40,40,40 | 0 |
| 55 | MG | 1A | 3629 | 1/1 | 0.98 | 0.07 | 32,32,32,32 | 0 |
| 55 | MG | 1A | 3738 | 1/1 | 0.98 | 0.06 | 34,34,34,34 | 0 |
| 55 | MG | 2A | 3016 | 1/1 | 0.98 | 0.05 | 40,40,40,40 | 0 |
| 55 | MG | 2A | 3249 | 1/1 | 0.98 | 0.05 | 59,59,59,59 | 0 |
| 55 | MG | 1A | 3143 | 1/1 | 0.98 | 0.03 | 28,28,28,28 | 0 |
| 55 | MG | 2E | 305 | 1/1 | 0.98 | 0.14 | 38,38,38,38 | 0 |
| 55 | MG | 1B | 218 | 1/1 | 0.98 | 0.07 | 20,20,20,20 | 0 |
| 55 | MG | 1A | 3396 | 1/1 | 0.98 | 0.16 | 31,31,31,31 | 0 |
| 55 | MG | 1A | 3959 | 1/1 | 0.98 | 0.08 | 40,40,40,40 | 0 |
| 55 | MG | 1A | 4044 | 1/1 | 0.98 | 0.06 | 57,57,57,57 | 0 |
| 55 | MG | 1B | 222 | 1/1 | 0.98 | 0.09 | 28,28,28,28 | 0 |
| 55 | MG | 1A | 3097 | 1/1 | 0.98 | 0.08 | 30,30,30,30 | 0 |
| 55 | MG | 1A | 3682 | 1/1 | 0.98 | 0.07 | 33,33,33,33 | 0 |
| 55 | MG | 1A | 3075 | 1/1 | 0.98 | 0.04 | 11,11,11,11 | 0 |
| 55 | MG | 1A | 3684 | 1/1 | 0.98 | 0.05 | 44,44,44,44 | 0 |
| 55 | MG | 2A | 3756 | 1/1 | 0.98 | 0.04 | 53,53,53,53 | 0 |
| 55 | MG | 2A | 3497 | 1/1 | 0.98 | 0.06 | 41,41,41,41 | 0 |
| 55 | MG | 1a | 1776 | 1/1 | 0.98 | 0.09 | 40,40,40,40 | 0 |
| 55 | MG | 2A | 3261 | 1/1 | 0.98 | 0.08 | 43,43,43,43 | 0 |
| 55 | MG | 1A | 3886 | 1/1 | 0.98 | 0.07 | 28,28,28,28 | 0 |
| 55 | MG | 2A | 3263 | 1/1 | 0.98 | 0.07 | 50,50,50,50 | 0 |
| 55 | MG | 1A | 3887 | 1/1 | 0.98 | 0.03 | 31,31,31,31 | 0 |
| 55 | MG | 2A | 3763 | 1/1 | 0.98 | 0.15 | 49,49,49,49 | 0 |
| 55 | MG | 1A | 4051 | 1/1 | 0.98 | 0.04 | 41,41,41,41 | 0 |
| 55 | MG | 1A | 3301 | 1/1 | 0.98 | 0.05 | 32,32,32,32 | 0 |
| 55 | MG | 2Q | 204 | 1/1 | 0.98 | 0.23 | 43,43,43,43 | 0 |
| 55 | MG | 1A | 3146 | 1/1 | 0.98 | 0.20 | 21,21,21,21 | 0 |
| 55 | MG | 1A | 3968 | 1/1 | 0.98 | 0.07 | 40,40,40,40 | 0 |
| 55 | MG | 2A | 3634 | 1/1 | 0.98 | 0.08 | 52,52,52,52 | 0 |
| 55 | MG | 1A | 3214 | 1/1 | 0.98 | 0.11 | 36,36,36,36 | 0 |
| 55 | MG | 1A | 3970 | 1/1 | 0.98 | 0.04 | 71,71,71,71 | 0 |
| 55 | MG | 1A | 3402 | 1/1 | 0.98 | 0.11 | 35,35,35,35 | 0 |
| 55 | MG | 1A | 3366 | 1/1 | 0.98 | 0.11 | 39,39,39,39 | 0 |
| 55 | MG | 2A | 3511 | 1/1 | 0.98 | 0.10 | 51,51,51,51 | 0 |
| 55 | MG | 1A | 3639 | 1/1 | 0.98 | 0.08 | 21,21,21,21 | 0 |
| 55 | MG | 1A | 3099 | 1/1 | 0.98 | 0.10 | 14,14,14,14 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 55 | MG | 1D | 306 | 1/1 | 0.98 | 0.13 | 45,45,45,45 | 0 |
| 55 | MG | 1A | 3148 | 1/1 | 0.98 | 0.04 | 31,31,31,31 | 0 |
| 55 | MG | 1A | 3113 | 1/1 | 0.98 | 0.10 | 34,34,34,34 | 0 |
| 55 | MG | 1A | 3754 | 1/1 | 0.98 | 0.09 | 30,30,30,30 | 0 |
| 55 | MG | 1A | 3978 | 1/1 | 0.98 | 0.06 | 40,40,40,40 | 0 |
| 55 | MG | 1a | 1687 | 1/1 | 0.98 | 0.16 | 52,52,52,52 | 0 |
| 55 | MG | 2A | 3048 | 1/1 | 0.98 | 0.05 | 52,52,52,52 | 0 |
| 55 | MG | 1A | 3562 | 1/1 | 0.98 | 0.08 | 17,17,17,17 | 0 |
| 55 | MG | 1A | 3275 | 1/1 | 0.98 | 0.34 | 28,28,28,28 | 0 |
| 55 | MG | 1D | 313 | 1/1 | 0.98 | 0.18 | 30,30,30,30 | 0 |
| 55 | MG | 2A | 3786 | 1/1 | 0.98 | 0.04 | 72,72,72,72 | 0 |
| 55 | MG | 1A | 3698 | 1/1 | 0.98 | 0.08 | 39,39,39,39 | 0 |
| 55 | MG | 1A | 3012 | 1/1 | 0.98 | 0.06 | 28,28,28,28 | 0 |
| 55 | MG | 1E | 303 | 1/1 | 0.98 | 0.14 | 27,27,27,27 | 0 |
| 55 | MG | 2A | 3790 | 1/1 | 0.98 | 0.05 | 59,59,59,59 | 0 |
| 55 | MG | 2a | 3003 | 1/1 | 0.98 | 0.17 | 49,49,49,49 | 0 |
| 55 | MG | 1A | 3061 | 1/1 | 0.98 | 0.08 | 31,31,31,31 | 0 |
| 55 | MG | 1A | 3701 | 1/1 | 0.98 | 0.06 | 18,18,18,18 | 0 |
| 55 | MG | 2A | 3530 | 1/1 | 0.98 | 0.16 | 41,41,41,41 | 0 |
| 55 | MG | 1A | 3986 | 1/1 | 0.98 | 0.06 | 24,24,24,24 | 0 |
| 55 | MG | 2A | 3532 | 1/1 | 0.98 | 0.17 | 42,42,42,42 | 0 |
| 55 | MG | 1A | 3116 | 1/1 | 0.98 | 0.06 | 30,30,30,30 | 0 |
| 55 | MG | 1A | 3153 | 1/1 | 0.98 | 0.09 | 49,49,49,49 | 0 |
| 55 | MG | 1A | 3281 | 1/1 | 0.98 | 0.14 | 36,36,36,36 | 0 |
| 55 | MG | 1a | 1700 | 1/1 | 0.98 | 0.06 | 42,42,42,42 | 0 |
| 55 | MG | 1A | 3175 | 1/1 | 0.98 | 0.05 | 20,20,20,20 | 0 |
| 55 | MG | 1A | 3909 | 1/1 | 0.98 | 0.07 | 37,37,37,37 | 0 |
| 55 | MG | 1A | 3707 | 1/1 | 0.98 | 0.12 | 18,18,18,18 | 0 |
| 55 | MG | 1F | 302 | 1/1 | 0.98 | 0.15 | 33,33,33,33 | 0 |
| 55 | MG | 2A | 3668 | 1/1 | 0.98 | 0.08 | 36,36,36,36 | 0 |
| 55 | MG | 1F | 303 | 1/1 | 0.98 | 0.09 | 30,30,30,30 | 0 |
| 55 | MG | 1A | 3224 | 1/1 | 0.98 | 0.10 | 35,35,35,35 | 0 |
| 55 | MG | 1a | 1817 | 1/1 | 0.98 | 0.04 | 68,68,68,68 | 0 |
| 55 | MG | 1A | 3653 | 1/1 | 0.98 | 0.05 | 40,40,40,40 | 0 |
| 55 | MG | 2A | 3811 | 1/1 | 0.98 | 0.14 | 35,35,35,35 | 0 |
| 55 | MG | 1A | 3379 | 1/1 | 0.98 | 0.06 | 16,16,16,16 | 0 |
| 55 | MG | 1A | 3711 | 1/1 | 0.98 | 0.04 | 31,31,31,31 | 0 |
| 55 | MG | 2A | 3814 | 1/1 | 0.98 | 0.06 | 48,48,48,48 | 0 |
| 55 | MG | 1A | 3176 | 1/1 | 0.98 | 0.05 | 24,24,24,24 | 0 |
| 55 | MG | 2A | 3073 | 1/1 | 0.98 | 0.24 | 43,43,43,43 | 0 |
| 55 | MG | 1A | 3010 | 1/1 | 0.98 | 0.07 | 24,24,24,24 | 0 |
| 55 | MG | 1A | 3774 | 1/1 | 0.98 | 0.05 | 37,37,37,37 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 55 | MG | 2A | 3309 | 1/1 | 0.98 | 0.06 | 63,63,63,63 | 0 |
| 55 | MG | 1A | 3457 | 1/1 | 0.98 | 0.05 | 21,21,21,21 | 0 |
| 55 | MG | 2A | 3428 | 1/1 | 0.98 | 0.16 | 32,32,32,32 | 0 |
| 55 | MG | 1A | 3200 | 1/1 | 0.98 | 0.06 | 22,22,22,22 | 0 |
| 55 | MG | 1A | 4003 | 1/1 | 0.98 | 0.04 | 48,48,48,48 | 0 |
| 55 | MG | 2A | 3825 | 1/1 | 0.98 | 0.05 | 42,42,42,42 | 0 |
| 55 | MG | 1A | 3660 | 1/1 | 0.98 | 0.09 | 22,22,22,22 | 0 |
| 55 | MG | 1A | 4095 | 1/1 | 0.98 | 0.05 | 31,31,31,31 | 0 |
| 55 | MG | 1A | 3201 | 1/1 | 0.98 | 0.09 | 32,32,32,32 | 0 |
| 55 | MG | 2A | 3687 | 1/1 | 0.98 | 0.07 | 53,53,53,53 | 0 |
| 55 | MG | 1a | 1617 | 1/1 | 0.98 | 0.07 | 63,63,63,63 | 0 |
| 55 | MG | 1A | 3718 | 1/1 | 0.98 | 0.07 | 19,19,19,19 | 0 |
| 55 | MG | 2A | 3561 | 1/1 | 0.98 | 0.09 | 46,46,46,46 | 0 |
| 55 | MG | 1A | 3118 | 1/1 | 0.98 | 0.08 | 26,26,26,26 | 0 |
| 55 | MG | 2A | 3692 | 1/1 | 0.98 | 0.08 | 54,54,54,54 | 0 |
| 55 | MG | 1A | 3782 | 1/1 | 0.98 | 0.08 | 38,38,38,38 | 0 |
| 55 | MG | 1A | 3783 | 1/1 | 0.98 | 0.07 | 26,26,26,26 | 0 |
| 55 | MG | 1A | 3720 | 1/1 | 0.98 | 0.07 | 31,31,31,31 | 0 |
| 55 | MG | 1A | 3663 | 1/1 | 0.98 | 0.03 | 23,23,23,23 | 0 |
| 55 | MG | 1A | 3786 | 1/1 | 0.98 | 0.09 | 38,38,38,38 | 0 |
| 55 | MG | 2A | 3091 | 1/1 | 0.98 | 0.14 | 37,37,37,37 | 0 |
| 55 | MG | 2A | 3700 | 1/1 | 0.98 | 0.06 | 51,51,51,51 | 0 |
| 55 | MG | 1A | 3787 | 1/1 | 0.98 | 0.07 | 13,13,13,13 | 0 |
| 55 | MG | 2A | 3843 | 1/1 | 0.98 | 0.14 | 37,37,37,37 | 0 |
| 55 | MG | 1A | 3664 | 1/1 | 0.98 | 0.06 | 18,18,18,18 | 0 |
| 55 | MG | 1A | 3665 | 1/1 | 0.98 | 0.07 | 25,25,25,25 | 0 |
| 55 | MG | 1A | 3724 | 1/1 | 0.98 | 0.11 | 12,12,12,12 | 0 |
| 55 | MG | 1A | 3230 | 1/1 | 0.98 | 0.18 | 44,44,44,44 | 0 |
| 55 | MG | 1A | 3792 | 1/1 | 0.98 | 0.07 | 20,20,20,20 | 0 |
| 55 | MG | 1A | 3864 | 1/1 | 0.98 | 0.11 | 43,43,43,43 | 0 |
| 55 | MG | 2A | 3708 | 1/1 | 0.98 | 0.04 | 36,36,36,36 | 0 |
| 55 | MG | 1A | 4111 | 1/1 | 0.98 | 0.04 | 51,51,51,51 | 0 |
| 55 | MG | 1Q | 207 | 1/1 | 0.98 | 0.18 | 39,39,39,39 | 0 |
| 55 | MG | 1A | 3386 | 1/1 | 0.98 | 0.22 | 23,23,23,23 | 0 |
| 55 | MG | 1A | 3090 | 1/1 | 0.98 | 0.09 | 29,29,29,29 | 0 |
| 55 | MG | 1A | 3795 | 1/1 | 0.98 | 0.06 | 21,21,21,21 | 0 |
| 55 | MG | 1A | 3941 | 1/1 | 0.98 | 0.05 | 54,54,54,54 | 0 |
| 55 | MG | 2A | 3105 | 1/1 | 0.98 | 0.05 | 30,30,30,30 | 0 |
| 55 | MG | 1A | 4025 | 1/1 | 0.98 | 0.08 | 25,25,25,25 | 0 |
| 55 | MG | 1A | 3728 | 1/1 | 0.98 | 0.04 | 31,31,31,31 | 0 |
| 55 | MG | 1U | 201 | 1/1 | 0.98 | 0.26 | 33,33,33,33 | 0 |
| 55 | MG | 2A | 3460 | 1/1 | 0.98 | 0.20 | 48,48,48,48 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 55 | MG | 1A | 3943 | 1/1 | 0.98 | 0.07 | 39,39,39,39 | 0 |
| 55 | MG | 1U | 203 | 1/1 | 0.98 | 0.02 | 22,22,22,22 | 0 |
| 55 | MG | 1B | 202 | 1/1 | 0.98 | 0.09 | 35,35,35,35 | 0 |
| 55 | MG | 1A | 4028 | 1/1 | 0.98 | 0.04 | 44,44,44,44 | 0 |
| 55 | MG | 1A | 3080 | 1/1 | 0.98 | 0.13 | 34,34,34,34 | 0 |
| 55 | MG | 2A | 3466 | 1/1 | 0.98 | 0.31 | 42,42,42,42 | 0 |
| 55 | MG | 1A | 3015 | 1/1 | 0.98 | 0.06 | 33,33,33,33 | 0 |
| 55 | MG | 1a | 1648 | 1/1 | 0.98 | 0.16 | 36,36,36,36 | 0 |
| 55 | MG | 1B | 206 | 1/1 | 0.98 | 0.12 | 40,40,40,40 | 0 |
| 55 | MG | 1A | 3544 | 1/1 | 0.98 | 0.10 | 30,30,30,30 | 0 |
| 55 | MG | 1A | 3003 | 1/1 | 0.98 | 0.07 | 22,22,22,22 | 0 |
| 55 | MG | 2A | 3004 | 1/1 | 0.98 | 0.04 | 43,43,43,43 | 0 |
| 55 | MG | 1A | 4033 | 1/1 | 0.98 | 0.04 | 36,36,36,36 | 0 |
| 55 | MG | 1A | 3802 | 1/1 | 0.98 | 0.04 | 32,32,32,32 | 0 |
| 55 | MG | 1A | 3023 | 1/1 | 0.98 | 0.07 | 35,35,35,35 | 0 |
| 55 | MG | 1a | 1756 | 1/1 | 0.98 | 0.04 | 41,41,41,41 | 0 |
| 55 | MG | 1A | 3034 | 1/1 | 0.98 | 0.09 | 24,24,24,24 | 0 |
| 56 | ZN | 14 | 501 | 1/1 | 0.98 | 0.07 | 109,109,109,109 | 0 |
| 55 | MG | 1a | 1759 | 1/1 | 0.98 | 0.06 | 40,40,40,40 | 0 |
| 55 | MG | 2A | 3126 | 1/1 | 0.98 | 0.16 | 34,34,34,34 | 0 |
| 55 | MG | 1a | 1760 | 1/1 | 0.98 | 0.14 | 39,39,39,39 | 0 |
| 55 | MG | 1A | 3085 | 1/1 | 0.98 | 0.07 | 24,24,24,24 | 0 |
| 58 | SF4 | 1d | 501 | 8/8 | 0.98 | 0.05 | 57,70,76,77 | 0 |
| 58 | SF4 | 2d | 303 | 8/8 | 0.98 | 0.05 | 58,77,87,92 | 0 |
| 55 | MG | 1A | 4070 | 1/1 | 0.99 | 0.07 | 19,19,19,19 | 0 |
| 55 | MG | 1A | 3985 | 1/1 | 0.99 | 0.05 | 24,24,24,24 | 0 |
| 55 | MG | 1A | 3689 | 1/1 | 0.99 | 0.09 | 28,28,28,28 | 0 |
| 55 | MG | 2A | 3822 | 1/1 | 0.99 | 0.11 | 26,26,26,26 | 0 |
| 55 | MG | 1A | 3690 | 1/1 | 0.99 | 0.16 | 35,35,35,35 | 0 |
| 55 | MG | 1A | 3640 | 1/1 | 0.99 | 0.05 | 28,28,28,28 | 0 |
| 55 | MG | 1A | 3490 | 1/1 | 0.99 | 0.12 | 28,28,28,28 | 0 |
| 55 | MG | 1A | 3990 | 1/1 | 0.99 | 0.06 | 56,56,56,56 | 0 |
| 55 | MG | 1A | 3846 | 1/1 | 0.99 | 0.03 | 28,28,28,28 | 0 |
| 55 | MG | 1A | 3666 | 1/1 | 0.99 | 0.07 | 22,22,22,22 | 0 |
| 55 | MG | 2A | 3694 | 1/1 | 0.99 | 0.06 | 24,24,24,24 | 0 |
| 55 | MG | 1A | 3953 | 1/1 | 0.99 | 0.03 | 19,19,19,19 | 0 |
| 55 | MG | 2A | 3186 | 1/1 | 0.99 | 0.15 | 40,40,40,40 | 0 |
| 55 | MG | 2A | 3187 | 1/1 | 0.99 | 0.05 | 53,53,53,53 | 0 |
| 55 | MG | 1A | 3491 | 1/1 | 0.99 | 0.16 | 29,29,29,29 | 0 |
| 55 | MG | 1A | 3437 | 1/1 | 0.99 | 0.03 | 36,36,36,36 | 0 |
| 55 | MG | 1a | 1757 | 1/1 | 0.99 | 0.12 | 47,47,47,47 | 0 |
| 55 | MG | 1A | 3956 | 1/1 | 0.99 | 0.08 | 24,24,24,24 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 55 | MG | 2P | 202 | 1/1 | 0.99 | 0.06 | 48,48,48,48 | 0 |
| 55 | MG | 1A | 3405 | 1/1 | 0.99 | 0.13 | 40,40,40,40 | 0 |
| 55 | MG | 1A | 3272 | 1/1 | 0.99 | 0.13 | 22,22,22,22 | 0 |
| 55 | MG | 1A | 4085 | 1/1 | 0.99 | 0.04 | 39,39,39,39 | 0 |
| 55 | MG | 1A | 3014 | 1/1 | 0.99 | 0.05 | 18,18,18,18 | 0 |
| 55 | MG | 1A | 4087 | 1/1 | 0.99 | 0.04 | 37,37,37,37 | 0 |
| 55 | MG | 2A | 3075 | 1/1 | 0.99 | 0.03 | 29,29,29,29 | 0 |
| 55 | MG | 1A | 3135 | 1/1 | 0.99 | 0.10 | 25,25,25,25 | 0 |
| 55 | MG | 2A | 3514 | 1/1 | 0.99 | 0.08 | 26,26,26,26 | 0 |
| 55 | MG | 1A | 3923 | 1/1 | 0.99 | 0.05 | 29,29,29,29 | 0 |
| 55 | MG | 2A | 3580 | 1/1 | 0.99 | 0.10 | 45,45,45,45 | 0 |
| 55 | MG | 2A | 3018 | 1/1 | 0.99 | 0.05 | 32,32,32,32 | 0 |
| 55 | MG | 1A | 3019 | 1/1 | 0.99 | 0.10 | 28,28,28,28 | 0 |
| 55 | MG | 1A | 3276 | 1/1 | 0.99 | 0.08 | 38,38,38,38 | 0 |
| 55 | MG | 1a | 1768 | 1/1 | 0.99 | 0.05 | 40,40,40,40 | 0 |
| 55 | MG | 1A | 3702 | 1/1 | 0.99 | 0.09 | 14,14,14,14 | 0 |
| 55 | MG | 1A | 3289 | 1/1 | 0.99 | 0.06 | 33,33,33,33 | 0 |
| 55 | MG | 1A | 3760 | 1/1 | 0.99 | 0.06 | 24,24,24,24 | 0 |
| 55 | MG | 2X | 102 | 1/1 | 0.99 | 0.10 | 52,52,52,52 | 0 |
| 55 | MG | 1A | 3761 | 1/1 | 0.99 | 0.08 | 14,14,14,14 | 0 |
| 55 | MG | 1A | 3066 | 1/1 | 0.99 | 0.07 | 26,26,26,26 | 0 |
| 55 | MG | 1A | 3173 | 1/1 | 0.99 | 0.03 | 24,24,24,24 | 0 |
| 55 | MG | 2A | 3210 | 1/1 | 0.99 | 0.12 | 35,35,35,35 | 0 |
| 55 | MG | 1A | 3222 | 1/1 | 0.99 | 0.11 | 28,28,28,28 | 0 |
| 55 | MG | 1A | 4052 | 1/1 | 0.99 | 0.04 | 24,24,24,24 | 0 |
| 55 | MG | 1A | 4053 | 1/1 | 0.99 | 0.04 | 29,29,29,29 | 0 |
| 55 | MG | 1A | 3933 | 1/1 | 0.99 | 0.03 | 24,24,24,24 | 0 |
| 55 | MG | 1A | 3022 | 1/1 | 0.99 | 0.04 | 29,29,29,29 | 0 |
| 55 | MG | 1A | 3830 | 1/1 | 0.99 | 0.06 | 31,31,31,31 | 0 |
| 55 | MG | 2A | 3034 | 1/1 | 0.99 | 0.09 | 36,36,36,36 | 0 |
| 55 | MG | 1e | 202 | 1/1 | 0.99 | 0.09 | 56,56,56,56 | 0 |
| 55 | MG | 1A | 3078 | 1/1 | 0.99 | 0.03 | 30,30,30,30 | 0 |
| 55 | MG | 1B | 235 | 1/1 | 0.99 | 0.04 | 23,23,23,23 | 0 |
| 55 | MG | 1A | 3656 | 1/1 | 0.99 | 0.06 | 20,20,20,20 | 0 |
| 55 | MG | 1A | 3799 | 1/1 | 0.99 | 0.04 | 41,41,41,41 | 0 |
| 55 | MG | 1a | 1785 | 1/1 | 0.99 | 0.06 | 51,51,51,51 | 0 |
| 55 | MG | 1D | 303 | 1/1 | 0.99 | 0.09 | 43,43,43,43 | 0 |
| 55 | MG | 2A | 3803 | 1/1 | 0.99 | 0.06 | 29,29,29,29 | 0 |
| 55 | MG | 1A | 3059 | 1/1 | 0.99 | 0.05 | 28,28,28,28 | 0 |
| 55 | MG | 1A | 3468 | 1/1 | 0.99 | 0.08 | 46,46,46,46 | 0 |
| 55 | MG | 1A | 3271 | 1/1 | 0.99 | 0.11 | 26,26,26,26 | 0 |
| 55 | MG | 1Q | 206 | 1/1 | 0.99 | 0.04 | 35,35,35,35 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 55 | MG | 2A | 3808 | 1/1 | 0.99 | 0.04 | 45,45,45,45 | 0 |
| 55 | MG | 1a | 1635 | 1/1 | 0.99 | 0.10 | 30,30,30,30 | 0 |
| 55 | MG | 1A | 4020 | 1/1 | 0.99 | 0.04 | 26,26,26,26 | 0 |
| 55 | MG | 1A | 3403 | 1/1 | 0.99 | 0.07 | 38,38,38,38 | 0 |
| 56 | ZN | 1Y | 205 | 1/1 | 0.99 | 0.02 | 57,57,57,57 | 0 |
| 55 | MG | 1A | 3571 | 1/1 | 0.99 | 0.09 | 32,32,32,32 | 0 |
| 56 | ZN | 15 | 106 | 1/1 | 0.99 | 0.03 | 46,46,46,46 | 0 |
| 56 | ZN | 16 | 102 | 1/1 | 0.99 | 0.04 | 41,41,41,41 | 0 |
| 56 | ZN | 19 | 102 | 1/1 | 0.99 | 0.05 | 41,41,41,41 | 0 |
| 56 | ZN | 1n | 103 | 1/1 | 0.99 | 0.03 | 69,69,69,69 | 0 |
| 56 | ZN | 2Y | 501 | 1/1 | 0.99 | 0.02 | 77,77,77,77 | 0 |
| 55 | MG | 1A | 3375 | 1/1 | 0.99 | 0.04 | 26,26,26,26 | 0 |
| 56 | ZN | 26 | 102 | 1/1 | 0.99 | 0.07 | 54,54,54,54 | 0 |
| 56 | ZN | 29 | 501 | 1/1 | 0.99 | 0.05 | 61,61,61,61 | 0 |
| 55 | MG | 1A | 3530 | 1/1 | 0.99 | 0.12 | 19,19,19,19 | 0 |
| 55 | MG | 1a | 1797 | 1/1 | 0.99 | 0.08 | 58,58,58,58 | 0 |
| 55 | MG | 1A | 4068 | 1/1 | 0.99 | 0.07 | 23,23,23,23 | 0 |
| 55 | MG | 1a | 1799 | 1/1 | 0.99 | 0.07 | 68,68,68,68 | 0 |
| 55 | MG | 1A | 3807 | 1/1 | 0.99 | 0.08 | 36,36,36,36 | 0 |
| 56 | ZN | 25 | 103 | 1/1 | 1.00 | 0.02 | 52,52,52,52 | 0 |
| 55 | MG | 1A | 3821 | 1/1 | 1.00 | 0.08 | 21,21,21,21 | 0 |
| 55 | MG | 1A | 3906 | 1/1 | 1.00 | 0.04 | 17,17,17,17 | 0 |
| 55 | MG | 1A | 3781 | 1/1 | 1.00 | 0.03 | 37,37,37,37 | 0 |

## 6.5 Other polymers (i)

There are no such residues in this entry.