



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 05:02 PM UTC

PDB ID : 9DFD / pdb_00009dfd
Title : Crystal structure of the wild-type *Thermus thermophilus* 70S ribosome in complex with lasso peptide lariocidin B, mRNA, aminoacylated A-site Phe-tRNA^{phe}, aminoacylated P-site fMet-tRNA^{met}, and deacylated E-site tRNA^{phe} at 2.60Å resolution
Authors : Aleksandrova, E.V.; Travin, D.Y.; Jangra, M.; Kaur, M.; Darwish, L.; Koteva, K.; Klepacki, D.; Wang, W.; Tiffany, M.; Sokaribo, A.; Coombes, B.K.; Vazquez-Laslop, N.; Wright, G.D.; Mankin, A.S.; Polikanov, Y.S.
Deposited on : 2024-08-29
Resolution : 2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

The types of validation reports are described at

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

The following versions of software and data (see [references ⓘ](#)) 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 |
| 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) |

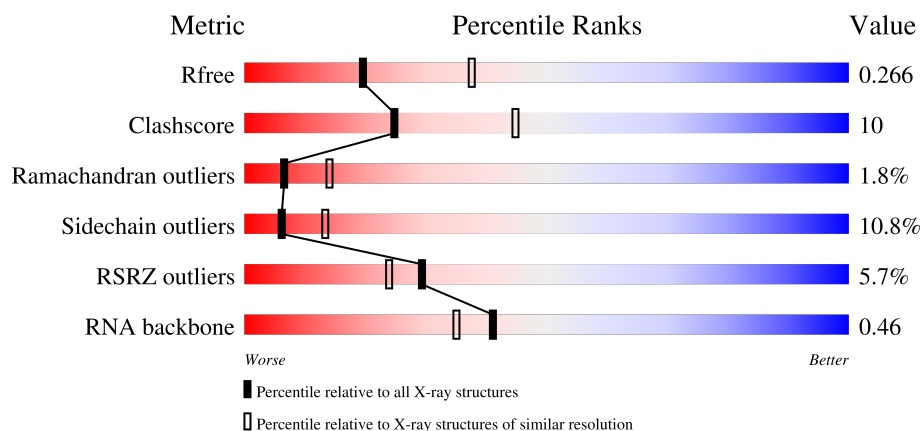
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

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



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




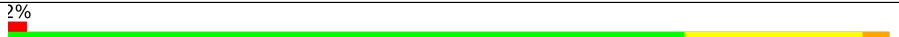
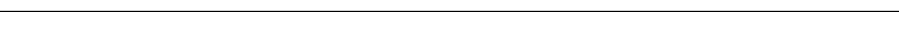
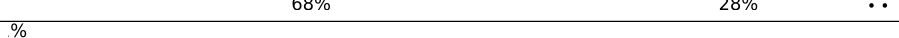
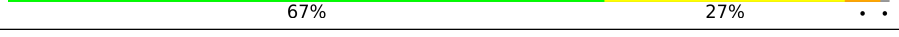




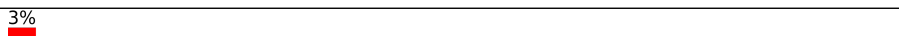

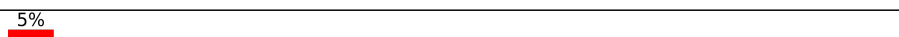





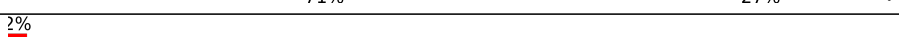





The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively.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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 1 | 1A | 2915 | <div> <div>6%</div> <div>63% 29% 7%</div> </div> |
| 1 | 2A | 2915 | <div> <div>6%</div> <div>57% 31% 7%</div> </div> |

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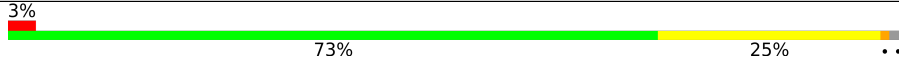
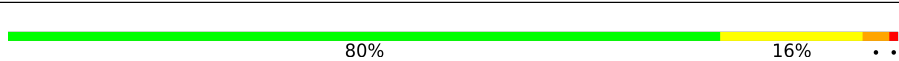
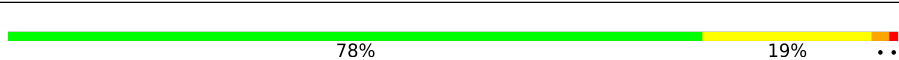
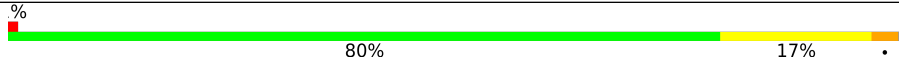
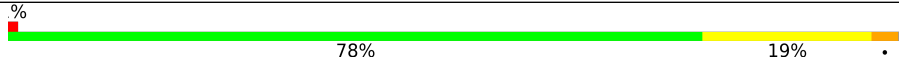
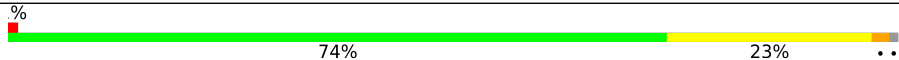
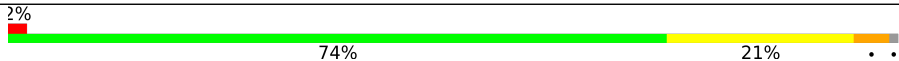
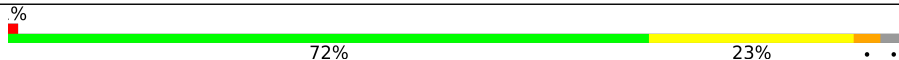

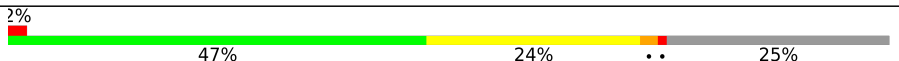
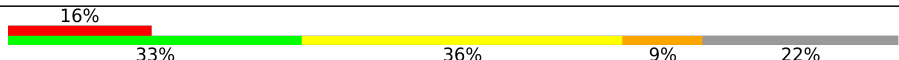
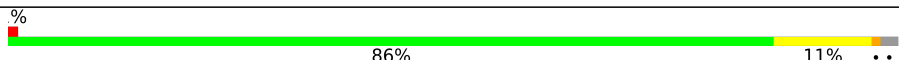
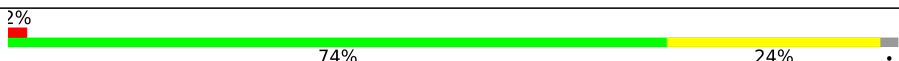
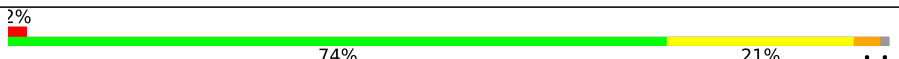
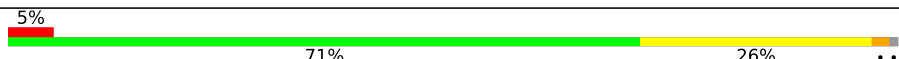

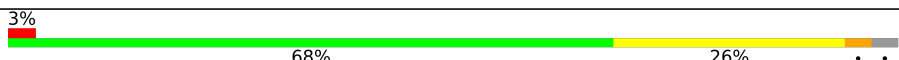
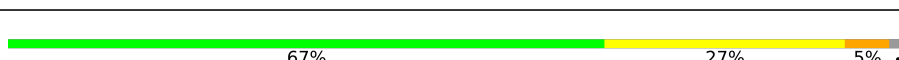
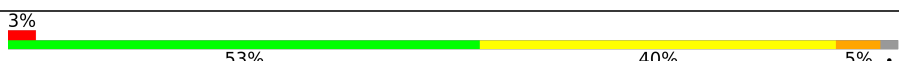
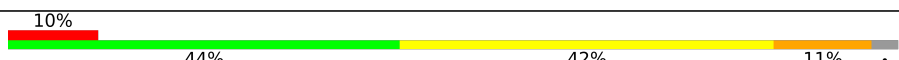
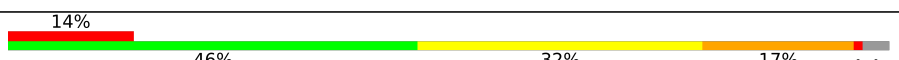
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 2 | 1B | 121 |  |
| 2 | 2B | 121 |  |
| 3 | 1D | 276 |  |
| 3 | 2D | 276 |  |
| 4 | 1E | 206 |  |
| 4 | 2E | 206 |  |
| 5 | 1F | 210 |  |
| 5 | 2F | 210 |  |
| 6 | 1G | 182 |  |
| 6 | 2G | 182 |  |
| 7 | 1H | 180 |  |
| 7 | 2H | 180 |  |
| 8 | 1I | 148 |  |
| 8 | 2I | 148 |  |
| 9 | 1N | 140 |  |
| 9 | 2N | 140 |  |
| 10 | 1O | 122 |  |
| 10 | 2O | 122 |  |
| 11 | 1P | 150 |  |
| 11 | 2P | 150 |  |
| 12 | 1Q | 141 |  |
| 12 | 2Q | 141 |  |
| 13 | 1R | 118 |  |
| 13 | 2R | 118 |  |
| 14 | 1S | 112 |  |


























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

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 27 | 15 | 60 |  |
| 27 | 25 | 60 |  |
| 28 | 16 | 54 |  |
| 28 | 26 | 54 |  |
| 29 | 17 | 49 |  |
| 29 | 27 | 49 |  |
| 30 | 18 | 65 |  |
| 30 | 28 | 65 |  |
| 31 | 19 | 37 |  |
| 31 | 29 | 37 |  |
| 32 | 1a | 1521 |  |
| 32 | 2a | 1521 |  |
| 33 | 1b | 256 |  |
| 33 | 2b | 256 |  |
| 34 | 1c | 239 |  |
| 34 | 2c | 239 |  |
| 35 | 1d | 209 |  |
| 35 | 2d | 209 |  |
| 36 | 1e | 162 |  |
| 36 | 2e | 162 |  |
| 37 | 1f | 101 |  |
| 37 | 2f | 101 |  |
| 38 | 1g | 156 |  |
| 38 | 2g | 156 |  |
| 39 | 1h | 138 |  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 39 | 2h | 138 | |
| 40 | 1i | 128 | |
| 40 | 2i | 128 | |
| 41 | 1j | 105 | |
| 41 | 2j | 105 | |
| 42 | 1k | 129 | |
| 42 | 2k | 129 | |
| 43 | 1l | 132 | |
| 43 | 2l | 132 | |
| 44 | 1m | 126 | |
| 44 | 2m | 126 | |
| 45 | 1n | 61 | |
| 45 | 2n | 61 | |
| 46 | 1o | 89 | |
| 46 | 2o | 89 | |
| 47 | 1p | 88 | |
| 47 | 2p | 88 | |
| 48 | 1q | 105 | |
| 48 | 2q | 105 | |
| 49 | 1r | 88 | |
| 49 | 2r | 88 | |
| 50 | 1s | 93 | |
| 50 | 2s | 93 | |
| 51 | 1t | 106 | |
| 51 | 2t | 106 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 52 | 1u | 27 | |
| 52 | 2u | 27 | |
| 53 | 1v | 24 | |
| 53 | 2v | 24 | |
| 54 | 1w | 76 | |
| 54 | 2w | 76 | |
| 55 | 1x | 77 | |
| 55 | 2x | 77 | |
| 56 | 1y | 76 | |
| 56 | 2y | 76 | |
| 57 | 1z | 17 | |
| 57 | 2z | 17 | |

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 |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 58 | MG | 29 | 101 | - | - | - | X |
| 61 | SF4 | 1d | 302 | - | - | X | - |

2 Entry composition

There are 62 unique types of molecules in this entry. The entry contains 300583 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 44 | 1m | 125 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 979 | 604 | 204 | 169 | 2 | | | |
| 44 | 2m | 122 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 950 | 586 | 197 | 165 | 2 | | | |

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 53 is a RNA chain called MET-PHE-mRNA.

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

- Molecule 54 is a RNA chain called A-site Aminoacylated Phe-tRNA^{phe}.

| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---|---------|---------|-------|
| 54 | 1w | 75 | Total | C | N | O | P | S | 0 | 0 | 0 |
| | | | 1623 | 731 | 289 | 526 | 75 | 2 | | | |
| 54 | 2w | 72 | Total | C | N | O | P | S | 0 | 0 | 0 |
| | | | 1555 | 699 | 280 | 502 | 72 | 2 | | | |

- Molecule 55 is a RNA chain called P-site Aminoacylated fMet-tRNA^{met}.

| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---|---------|---------|-------|
| 55 | 1x | 77 | Total | C | N | O | P | S | 0 | 0 | 0 |
| | | | 1656 | 740 | 299 | 538 | 77 | 2 | | | |
| 55 | 2x | 77 | Total | C | N | O | P | S | 0 | 0 | 0 |
| | | | 1656 | 740 | 299 | 538 | 77 | 2 | | | |

- Molecule 56 is a RNA chain called E-site Deacylated tRNA^{phe}.

| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---|---------|---------|-------|
| 56 | 1y | 74 | Total | C | N | O | P | S | 0 | 0 | 0 |
| | | | 1585 | 707 | 285 | 518 | 74 | 1 | | | |
| 56 | 2y | 73 | Total | C | N | O | P | S | 0 | 0 | 0 |
| | | | 1565 | 698 | 283 | 510 | 73 | 1 | | | |

- Molecule 57 is a protein called Lasso peptide lariocidin B.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---------|---------|-------|
| 57 | 1z | 17 | Total | C | N | O | 0 | 0 | 0 |
| | | | 127 | 79 | 28 | 20 | | | |
| 57 | 2z | 17 | Total | C | N | O | 0 | 0 | 0 |
| | | | 127 | 79 | 28 | 20 | | | |

- Molecule 58 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|------|---------|---------|
| 58 | 1A | 1105 | Total | Mg | 0 | 0 |
| | | | 1105 | 1105 | | |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|----------|---------|---------|
| 58 | 1B | 37 | Total 37 | Mg 37 | 0 | 0 |
| 58 | 1D | 12 | Total 12 | Mg 12 | 0 | 0 |
| 58 | 1E | 14 | Total 14 | Mg 14 | 0 | 0 |
| 58 | 1F | 13 | Total 13 | Mg 13 | 0 | 0 |
| 58 | 1G | 5 | Total 5 | Mg 5 | 0 | 0 |
| 58 | 1I | 1 | Total 1 | Mg 1 | 0 | 0 |
| 58 | 1N | 7 | Total 7 | Mg 7 | 0 | 0 |
| 58 | 1O | 5 | Total 5 | Mg 5 | 0 | 0 |
| 58 | 1P | 4 | Total 4 | Mg 4 | 0 | 0 |
| 58 | 1Q | 7 | Total 7 | Mg 7 | 0 | 0 |
| 58 | 1R | 4 | Total 4 | Mg 4 | 0 | 0 |
| 58 | 1S | 3 | Total 3 | Mg 3 | 0 | 0 |
| 58 | 1T | 3 | Total 3 | Mg 3 | 0 | 0 |
| 58 | 1U | 11 | Total 11 | Mg 11 | 0 | 0 |
| 58 | 1V | 7 | Total 7 | Mg 7 | 0 | 0 |
| 58 | 1W | 8 | Total 8 | Mg 8 | 0 | 0 |
| 58 | 1X | 6 | Total 6 | Mg 6 | 0 | 0 |
| 58 | 1Y | 3 | Total 3 | Mg 3 | 0 | 0 |
| 58 | 1Z | 3 | Total 3 | Mg 3 | 0 | 0 |
| 58 | 10 | 9 | Total 9 | Mg 9 | 0 | 0 |
| 58 | 11 | 6 | Total 6 | Mg 6 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|-----------|---------|---------|
| 58 | 12 | 2 | Total 2 | Mg 2 | 0 | 0 |
| 58 | 13 | 3 | Total 3 | Mg 3 | 0 | 0 |
| 58 | 15 | 9 | Total 9 | Mg 9 | 0 | 0 |
| 58 | 16 | 2 | Total 2 | Mg 2 | 0 | 0 |
| 58 | 17 | 3 | Total 3 | Mg 3 | 0 | 0 |
| 58 | 18 | 5 | Total 5 | Mg 5 | 0 | 0 |
| 58 | 19 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 58 | 1a | 218 | Total 218 | Mg 218 | 0 | 0 |
| 58 | 1b | 1 | Total 1 | Mg 1 | 0 | 0 |
| 58 | 1d | 1 | Total 1 | Mg 1 | 0 | 0 |
| 58 | 1e | 2 | Total 2 | Mg 2 | 0 | 0 |
| 58 | 1f | 2 | Total 2 | Mg 2 | 0 | 0 |
| 58 | 1h | 1 | Total 1 | Mg 1 | 0 | 0 |
| 58 | 1l | 2 | Total 2 | Mg 2 | 0 | 0 |
| 58 | 1m | 1 | Total 1 | Mg 1 | 0 | 0 |
| 58 | 1n | 1 | Total 1 | Mg 1 | 0 | 0 |
| 58 | 1p | 1 | Total 1 | Mg 1 | 0 | 0 |
| 58 | 1s | 1 | Total 1 | Mg 1 | 0 | 0 |
| 58 | 1t | 1 | Total 1 | Mg 1 | 0 | 0 |
| 58 | 1v | 2 | Total 2 | Mg 2 | 0 | 0 |
| 58 | 1w | 8 | Total 8 | Mg 8 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|---------------------|---------|---------|
| 58 | 1x | 13 | Total 13 Mg 13 | 0 | 0 |
| 58 | 1y | 1 | Total 1 Mg 1 | 0 | 0 |
| 58 | 2A | 883 | Total 883 Mg 883 | 0 | 0 |
| 58 | 2B | 19 | Total 19 Mg 19 | 0 | 0 |
| 58 | 2D | 7 | Total 7 Mg 7 | 0 | 0 |
| 58 | 2E | 11 | Total 11 Mg 11 | 0 | 0 |
| 58 | 2F | 9 | Total 9 Mg 9 | 0 | 0 |
| 58 | 2G | 1 | Total 1 Mg 1 | 0 | 0 |
| 58 | 2N | 1 | Total 1 Mg 1 | 0 | 0 |
| 58 | 2O | 1 | Total 1 Mg 1 | 0 | 0 |
| 58 | 2Q | 3 | Total 3 Mg 3 | 0 | 0 |
| 58 | 2R | 3 | Total 3 Mg 3 | 0 | 0 |
| 58 | 2S | 1 | Total 1 Mg 1 | 0 | 0 |
| 58 | 2T | 3 | Total 3 Mg 3 | 0 | 0 |
| 58 | 2U | 2 | Total 2 Mg 2 | 0 | 0 |
| 58 | 2V | 2 | Total 2 Mg 2 | 0 | 0 |
| 58 | 2W | 2 | Total 2 Mg 2 | 0 | 0 |
| 58 | 2X | 1 | Total 1 Mg 1 | 0 | 0 |
| 58 | 2Z | 1 | Total 1 Mg 1 | 0 | 0 |
| 58 | 21 | 1 | Total 1 Mg 1 | 0 | 0 |
| 58 | 23 | 1 | Total 1 Mg 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|-----------|---------|---------|
| 58 | 25 | 4 | Total 4 | Mg 4 | 0 | 0 |
| 58 | 26 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 58 | 27 | 3 | Total 3 | Mg 3 | 0 | 0 |
| 58 | 28 | 4 | Total 4 | Mg 4 | 0 | 0 |
| 58 | 29 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 58 | 2a | 242 | Total 242 | Mg 242 | 0 | 0 |
| 58 | 2d | 1 | Total 1 | Mg 1 | 0 | 0 |
| 58 | 2e | 1 | Total 1 | Mg 1 | 0 | 0 |
| 58 | 2f | 2 | Total 2 | Mg 2 | 0 | 0 |
| 58 | 2g | 1 | Total 1 | Mg 1 | 0 | 0 |
| 58 | 2i | 1 | Total 1 | Mg 1 | 0 | 0 |
| 58 | 2j | 1 | Total 1 | Mg 1 | 0 | 0 |
| 58 | 2l | 5 | Total 5 | Mg 5 | 0 | 0 |
| 58 | 2p | 1 | Total 1 | Mg 1 | 0 | 0 |
| 58 | 2q | 2 | Total 2 | Mg 2 | 0 | 0 |
| 58 | 2r | 1 | Total 1 | Mg 1 | 0 | 0 |
| 58 | 2t | 1 | Total 1 | Mg 1 | 0 | 0 |
| 58 | 2v | 3 | Total 3 | Mg 3 | 0 | 0 |
| 58 | 2w | 12 | Total 12 | Mg 12 | 0 | 0 |
| 58 | 2x | 5 | Total 5 | Mg 5 | 0 | 0 |
| 58 | 2y | 6 | Total 6 | Mg 6 | 0 | 0 |

- Molecule 59 is POTASSIUM ION (CCD ID: K) (formula: K).

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|----------------|---------|---------|
| 59 | 1A | 1 | Total K 1 1 | 0 | 0 |
| 59 | 2x | 1 | Total K 1 1 | 0 | 0 |

- Molecule 60 is ZINC ION (CCD ID: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 60 | 1Y | 1 | Total Zn 1 1 | 0 | 0 |
| 60 | 14 | 1 | Total Zn 1 1 | 0 | 0 |
| 60 | 15 | 1 | Total Zn 1 1 | 0 | 0 |
| 60 | 16 | 1 | Total Zn 1 1 | 0 | 0 |
| 60 | 19 | 1 | Total Zn 1 1 | 0 | 0 |
| 60 | 1n | 1 | Total Zn 1 1 | 0 | 0 |
| 60 | 2Y | 1 | Total Zn 1 1 | 0 | 0 |
| 60 | 24 | 1 | Total Zn 1 1 | 0 | 0 |
| 60 | 25 | 1 | Total Zn 1 1 | 0 | 0 |
| 60 | 26 | 1 | Total Zn 1 1 | 0 | 0 |
| 60 | 29 | 1 | Total Zn 1 1 | 0 | 0 |
| 60 | 2n | 1 | Total Zn 1 1 | 0 | 0 |

- Molecule 61 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 61 | 1d | 1 | Total | Fe | S | 0 | 0 |
| | | | 8 | 4 | 4 | | |
| 61 | 2d | 1 | Total | Fe | S | 0 | 0 |
| | | | 8 | 4 | 4 | | |

- Molecule 62 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|------|---------|---------|
| 62 | 1A | 2019 | Total | O | 0 | 0 |
| | | | 2019 | 2019 | | |
| 62 | 1B | 63 | Total | O | 0 | 0 |
| | | | 63 | 63 | | |
| 62 | 1D | 24 | Total | O | 0 | 0 |
| | | | 24 | 24 | | |
| 62 | 1E | 24 | Total | O | 0 | 0 |
| | | | 24 | 24 | | |
| 62 | 1F | 15 | Total | O | 0 | 0 |
| | | | 15 | 15 | | |
| 62 | 1G | 2 | Total | O | 0 | 0 |
| | | | 2 | 2 | | |
| 62 | 1H | 2 | Total | O | 0 | 0 |
| | | | 2 | 2 | | |
| 62 | 1I | 1 | Total | O | 0 | 0 |
| | | | 1 | 1 | | |
| 62 | 1N | 5 | Total | O | 0 | 0 |
| | | | 5 | 5 | | |
| 62 | 1O | 6 | Total | O | 0 | 0 |
| | | | 6 | 6 | | |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 62 | 1P | 19 | Total 19 | O 19 | 0 | 0 |
| 62 | 1Q | 8 | Total 8 | O 8 | 0 | 0 |
| 62 | 1R | 12 | Total 12 | O 12 | 0 | 0 |
| 62 | 1S | 5 | Total 5 | O 5 | 0 | 0 |
| 62 | 1T | 9 | Total 9 | O 9 | 0 | 0 |
| 62 | 1U | 15 | Total 15 | O 15 | 0 | 0 |
| 62 | 1V | 8 | Total 8 | O 8 | 0 | 0 |
| 62 | 1W | 9 | Total 9 | O 9 | 0 | 0 |
| 62 | 1X | 4 | Total 4 | O 4 | 0 | 0 |
| 62 | 1Y | 3 | Total 3 | O 3 | 0 | 0 |
| 62 | 1Z | 1 | Total 1 | O 1 | 0 | 0 |
| 62 | 10 | 13 | Total 13 | O 13 | 0 | 0 |
| 62 | 11 | 11 | Total 11 | O 11 | 0 | 0 |
| 62 | 12 | 4 | Total 4 | O 4 | 0 | 0 |
| 62 | 13 | 5 | Total 5 | O 5 | 0 | 0 |
| 62 | 14 | 1 | Total 1 | O 1 | 0 | 0 |
| 62 | 15 | 5 | Total 5 | O 5 | 0 | 0 |
| 62 | 16 | 4 | Total 4 | O 4 | 0 | 0 |
| 62 | 17 | 7 | Total 7 | O 7 | 0 | 0 |
| 62 | 18 | 9 | Total 9 | O 9 | 0 | 0 |
| 62 | 1a | 388 | Total 388 | O 388 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|---------------|-----------|---------|---------|
| 62 | 1b | 1 | Total 1 | O 1 | 0 | 0 |
| 62 | 1f | 1 | Total 1 | O 1 | 0 | 0 |
| 62 | 1l | 8 | Total 8 | O 8 | 0 | 0 |
| 62 | 1m | 2 | Total 2 | O 2 | 0 | 0 |
| 62 | 1n | 1 | Total 1 | O 1 | 0 | 0 |
| 62 | 1o | 1 | Total 1 | O 1 | 0 | 0 |
| 62 | 1p | 1 | Total 1 | O 1 | 0 | 0 |
| 62 | 1q | 2 | Total 2 | O 2 | 0 | 0 |
| 62 | 1u | 1 | Total 1 | O 1 | 0 | 0 |
| 62 | 1v | 6 | Total 6 | O 6 | 0 | 0 |
| 62 | 1w | 20 | Total 20 | O 20 | 0 | 0 |
| 62 | 1x | 15 | Total 15 | O 15 | 0 | 0 |
| 62 | 1y | 2 | Total 2 | O 2 | 0 | 0 |
| 62 | 1z | 1 | Total 1 | O 1 | 0 | 0 |
| 62 | 2A | 1153 | Total 1153 | O 1153 | 0 | 0 |
| 62 | 2B | 23 | Total 23 | O 23 | 0 | 0 |
| 62 | 2D | 24 | Total 24 | O 24 | 0 | 0 |
| 62 | 2E | 14 | Total 14 | O 14 | 0 | 0 |
| 62 | 2F | 13 | Total 13 | O 13 | 0 | 0 |
| 62 | 2I | 2 | Total 2 | O 2 | 0 | 0 |
| 62 | 2N | 3 | Total 3 | O 3 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 62 | 2O | 3 | Total 3 | O 3 | 0 | 0 |
| 62 | 2P | 14 | Total 14 | O 14 | 0 | 0 |
| 62 | 2Q | 3 | Total 3 | O 3 | 0 | 0 |
| 62 | 2R | 3 | Total 3 | O 3 | 0 | 0 |
| 62 | 2T | 4 | Total 4 | O 4 | 0 | 0 |
| 62 | 2U | 2 | Total 2 | O 2 | 0 | 0 |
| 62 | 2W | 2 | Total 2 | O 2 | 0 | 0 |
| 62 | 2X | 2 | Total 2 | O 2 | 0 | 0 |
| 62 | 2Y | 1 | Total 1 | O 1 | 0 | 0 |
| 62 | 2Z | 1 | Total 1 | O 1 | 0 | 0 |
| 62 | 20 | 3 | Total 3 | O 3 | 0 | 0 |
| 62 | 21 | 13 | Total 13 | O 13 | 0 | 0 |
| 62 | 23 | 1 | Total 1 | O 1 | 0 | 0 |
| 62 | 25 | 1 | Total 1 | O 1 | 0 | 0 |
| 62 | 27 | 5 | Total 5 | O 5 | 0 | 0 |
| 62 | 28 | 4 | Total 4 | O 4 | 0 | 0 |
| 62 | 29 | 1 | Total 1 | O 1 | 0 | 0 |
| 62 | 2a | 283 | Total 283 | O 283 | 0 | 0 |
| 62 | 2c | 2 | Total 2 | O 2 | 0 | 0 |
| 62 | 2d | 2 | Total 2 | O 2 | 0 | 0 |
| 62 | 2e | 1 | Total 1 | O 1 | 0 | 0 |

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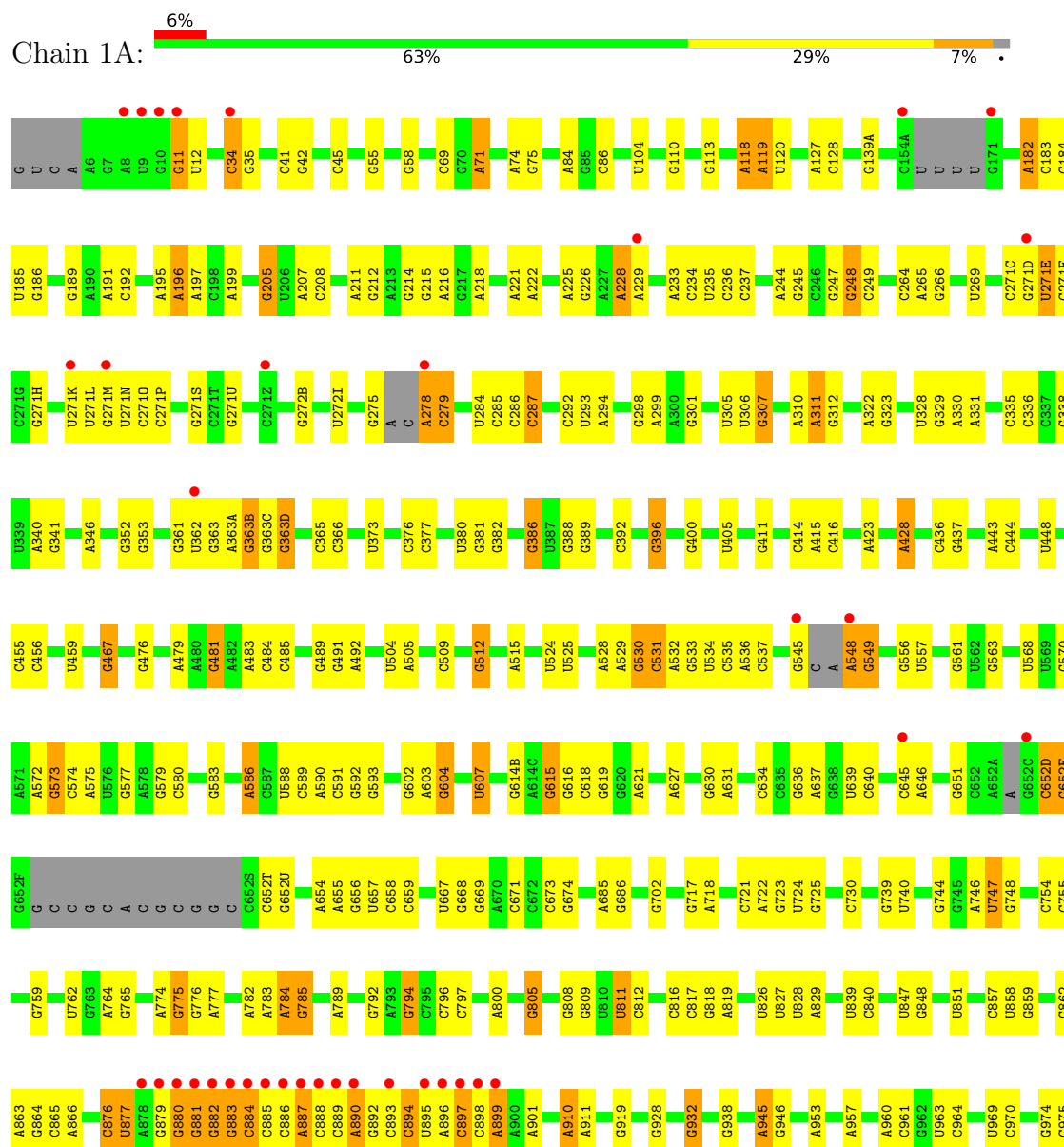
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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|
| 62 | 2j | 3 | Total 3 | O 3 | 0 | 0 |
| 62 | 2l | 6 | Total 6 | O 6 | 0 | 0 |
| 62 | 2p | 1 | Total 1 | O 1 | 0 | 0 |
| 62 | 2r | 1 | Total 1 | O 1 | 0 | 0 |
| 62 | 2t | 1 | Total 1 | O 1 | 0 | 0 |
| 62 | 2v | 2 | Total 2 | O 2 | 0 | 0 |
| 62 | 2w | 10 | Total 10 | O 10 | 0 | 0 |
| 62 | 2x | 6 | Total 6 | O 6 | 0 | 0 |
| 62 | 2y | 9 | Total 9 | O 9 | 0 | 0 |

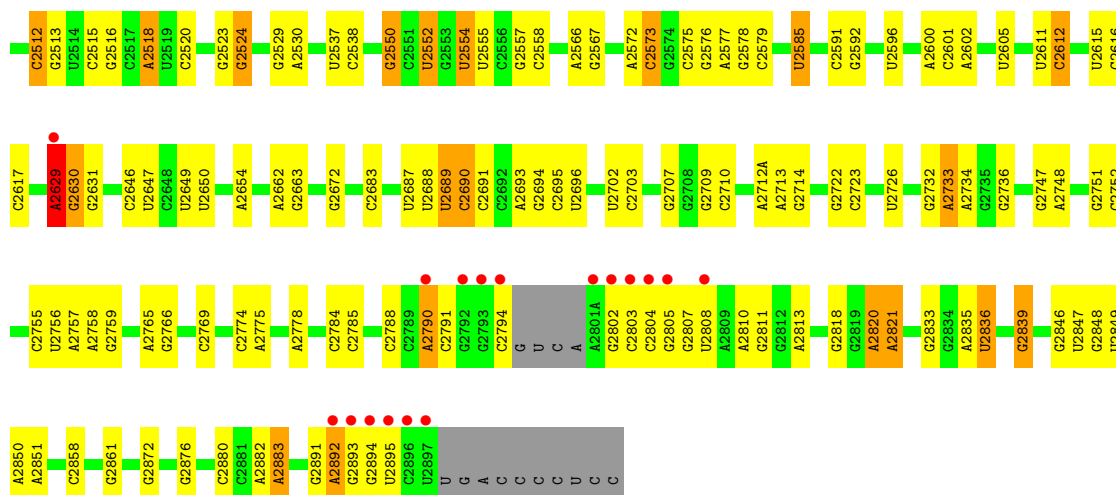
3 Residue-property plots

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.

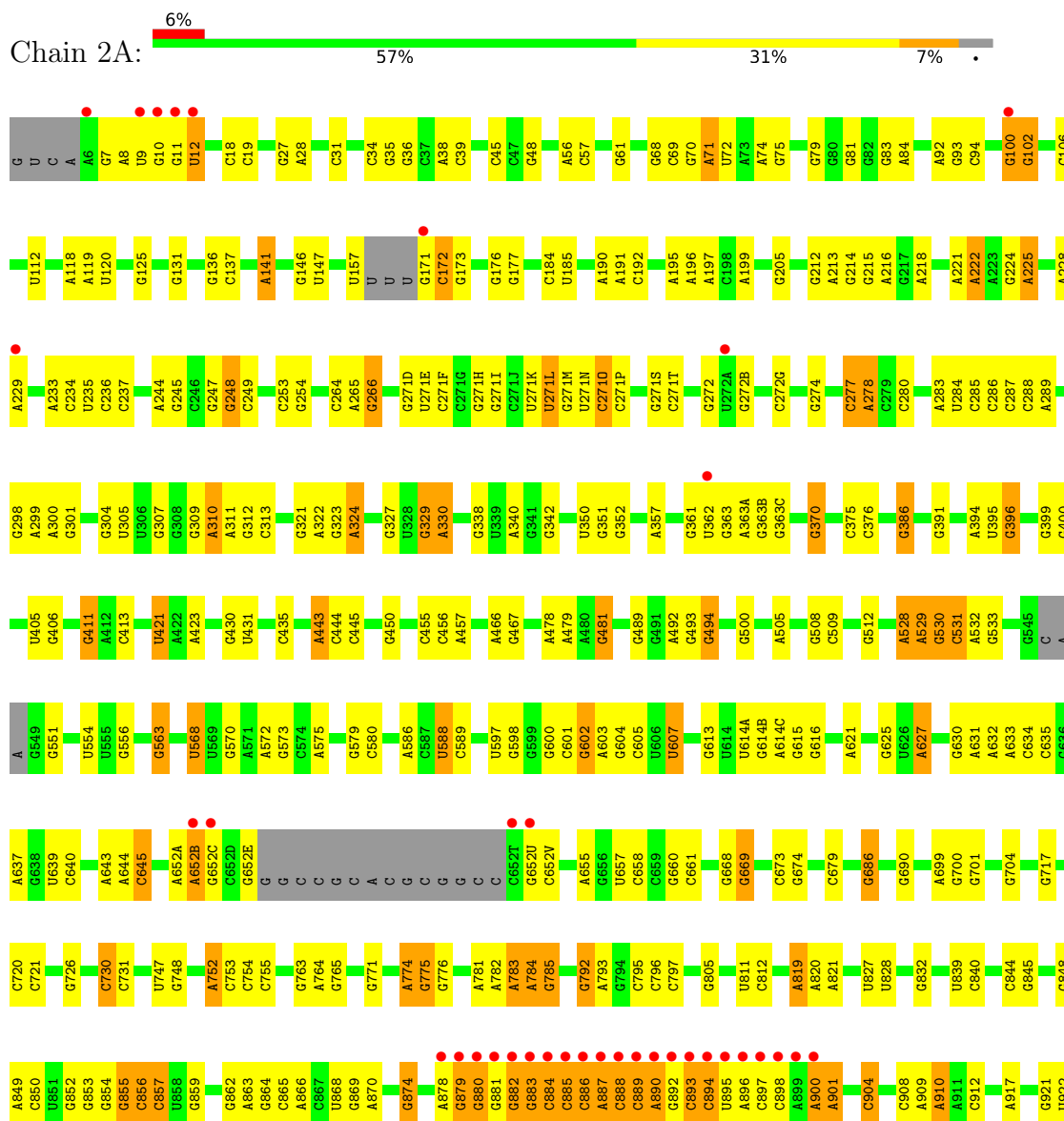
• Molecule 1: 23S Ribosomal RNA



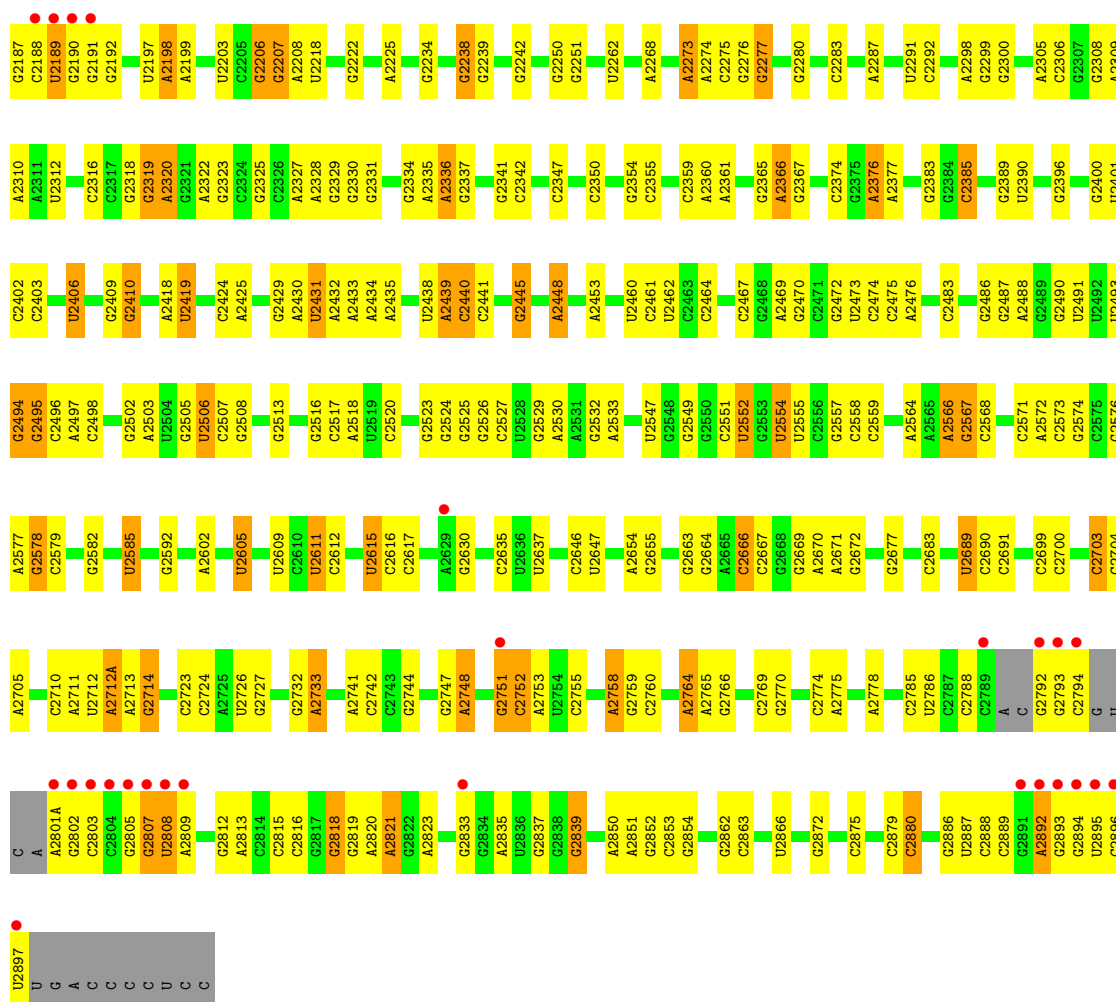
| | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
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| C2381 | C2382 | C2383 | C2384 | C2385 | C2386 | U2387 | G2396 | G2400 | C2404 | G2405 | U2406 | G2407 | G2410 | G2414 | A2422 | U2423 | C2424 | A2425 | A2426 | G2427 | G2428 | G2429 | A2430 | A2435 | A2439 | C2440 | C2441 | A2448 | C2464 | C2467 | G2470 | C2474 | C2475 | A2476 | U2491 | U2492 | U2493 | C2498 | G2502 | A2503 | U2504 | G2505 | U2506 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| U2291 | C2292 | C2295 | C2296 | A2298 | C2299 | A2305 | C2306 | G2307 | G2308 | U2312 | G2313 | C2314 | G2315 | G2316 | G2319 | A2320 | C2324 | G2325 | C2326 | A2327 | A2328 | G2329 | G2334 | A2335 | A2336 | G2337 | G2340 | C2347 | U2348 | G2349 | C2350 | G2354 | C2355 | C2356 | U2357 | G2358 | C2359 | A2360 | A2361 | C2364 | G2365 | G2372 | A2376 | A2377 | U2378 | G2379 | C2380 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| C2177 | C2178 | C2179 | U2180 | G2181 | G2182 | C2183 | G2184 | C2185 | U2186 | G2187 | C2188 | U2189 | G2190 | G2191 | G2192 | C2196 | U2197 | A2198 | G2206 | U2207 | A2208 | U2218 | A2225 | G2228 | G2235 | G2238 | G2239 | U2243 | U2244 | C2248 | G2251 | G2259 | U2262 | A2268 | A2269 | G2277 | G2280 | C2283 | C2284 | C2285 | A2286 | A2287 | A2288 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| U2117 | U2118 | A2119 | G2120 | G2121 | U2122 | G2123 | G2124 | G2125 | A2126 | G2127 | C2128 | G2129 | U2130 | U2131 | U2132 | G2133 | A2134 | A2135 | C2136 | G2137 | C2138 | C2139 | G2140 | G2141 | C2142 | C2143 | C2144 | G2145 | G2146 | G2147 | G2148 | G2149 | U2150 | G2151 | G2152 | G2153 | G2154 | G2155 | G2156 | G2157 | A2158 | G2159 | G2160 | C2161 | G2162 | C2163 | C2164 | G2165 | G2166 | U2167 | C2168 | A2169 | A2170 | A2171 | C2172 | U2173 | U2174 | U2175 | U2176 | U2177 | U2178 | U2179 | U2180 | U2181 | U2182 | U2183 | U2184 | U2185 | U2186 | U2187 | U2188 | U2189 | U2190 | U2191 | U2192 | U2193 | U2194 | U2195 | U2196 | U2197 | U2198 | U2199 | U2200 | U2201 | U2202 | U2203 | U2204 | U2205 | U2206 | U2207 | U2208 | U2209 | U2210 | U2211 | U2212 | U2213 | U2214 | U2215 | U2216 | U2217 | U2218 | U2219 | U2220 | U2221 | U2222 | U2223 | U2224 | U2225 | U2226 | U2227 | U2228 | U2229 | U2230 | U2231 | U2232 | U2233 | U2234 | U2235 | U2236 | U2237 | U2238 | U2239 | U2240 | U2241 | U2242 | U2243 | U2244 | U2245 | U2246 | U2247 | U2248 | U2249 | U2250 | U2251 | U2252 | U2253 | U2254 | U2255 | U2256 | U2257 | U2258 | U2259 | U2260 | U2261 | U2262 | U2263 | U2264 | U2265 | U2266 | U2267 | U2268 | U2269 | U2270 | U2271 | U2272 | U2273 | U2274 | U2275 | U2276 | U2277 | U2278 | U2279 | U2280 | U2281 | U2282 | U2283 | U2284 | U2285 | U2286 | U2287 | U2288 | U2289 | U2290 | U2291 | U2292 | U2293 | U2294 | U2295 | U2296 | U2297 | U2298 | U2299 | U2300 | U2301 | U2302 | U2303 | U2304 | U2305 | U2306 | U2307 | U2308 | U2309 | U2310 | U2311 | U2312 | U2313 | U2314 | U2315 | U2316 | U2317 | U2318 | U2319 | U2320 | U2321 | U2322 | U2323 | U2324 | U2325 | U2326 | U2327 | U2328 | U2329 | U2330 | U2331 | U2332 | U2333 | U2334 | U2335 | U2336 | U2337 | U2338 | U2339 | U2340 | U2341 | U2342 | U2343 | U2344 | U2345 | U2346 | U2347 | U2348 | U2349 | U2350 | U2351 | U2352 | U2353 | U2354 | U2355 | U2356 | U2357 | U2358 | U2359 | U2360 | U2361 | U2362 | U2363 | U2364 | U2365 | U2366 | U2367 | U2368 | U2369 | U2370 | U2371 | U2372 | U2373 | U2374 | U2375 | U2376 | U2377 | U2378 | U2379 | U2380 | U2381 | U2382 | U2383 | U2384 | U2385 | U2386 | U2387 | U2388 | U2389 | U2390 | U2391 | U2392 | U2393 | U2394 | U2395 | U2396 | U2397 | U2398 | U2399 | U2400 | U2401 | U2402 | U2403 | U2404 | U2405 | U2406 | U2407 | U2408 | U2409 | U2410 | U2411 | U2412 | U2413 | U2414 | U2415 | U2416 | U2417 | U2418 | U2419 | U2420 | U2421 | U2422 | U2423 | U2424 | U2425 | U2426 | U2427 | U2428 | U2429 | U2430 | U2431 | U2432 | U2433 | U2434 | U2435 | U2436 | U2437 | U2438 | U2439 | U2440 | U2441 | U2442 | U2443 | U2444 | U2445 | U2446 | U2447 | U2448 | U2449 | U2450 | U2451 | U2452 | U2453 | U2454 | U2455 | U2456 | U2457 | U2458 | U2459 | U2460 | U2461 | U2462 | U2463 | U2464 | U2465 | U2466 | U2467 | U2468 | U2469 | U2470 | U2471 | U2472 | U2473 | U2474 | U2475 | U2476 | U2477 | U2478 | U2479 | U2480 | U2481 | U2482 | U2483 | U2484 | U2485 | U2486 | U2487 | U2488 | U2489 | U2490 | U2491 | U2492 | U2493 | U2494 | U2495 | U2496 | U2497 | U2498 | U2499 | U2500 | U2501 | U2502 | U2503 | U2504 | U2505 | U2506 | U2507 | U2508 | U2509 | U2510 | U2511 | U2512 | U2513 | U2514 | U2515 | U2516 | U2517 | U2518 | U2519 | U2520 | U2521 | U2522 | U2523 | U2524 | U2525 | U2526 | U2527 | U2528 | U2529 | U2530 | U2531 | U2532 | U2533 | U2534 | U2535 | U2536 | U2537 | U2538 | U2539 | U2540 | U2541 | U2542 | U2543 | U2544 | U2545 | U2546 | U2547 | U2548 | U2549 | U2550 | U2551 | U2552 | U2553 | U2554 | U2555 | U2556 | U2557 | U2558 | U2559 | U2560 | U2561 | U2562 | U2563 | U2564 | U2565 | U2566 | U2567 | U2568 | U2569 | U2570 | U2571 | U2572 | U2573 | U2574 | U2575 | U2576 | U2577 | U2578 | U2579 | U2580 | U2581 | U2582 | U2583 | U2584 | U2585 | U2586 | U2587 | U2588 | U2589 | U2590 | U2591 | U2592 | U2593 | U2594 | U2595 | U2596 | U2597 | U2598 | U2599 | U2600 | U2601 | U2602 | U2603 | U2604 | U2605 | U2606 | U2607 | U2608 | U2609 | U2610 | U2611 | U2612 | U2613 | U2614 | U2615 | U2616 | U2617 | U2618 | U2619 | U2620 | U2621 | U2622 | U2623 | U2624 | U2625 | U2626 | U2627 | U2628 | U2629 | U2630 | U2631 | U2632 | U2633 | U2634 | U2635 | U2636 | U2637 | U2638 | U2639 | U2640 | U2641 | U2642 | U2643 | U2644 | U2645 | U2646 | U2647 | U2648 | U2649 | U2650 | U2651 | U2652 | U2653 | U2654 | U2655 | U2656 | U2657 | U2658 | U2659 | U2660 | U2661 | U2662 | U2663 | U2664 | U2665 | U2666 | U2667 | U2668 | U2669 | U2670 | U2671 | U2672 | U2673 | U2674 | U2675 | U2676 | U2677 | U2678 | U2679 | U2680 | U2681 | U2682 | U2683 | U2684 | U2685 | U2686 | U2687 | U2688 | U2689 | U2690 | U2691 | U2692 | U2693 | U2694 | U2695 | U2696 | U2697 | U2698 | U2699 | U2700 | U2701 | U2702 | U2703 | U2704 | U2705 | U2706 | U2707 | U2708 | U2709 | U2710 | U2711 | U2712 | U2713 | U2714 | U2715 | U2716 | U2717 | U2718 | U2719 | U2720 | U2721 | U2722 | U2723 | U2724 | U2725 | U2726 | U2727 | U2728 | U2729 | U2730 | U2731 | U2732 | U2733 | U2734 | U2735 | U2736 | U2737 | U2738 | U2739 | U2740 | U2741 | U2742 | U2743 | U2744 | U2745 | U2746 | U2747 | U2748 | U2749 | U2750 | U2751 | U2752 | U2753 | U2754 | U2755 | U2756 | U2757 | U2758 | U2759 | U2760 | U2761 | U2762 | U2763 | U2764 | U2765 | U2766 | U2767 | U2768 | U2769 | U2770 | U2771 | U2772 | U2773 | U2774 | U2775 | U2776 | U2777 | U2778 | U2779 | U2780 | U2781 | U2782 | U2783 | U2784 | U2785 | U2786 | U2787 | U2788 | U2789 | U2790 | U2791 | U2792 | U2793 | U2794 | U2795 | U2796 | U2797 | U2798 | U2799 | U2800 | U2801 | U2802 | U2803 | U2804 | U2805 | U2806 | U2807 | U2808 | U2809 | U2810 | U2811 | U2812 | U2813 | U2814 | U2815 | U2816 | U2817 | U2818 | U2819 | U2820 | U2821 | U2822 | U2823 | U2824 | U2825 | U2826 | U2827 | U2828 | U2829 | U2830 | U2831 | U2832 | U2833 | U2834 | U2835 | U2836 | U2837 | U2838 | U2839 | U2840 | U2841 | U2842 | U2843 | U2844 | U2845 | U2846 | U2847 | U2848 | U2849 | U2850 | U2851 | U2852 | U2853 | U2854 | U2855 | U2856 | U2857 | U2858 | U2859 | U2860 | U2861 | U2862 | U2863 | U2864 | U2865 | U2866 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• Molecule 1: 23S Ribosomal RNA

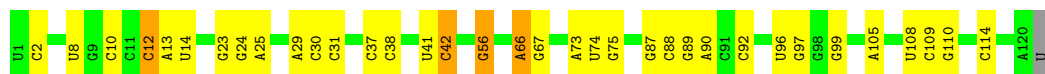






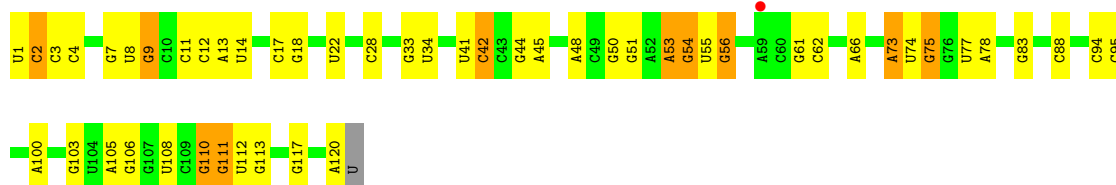
• Molecule 2: 5S Ribosomal RNA

Chain 1B: 70% 26%



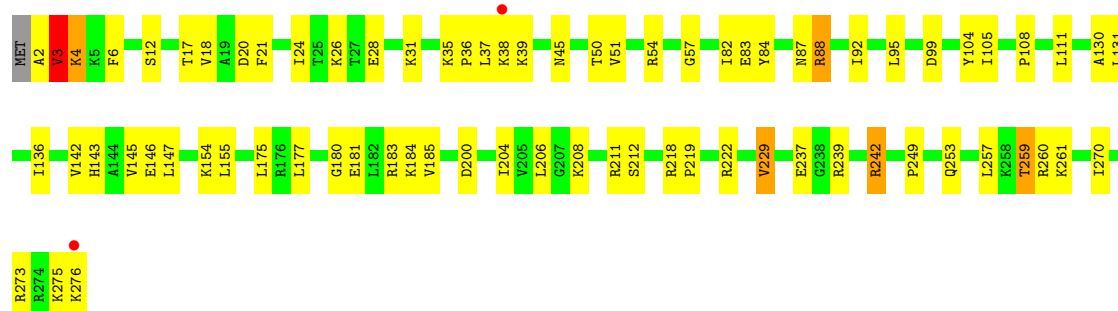
• Molecule 2: 5S Ribosomal RNA

Chain 2B: 57% 34% 8%

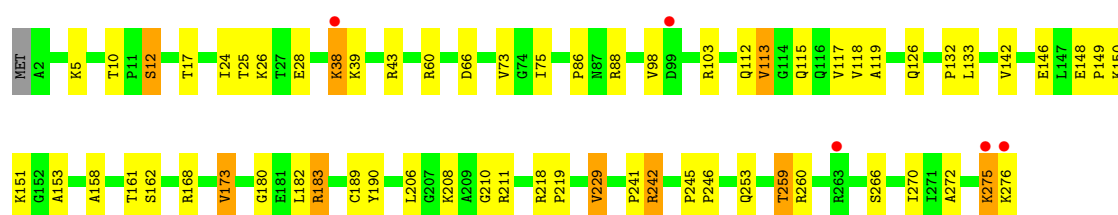
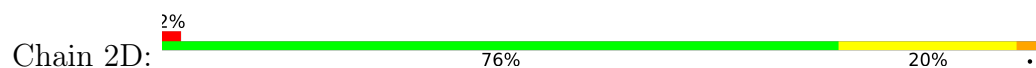


• Molecule 3: 50S ribosomal protein L2

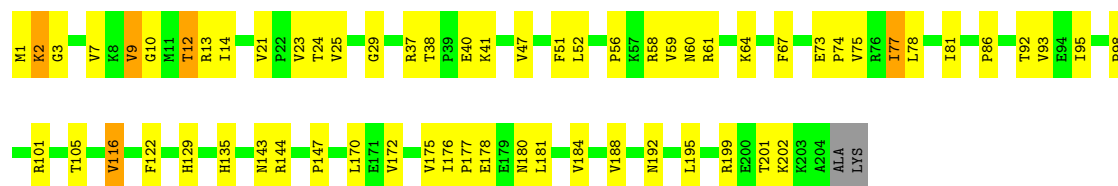
Chain 1D: 72% 25%



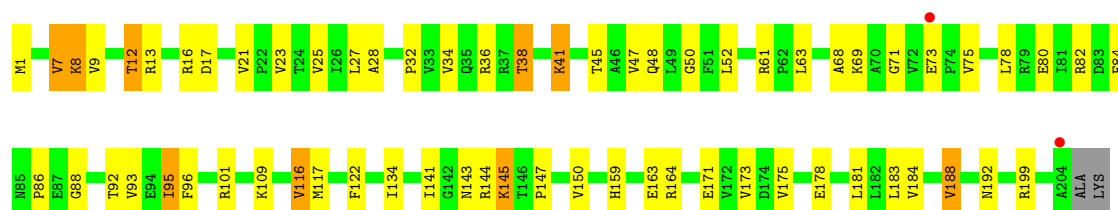
• Molecule 3: 50S ribosomal protein L2



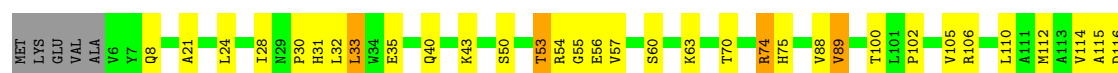
• Molecule 4: 50S ribosomal protein L3



• Molecule 4: 50S ribosomal protein L3

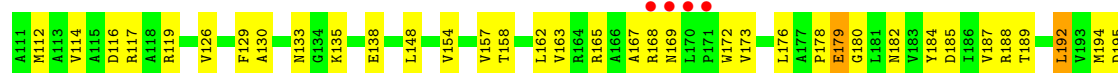


• Molecule 5: 50S ribosomal protein L4

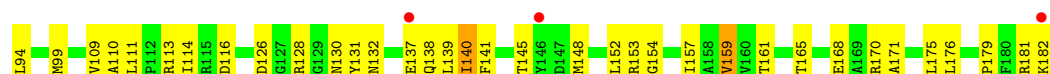




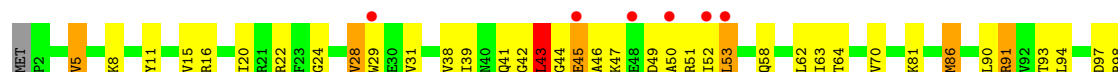
• Molecule 5: 50S ribosomal protein L4



• Molecule 6: 50S ribosomal protein L5



• Molecule 6: 50S ribosomal protein L5

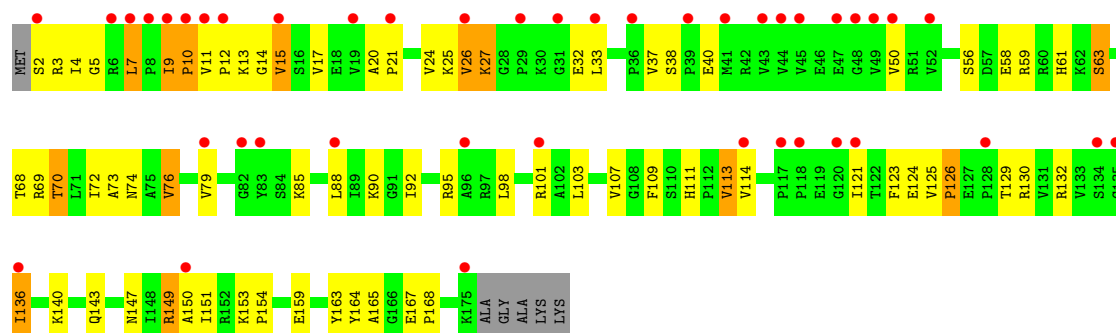


• Molecule 7: 50S ribosomal protein L6

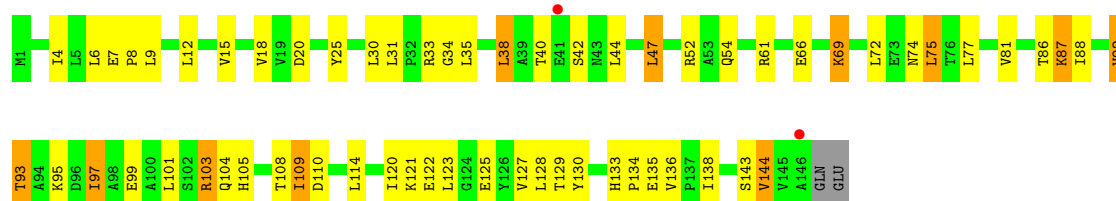




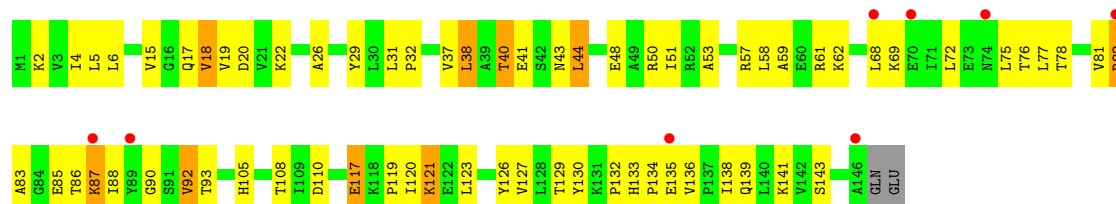
• Molecule 7: 50S ribosomal protein L6



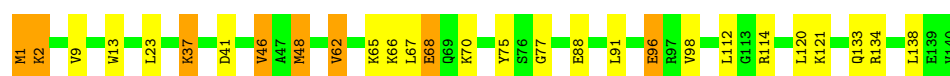
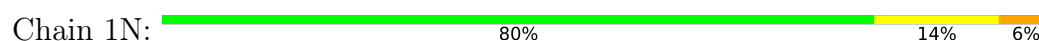
• Molecule 8: 50S ribosomal protein L9



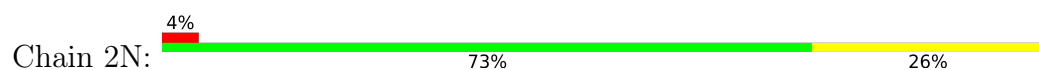
• Molecule 8: 50S ribosomal protein L9



• Molecule 9: 50S ribosomal protein L13



• Molecule 9: 50S ribosomal protein L13

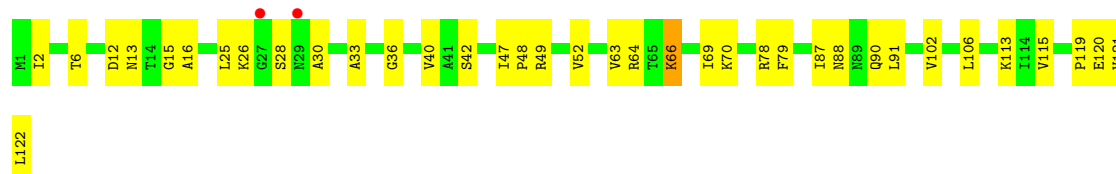




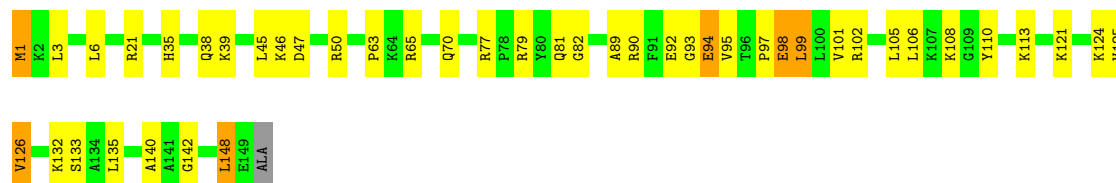
- Molecule 10: 50S ribosomal protein L14



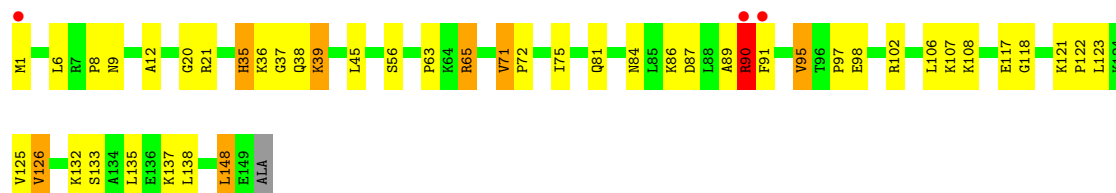
- Molecule 10: 50S ribosomal protein L14



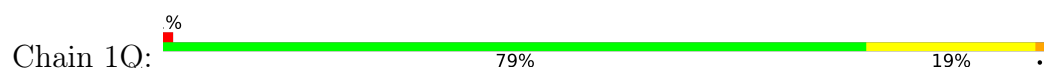
- Molecule 11: 50S ribosomal protein L15



- Molecule 11: 50S ribosomal protein L15

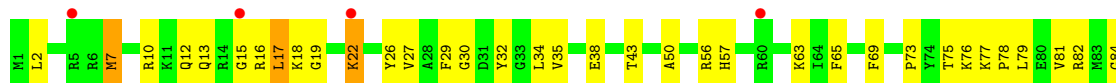


- Molecule 12: 50S ribosomal protein L16

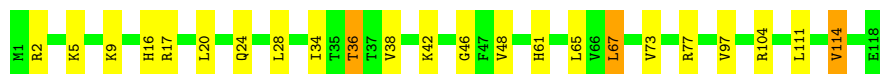
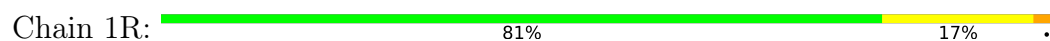




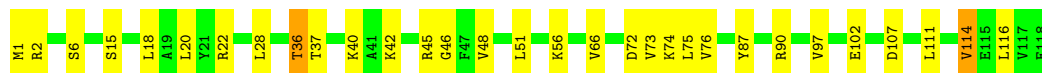
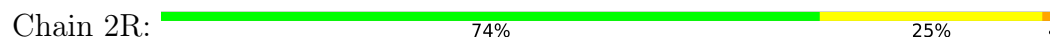
- Molecule 12: 50S ribosomal protein L16



- Molecule 13: 50S ribosomal protein L17



- Molecule 13: 50S ribosomal protein L17



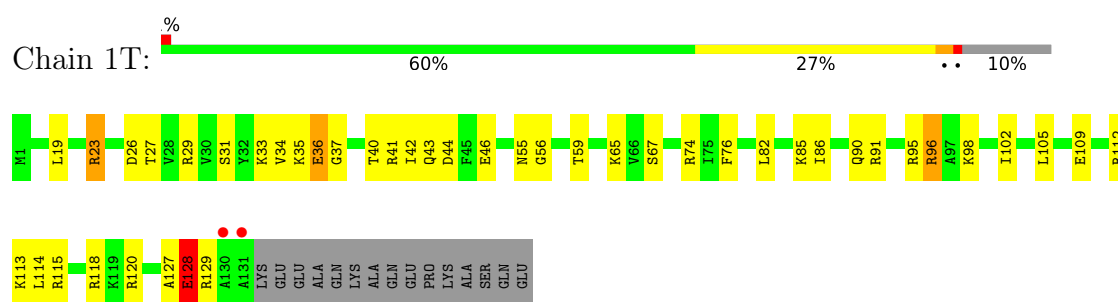
- Molecule 14: 50S ribosomal protein L18



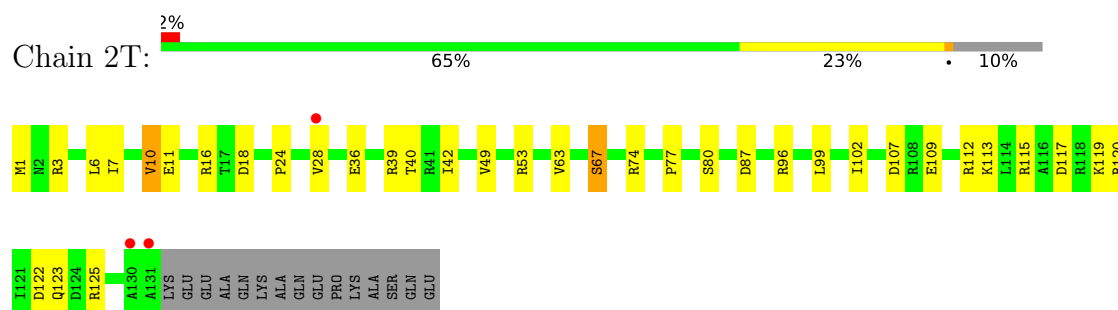
- Molecule 14: 50S ribosomal protein L18



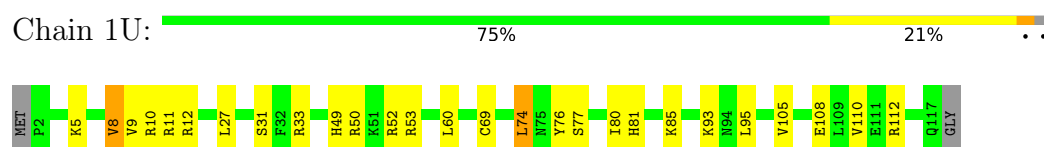
- Molecule 15: 50S ribosomal protein L19



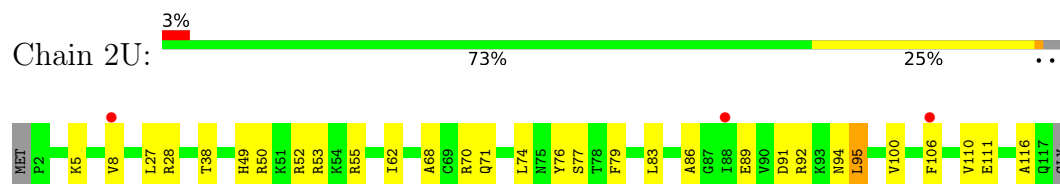
- Molecule 15: 50S ribosomal protein L19



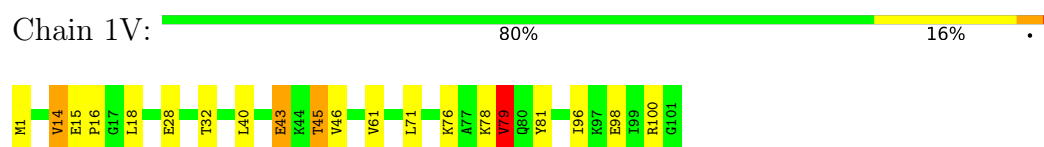
- Molecule 16: 50S ribosomal protein L20



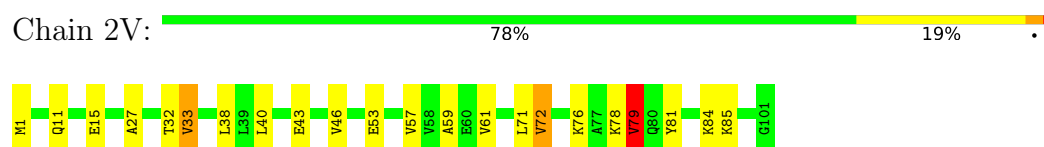
- Molecule 16: 50S ribosomal protein L20



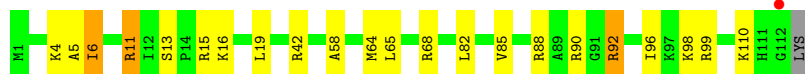
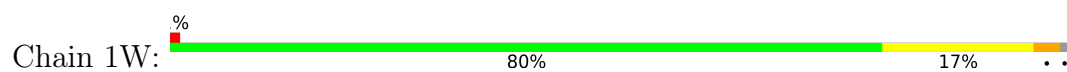
- Molecule 17: 50S ribosomal protein L21



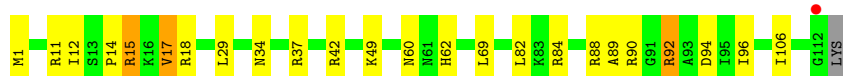
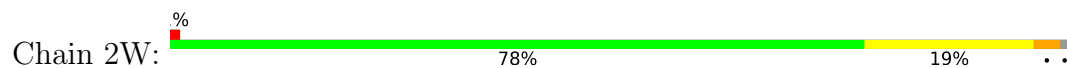
- Molecule 17: 50S ribosomal protein L21



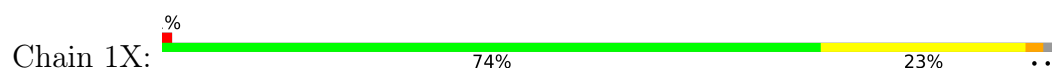
- Molecule 18: 50S ribosomal protein L22



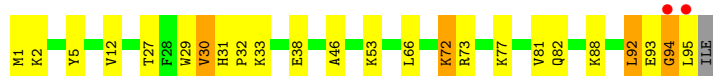
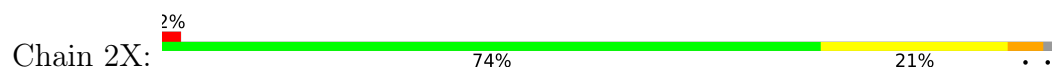
- Molecule 18: 50S ribosomal protein L22



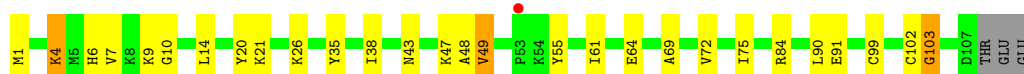
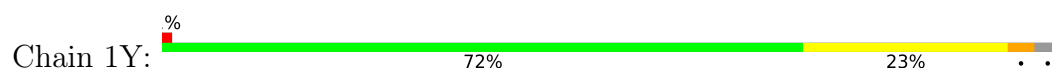
- Molecule 19: 50S ribosomal protein L23



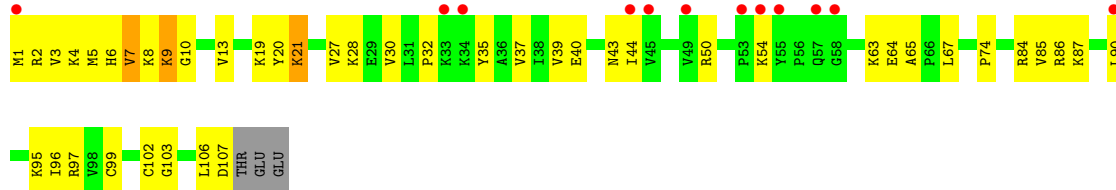
- Molecule 19: 50S ribosomal protein L23



- Molecule 20: 50S ribosomal protein L24

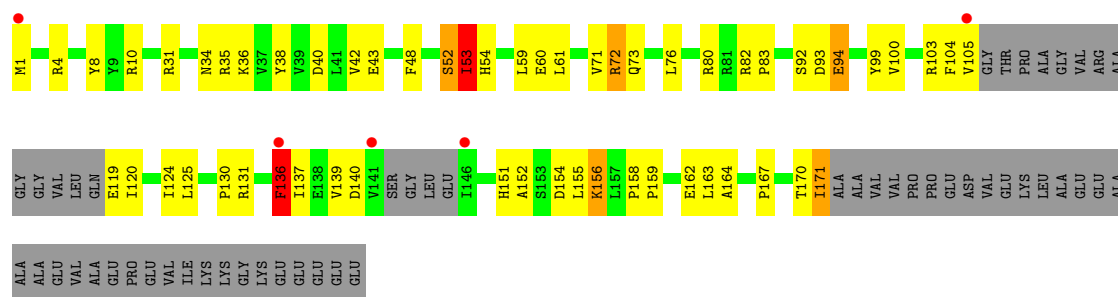


- Molecule 20: 50S ribosomal protein L24

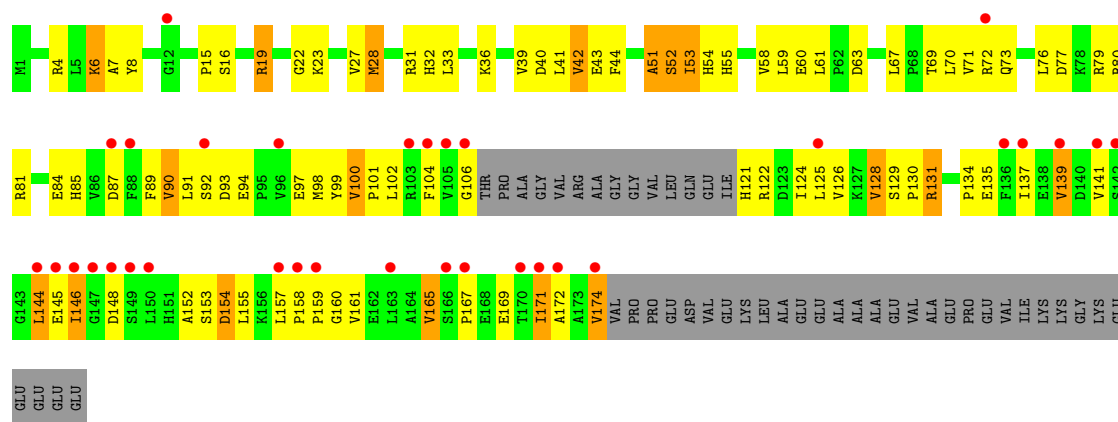


- Molecule 21: 50S ribosomal protein L25

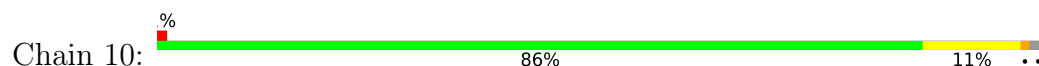




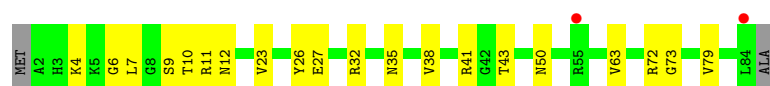
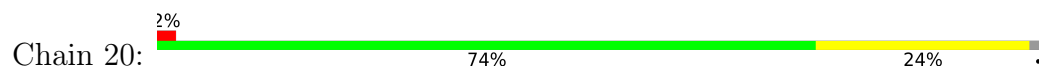
• Molecule 21: 50S ribosomal protein L25



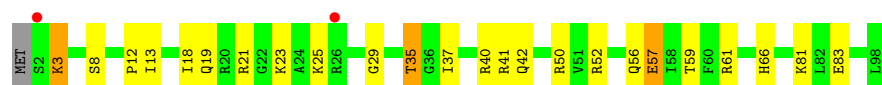
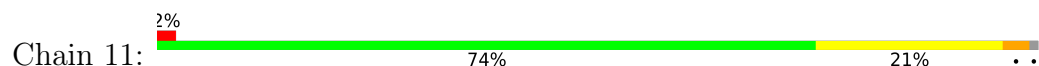
• Molecule 22: 50S ribosomal protein L27



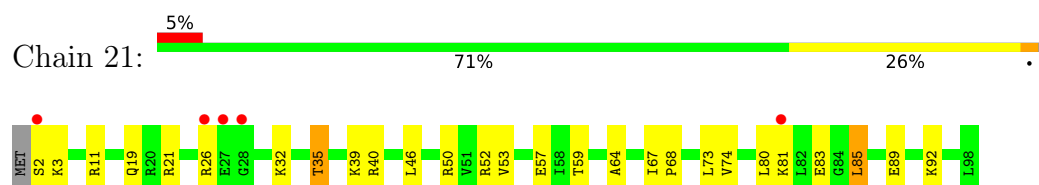
• Molecule 22: 50S ribosomal protein L27



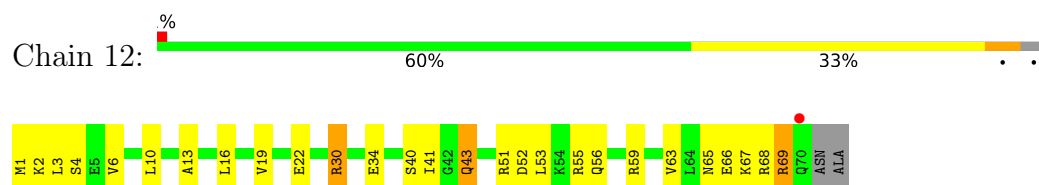
• Molecule 23: 50S ribosomal protein L28



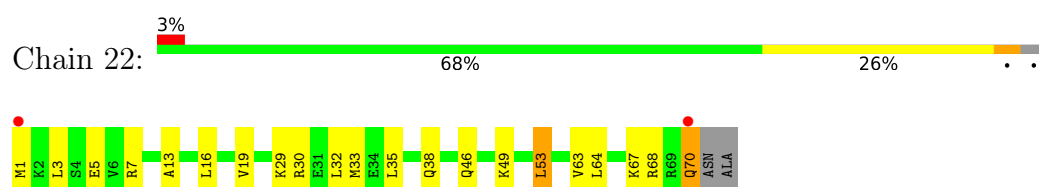
• Molecule 23: 50S ribosomal protein L28



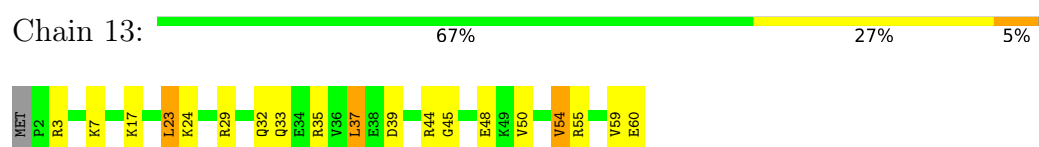
- Molecule 24: 50S ribosomal protein L29



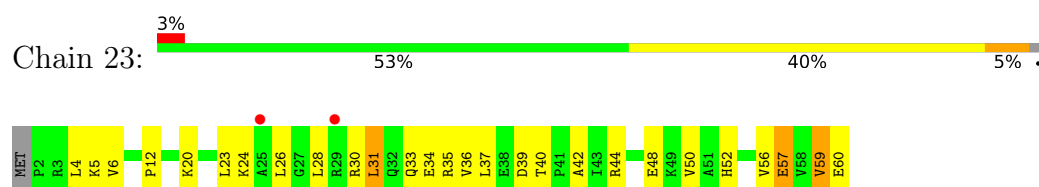
- Molecule 24: 50S ribosomal protein L29



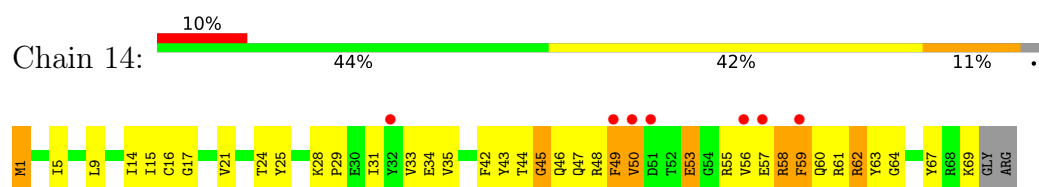
- Molecule 25: 50S ribosomal protein L30



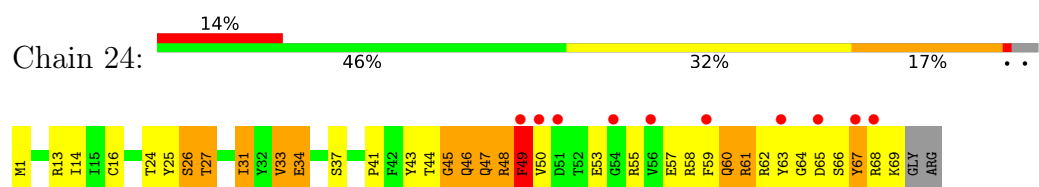
- Molecule 25: 50S ribosomal protein L30




- Molecule 26: 50S ribosomal protein L31



- Molecule 26: 50S ribosomal protein L31




- Molecule 27: 50S ribosomal protein L32

Chain 15:  75% 22% ..



- Molecule 27: 50S ribosomal protein L32

Chain 25:  82% 17% .



- Molecule 28: 50S ribosomal protein L33

Chain 16:  69% 28% ..




- Molecule 28: 50S ribosomal protein L33

Chain 26:  2% 65% 26% 7% .



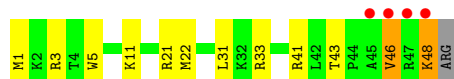
- Molecule 29: 50S ribosomal protein L34

Chain 17:  4% 76% 18% ..



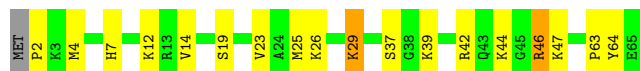
- Molecule 29: 50S ribosomal protein L34

Chain 27:  8% 73% 20% ..



- Molecule 30: 50S ribosomal protein L35

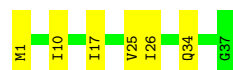
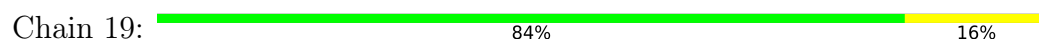
Chain 18:  71% 25% ..



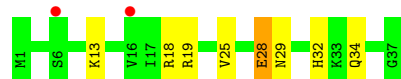
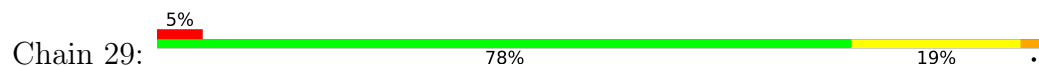
- Molecule 30: 50S ribosomal protein L35



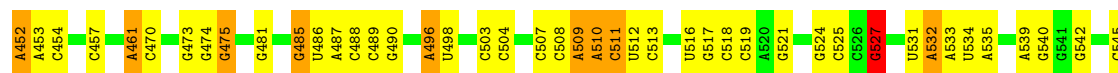
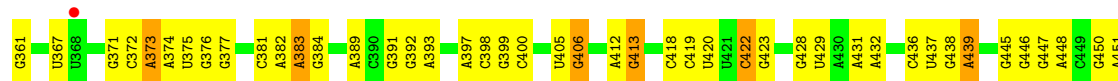
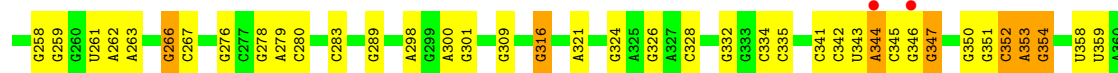
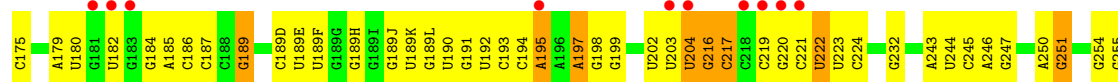
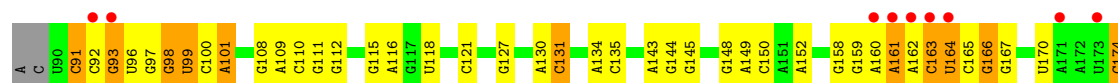
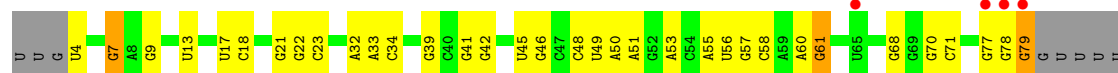
- Molecule 31: 50S ribosomal protein L36

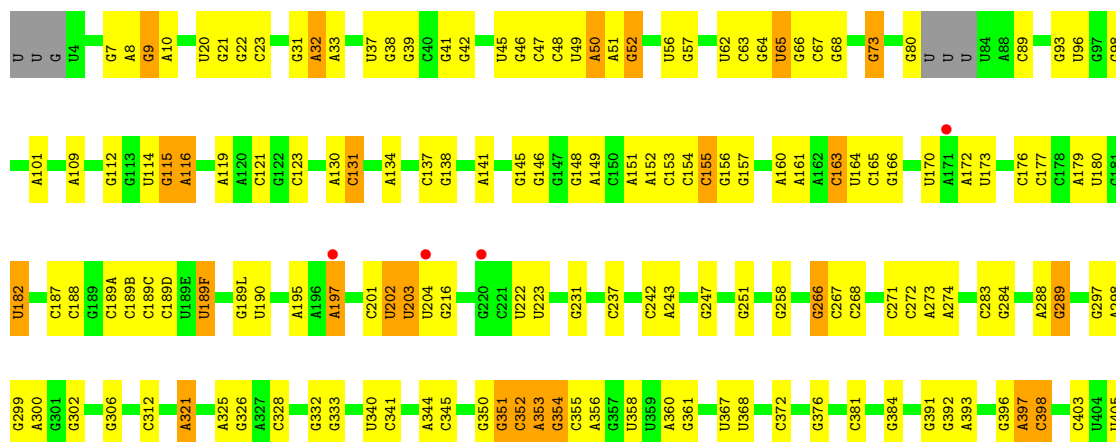
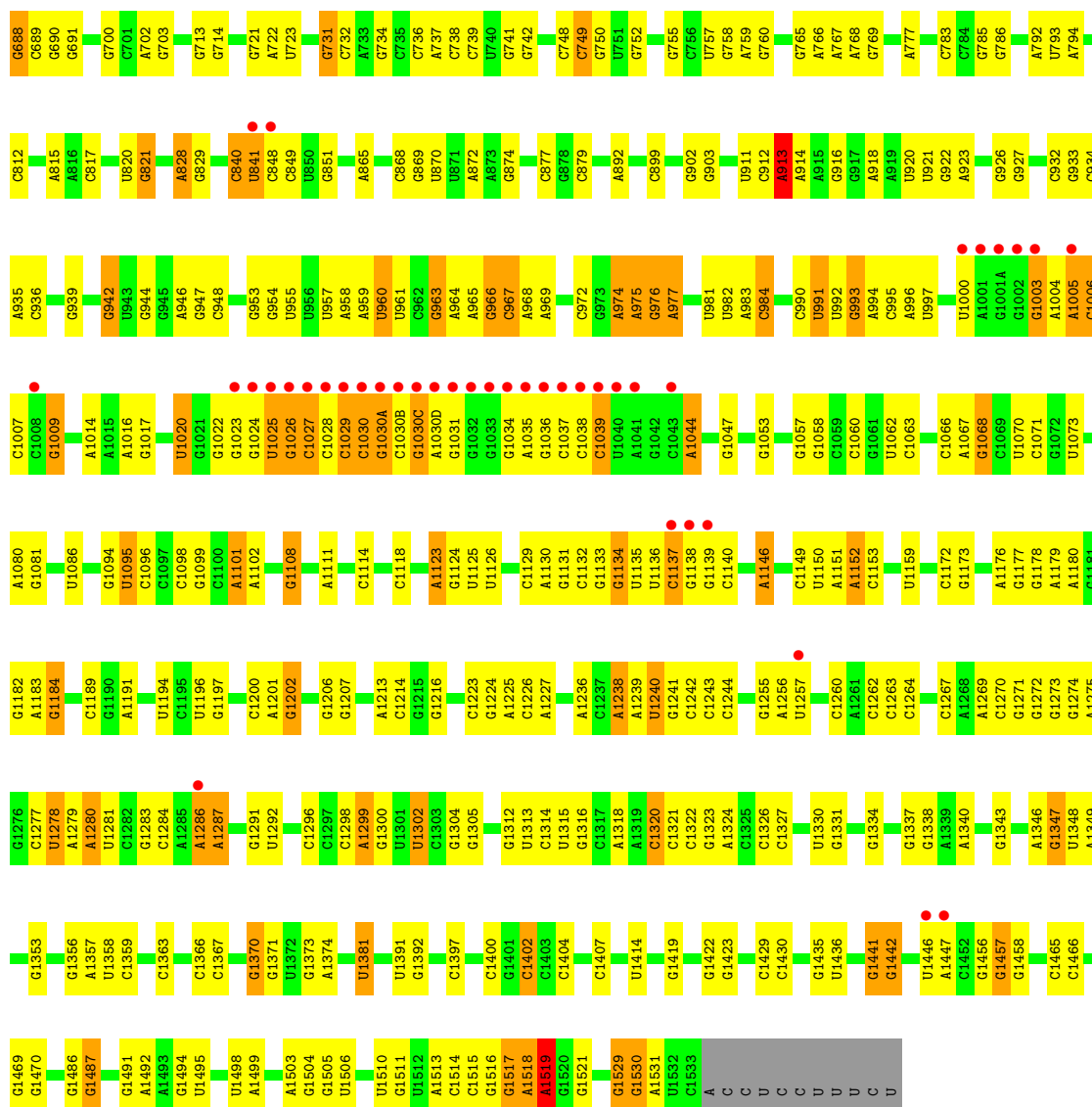


- Molecule 31: 50S ribosomal protein L36

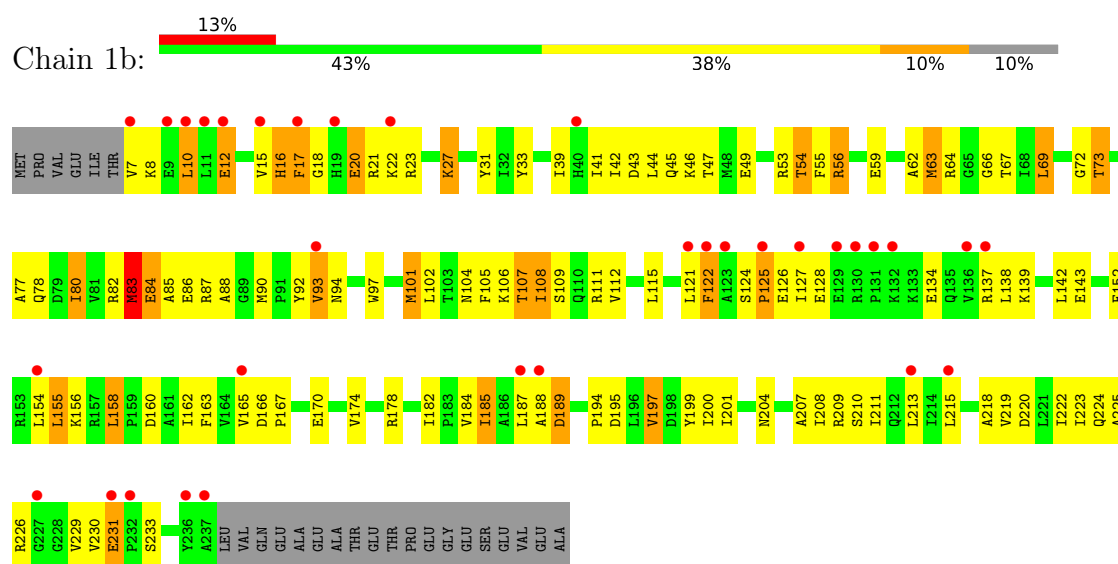


- Molecule 32: 16S Ribosomal RNA

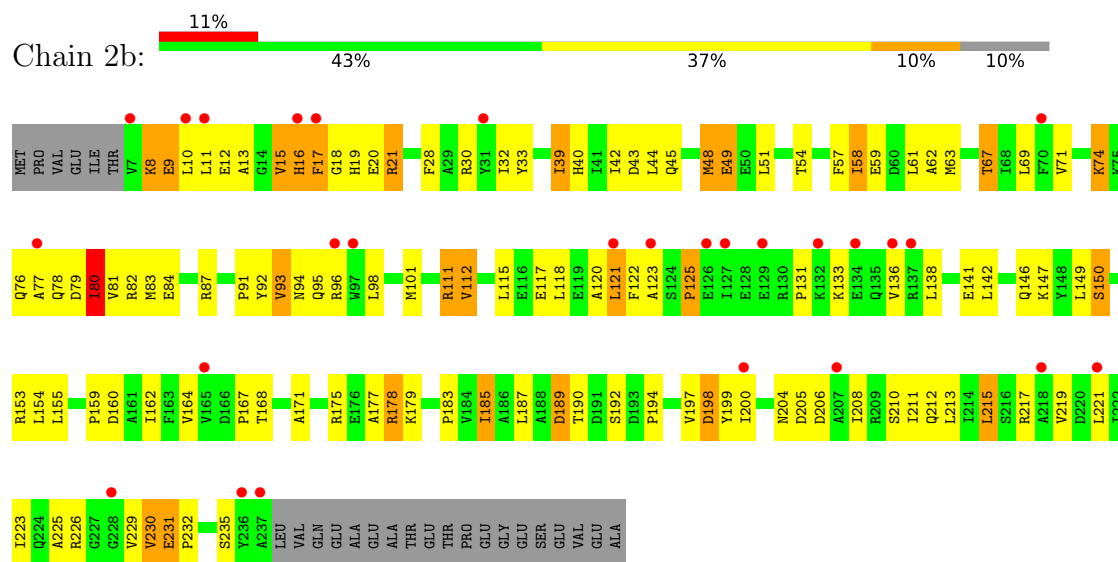




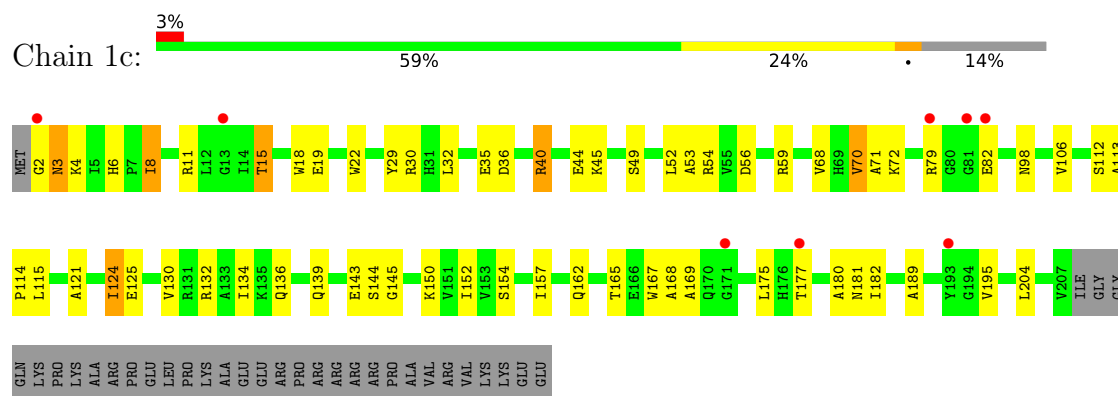
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| C | G1417 | A1268 | A1288 | G1131 | C1059 | A1001 | A935 | U793 | U677 | G585 | C508 | G407 |
| U | A1418 | A1333 | C1269 | U1135 | C1060 | G1001A | C936 | A794 | A687 | C586 | A509 | G410 |
| U | G1419 | G1334 | C1270 | U1136 | G1061 | G1002 | A937 | A807 | A688 | C590 | A510 | A411 |
| C | G1422 | C1342 | A1201 | G1137 | U1062 | G1003 | A938 | C808 | C689 | C593 | C511 | G412 |
| U | G1423 | G1202 | G1203 | G1138 | G1063 | A1004 | C939 | C809 | C690 | G594 | U512 | G413 |
| | | G1204 | G1205 | G1139 | G1064 | A1005 | C940 | | G691 | G595 | C513 | A414 |
| | | G1206 | G1207 | G1140 | U1065 | C1007 | G941 | C612 | G692 | G596 | U516 | A415 |
| | | G1207 | | G1141 | A1067 | G1008 | G942 | C817 | G693 | C597 | C517 | G416 |
| | | U1212 | | G1142 | G1068 | G1009 | G944 | G818 | G694 | G598 | C518 | C417 |
| | | A1213 | | G1143 | U1069 | G1010 | G945 | A819 | A695 | C599 | C519 | C418 |
| | | G1214 | | G1144 | C1070 | G1011 | A946 | U820 | | U420 | A520 | U421 |
| | | G1215 | | G1145 | C1071 | U1012 | G947 | G821 | C701 | G603 | G521 | U422 |
| | | G1216 | | A1146 | U1072 | G1013 | U952 | C826 | A706 | G604 | C522 | U427 |
| | | G1217 | | U1147 | U1073 | A1014 | G953 | U827 | G713 | A611 | A523 | G428 |
| | | G1218 | | U1148 | C1076 | A1015 | G954 | A828 | G719 | G612 | G527 | U429 |
| | | G1219 | | U1149 | U1077 | G1016 | U955 | G829 | | G613 | G528 | C433 |
| | | G1220 | | U1150 | U1078 | C1017 | U956 | | | A614 | G529 | U434 |
| | | G1221 | | A1151 | G1081 | C1018 | U957 | U833 | | C615 | U531 | C435 |
| | | G1222 | | U1152 | U1082 | G1019 | A958 | G836 | | C616 | A532 | G438 |
| | | G1223 | | G1153 | U1083 | U1020 | U959 | | | C617 | A533 | A439 |
| | | G1224 | | G1154 | U1084 | G1021 | A960 | G840 | | C618 | U534 | A441 |
| | | G1225 | | G1155 | U1085 | G1022 | U961 | U841 | | U619 | G544 | A448 |
| | | G1226 | | U1156 | U1086 | U1023 | C962 | | | C620 | C545 | A451 |
| | | G1227 | | A1157 | U1087 | G1024 | G963 | | | A621 | G546 | A452 |
| | | G1228 | | U1158 | U1088 | U1025 | A964 | | | C621 | U547 | C454 |
| | | U1232 | | U1159 | U1089 | G1026 | A965 | | | C622 | G548 | C457 |
| | | A1236 | | G1160 | U1090 | C1027 | A966 | | | C623 | C554 | C458 |
| | | C1237 | | G1161 | U1091 | G1028 | A967 | | | C624 | C555 | G460 |
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| | | U1302 | | C1163 | U1093 | G1030 | A968 | | | U626 | C557 | C470 |
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| | | A1238 | | U1168 | C1098 | C1030B | C970 | | | C628 | C559 | A472 |
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| | | | | G1180 | C1116 | U1040 | U982 | | | U657 | C571 | |
| | | | | G1181 | G1117 | A1041 | A983 | | | C658 | C572 | |
| | | | | G1182 | C1118 | G1042 | C984 | | | U659 | C573 | |
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| | | | | G1190 | U1126 | C1054 | A996 | | | G667 | C581 | |
| | | | | A1191 | U1127 | A1055 | U997 | | | C668 | C582 | |
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| | | | | | | | | | | C729 | C643 | |
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| | | | | | | | | | | C749 | C663 | |
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| | | | | | | | | | | C751 | C665 | |
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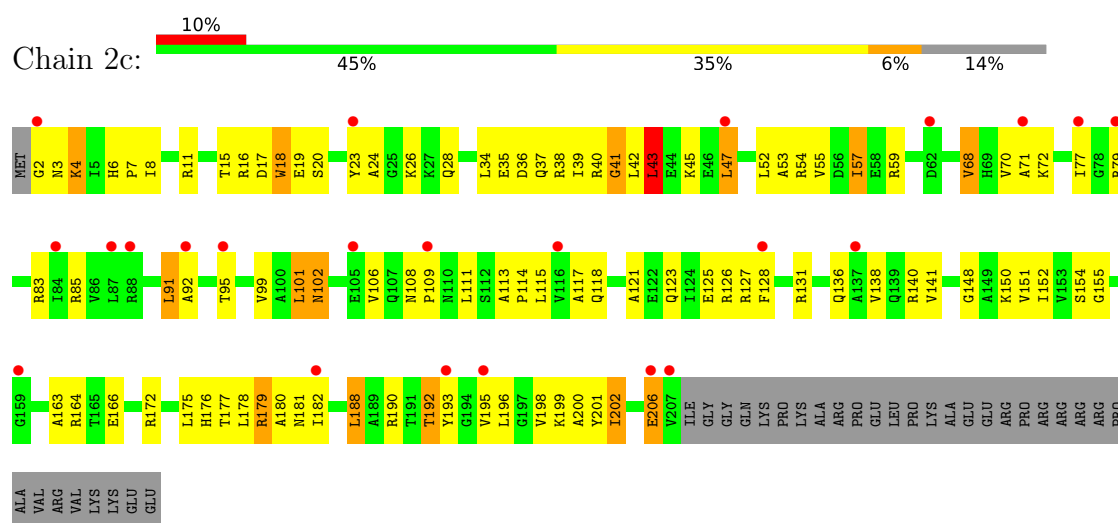
• Molecule 33: 30S ribosomal protein S2



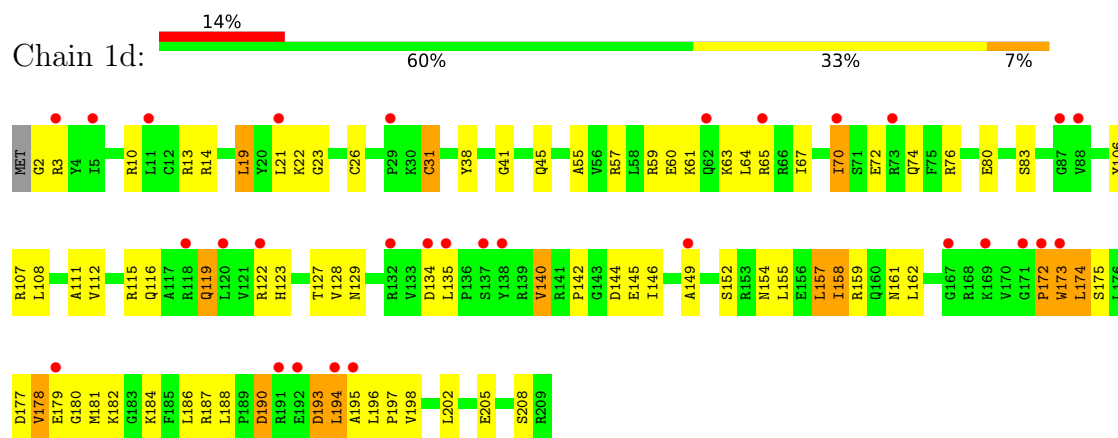
• Molecule 34: 30S ribosomal protein S3



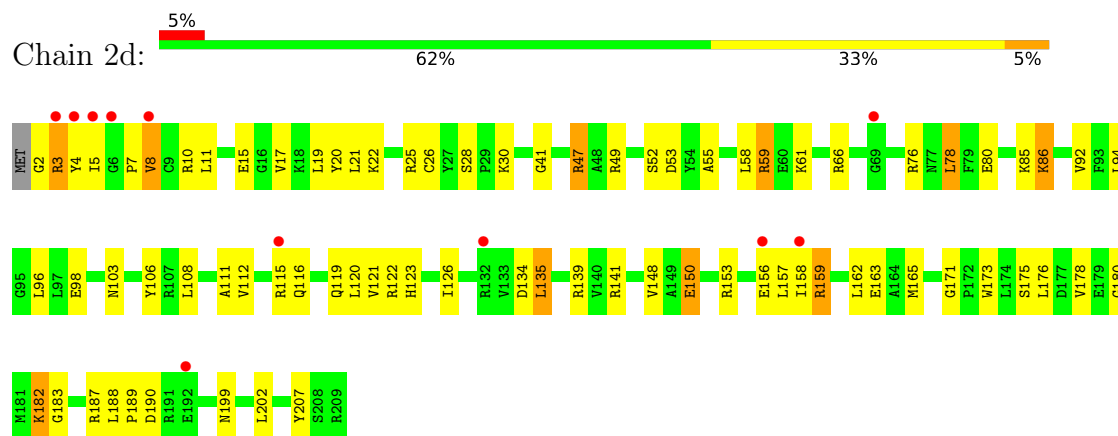
• Molecule 34: 30S ribosomal protein S3



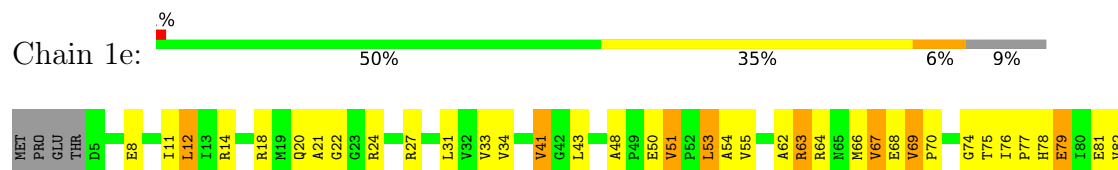
- Molecule 35: 30S ribosomal protein S4



- Molecule 35: 30S ribosomal protein S4

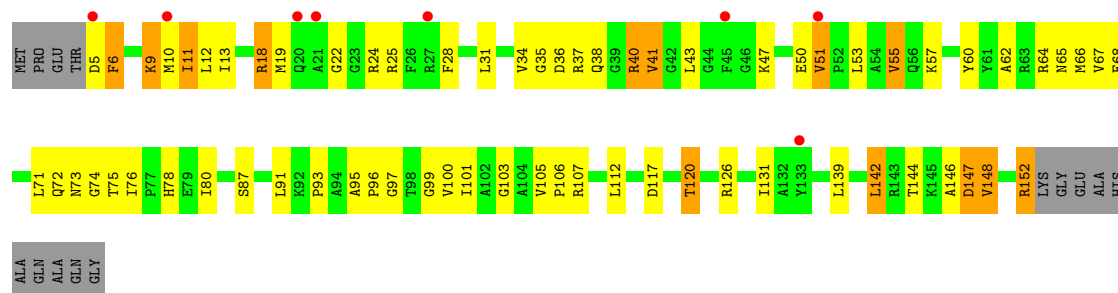


- Molecule 36: 30S ribosomal protein S5

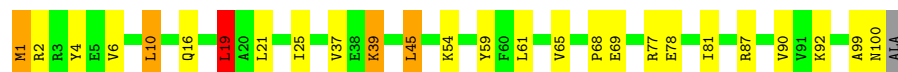




- Molecule 36: 30S ribosomal protein S5



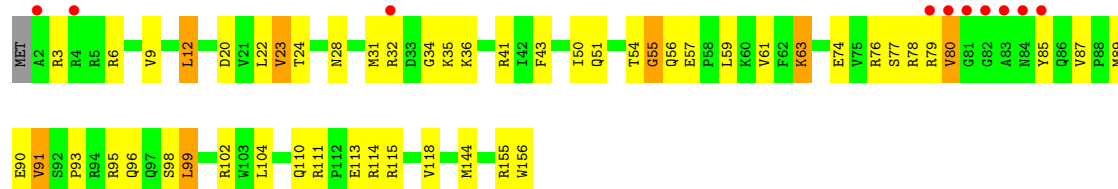
- Molecule 37: 30S ribosomal protein S6



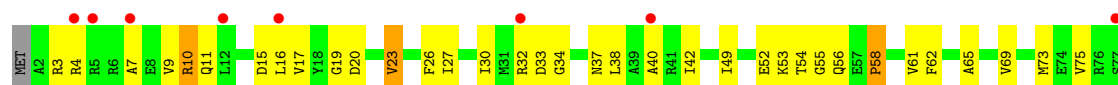
- Molecule 37: 30S ribosomal protein S6



- Molecule 38: 30S ribosomal protein S7

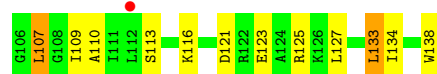
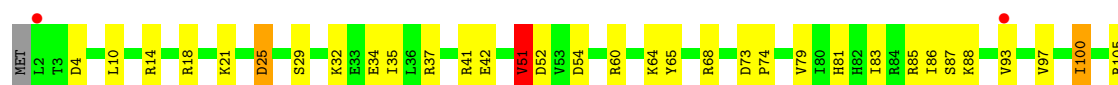


- Molecule 38: 30S ribosomal protein S7

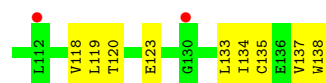
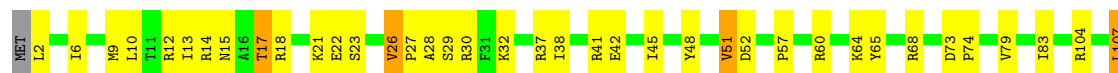




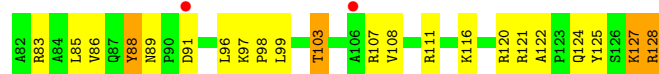
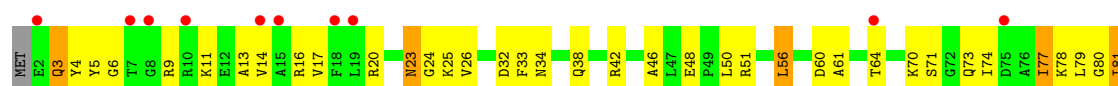
- Molecule 39: 30S ribosomal protein S8



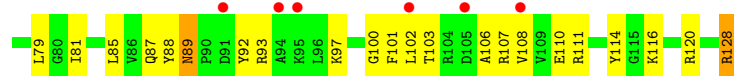
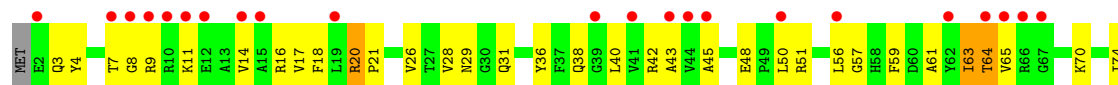
- Molecule 39: 30S ribosomal protein S8



- Molecule 40: 30S ribosomal protein S9

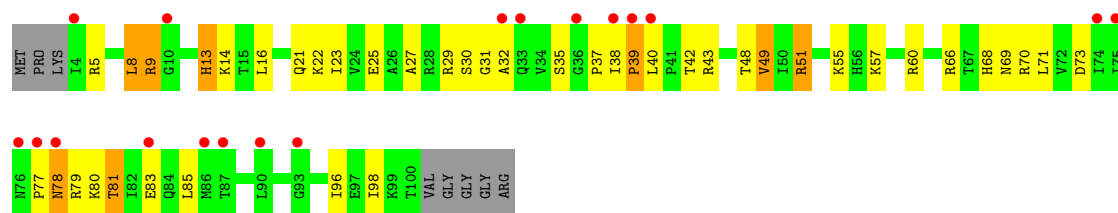


- Molecule 40: 30S ribosomal protein S9

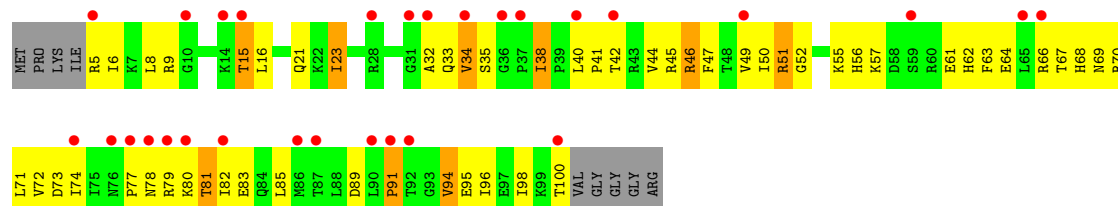


- Molecule 41: 30S ribosomal protein S10

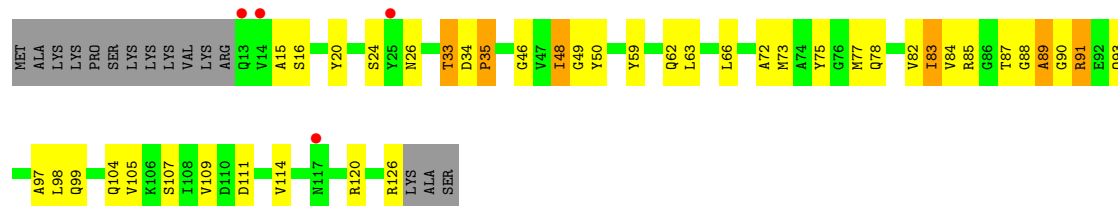




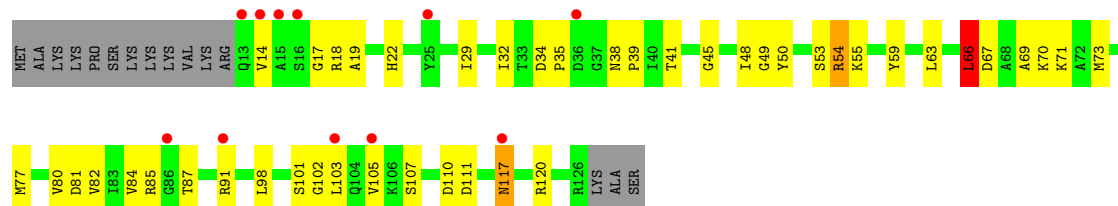
- Molecule 41: 30S ribosomal protein S10



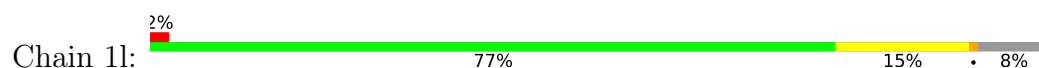
- Molecule 42: 30S ribosomal protein S11



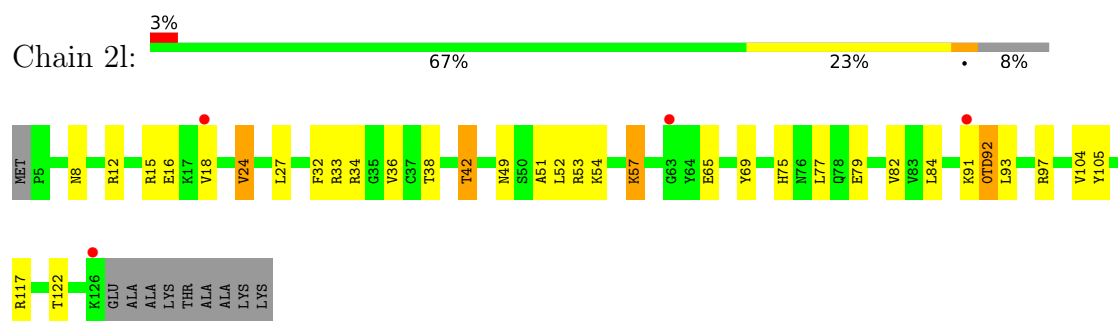
- Molecule 42: 30S ribosomal protein S11



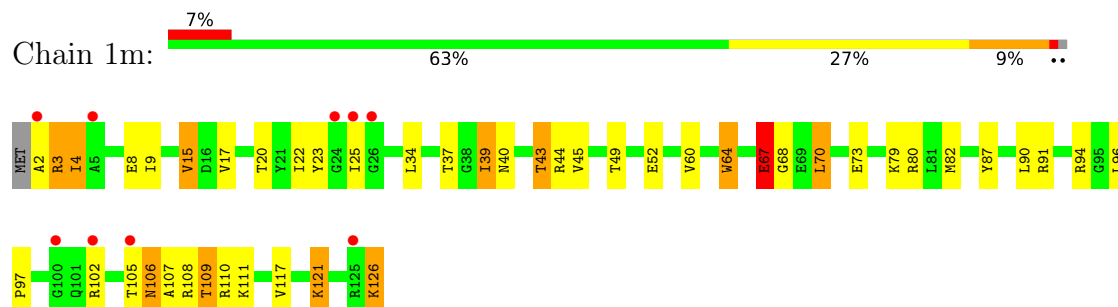
- Molecule 43: 30S ribosomal protein S12



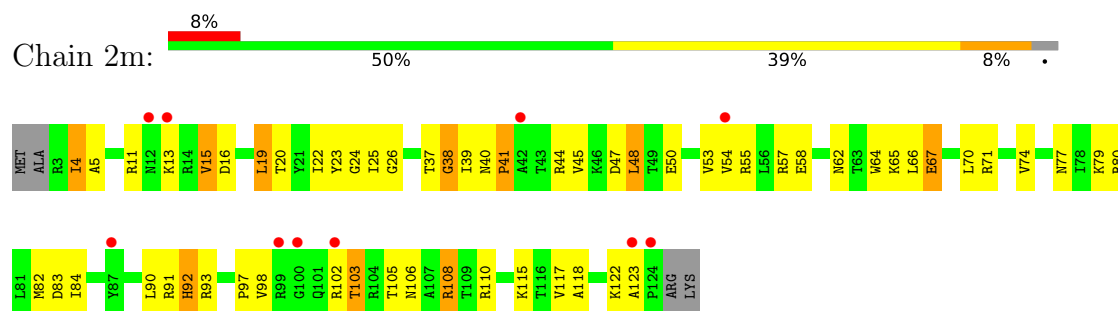
- Molecule 43: 30S ribosomal protein S12



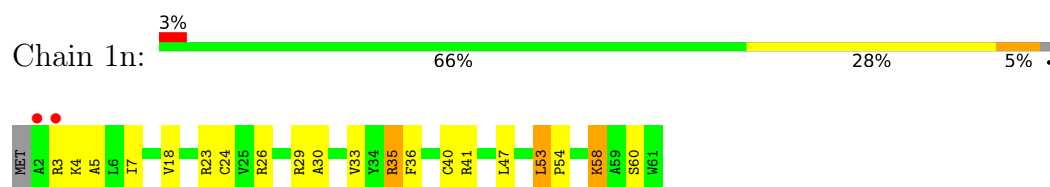
- Molecule 44: 30S ribosomal protein S13



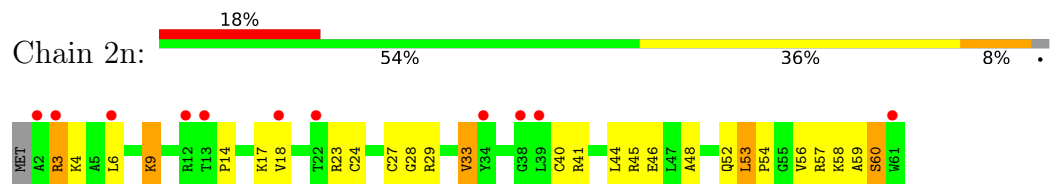
- Molecule 44: 30S ribosomal protein S13



- Molecule 45: 30S ribosomal protein S14 type Z

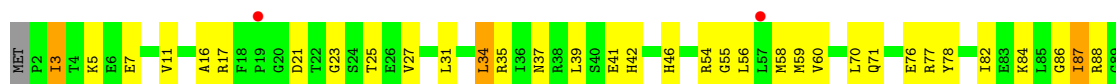


- Molecule 45: 30S ribosomal protein S14 type Z



- Molecule 46: 30S ribosomal protein S15





- Molecule 46: 30S ribosomal protein S15

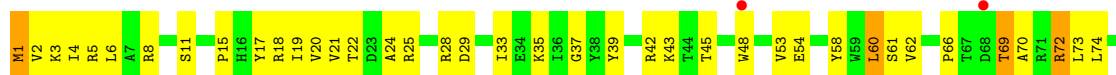


- Molecule 47: 30S ribosomal protein S16



GLY
ALA

- Molecule 47: 30S ribosomal protein S16



V79
Q82
GLY
ALA
ARG
GLY
GLY
ALA

- Molecule 48: 30S ribosomal protein S17

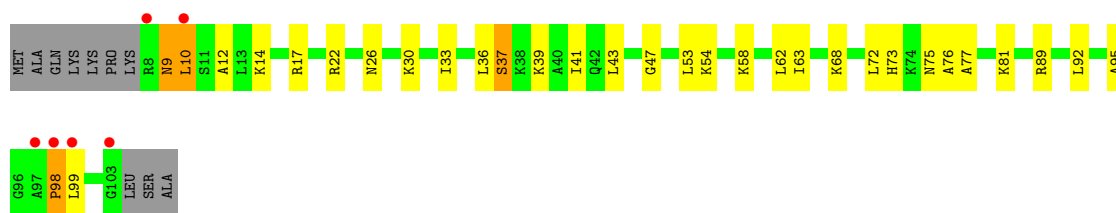


- Molecule 48: 30S ribosomal protein S17

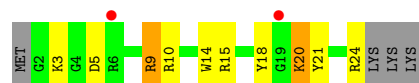


K100
ARG
GLY
GLY
LYS
ALA

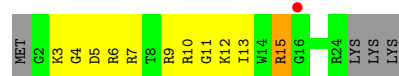
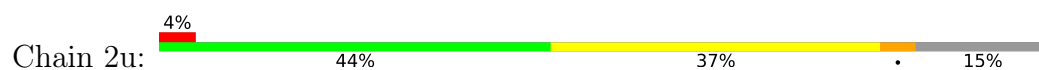
- Chain 2t:  6% 60% 26% 9%



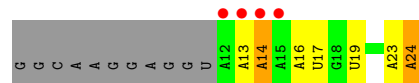
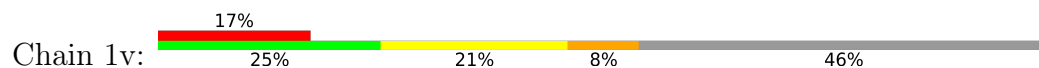
- Molecule 52: 30S ribosomal protein Thx



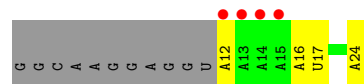
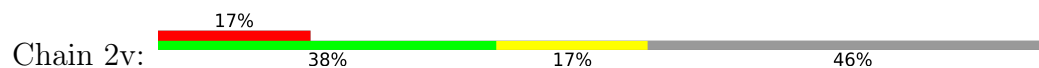
- Molecule 52: 30S ribosomal protein Thx



- Molecule 53: MET-PHE-mRNA



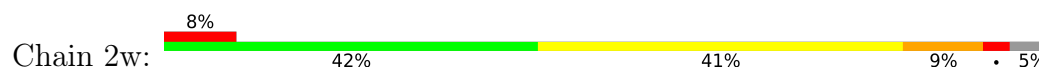
- Molecule 53: MET-PHE-mRNA

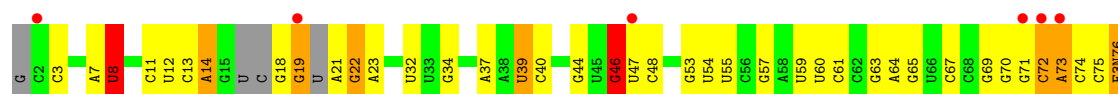


- Molecule 54: A-site Aminoacylated Phe-tRNAphe

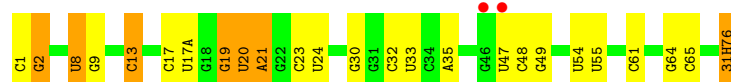


- Molecule 54: A-site Aminoacylated Phe-tRNAphe





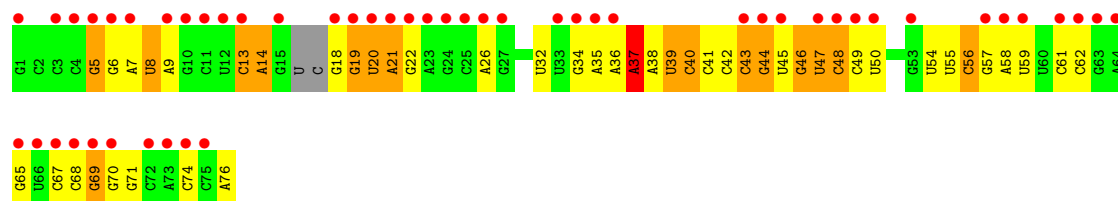
- Molecule 55: P-site Aminoacylated fMet-tRNA^{Met}



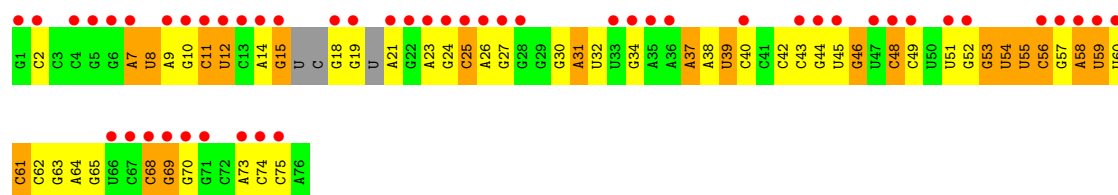
- Molecule 55: P-site Aminoacylated fMet-tRNA^{Met}



- Molecule 56: E-site Deacylated tRNA^{Phe}



- Molecule 56: E-site Deacylated tRNA^{Phe}



- Molecule 57: Lasso peptide lariocidin B



- Molecule 57: Lasso peptide lariocidin B



4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 21 21 21 | Depositor |
| Cell constants a, b, c, α , β , γ | 210.29Å 450.05Å 626.34Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 365.48 – 2.60 365.48 – 2.60 | Depositor EDS |
| % Data completeness (in resolution range) | 99.7 (365.48-2.60) 99.8 (365.48-2.60) | Depositor EDS |
| R_{merge} | 0.26 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 1.25 (at 2.62Å) | Xtriage |
| Refinement program | PHENIX 1.8.2 | Depositor |
| R, R_{free} | 0.215 , 0.266 0.218 , 0.266 | Depositor DCC |
| R_{free} test set | 89929 reflections (5.01%) | wwPDB-VP |
| Wilson B-factor (Å ²) | 45.8 | Xtriage |
| Anisotropy | 0.141 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.39 , 93.0 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| F_o, F_c correlation | 0.88 | EDS |
| Total number of atoms | 300583 | wwPDB-VP |
| Average B, all atoms (Å ²) | 47.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.52% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: K, M2G, 5MC, OMU, UR3, MIA, F3N, MG, 4OC, ZN, 5MU, SF4, MA6, PSU, 0TD, OMC, 31H, G7M, 4SU, 2MA, OMG, 2MG

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 | 0.54 | 0/69011 | 0.71 | 9/107720 (0.0%) |
| 1 | 2A | 0.43 | 0/67295 | 0.62 | 6/105042 (0.0%) |
| 2 | 1B | 0.44 | 0/2882 | 0.66 | 0/4494 |
| 2 | 2B | 0.37 | 0/2879 | 0.58 | 0/4487 |
| 3 | 1D | 0.52 | 0/2186 | 0.72 | 0/2944 |
| 3 | 2D | 0.46 | 0/2186 | 0.66 | 0/2944 |
| 4 | 1E | 0.50 | 0/1592 | 0.72 | 0/2149 |
| 4 | 2E | 0.39 | 0/1592 | 0.60 | 0/2149 |
| 5 | 1F | 0.51 | 0/1619 | 0.78 | 2/2193 (0.1%) |
| 5 | 2F | 0.42 | 0/1615 | 0.65 | 2/2188 (0.1%) |
| 6 | 1G | 0.44 | 0/1448 | 0.64 | 0/1957 |
| 6 | 2G | 0.36 | 0/1453 | 0.59 | 0/1963 |
| 7 | 1H | 0.45 | 0/1356 | 0.64 | 0/1834 |
| 7 | 2H | 0.35 | 0/1356 | 0.53 | 0/1834 |
| 8 | 1I | 0.39 | 0/1112 | 0.57 | 0/1514 |
| 8 | 2I | 0.37 | 0/1079 | 0.61 | 0/1475 |
| 9 | 1N | 0.52 | 0/1144 | 0.69 | 0/1543 |
| 9 | 2N | 0.39 | 0/1144 | 0.61 | 0/1543 |
| 10 | 1O | 0.50 | 0/943 | 0.66 | 0/1269 |
| 10 | 2O | 0.38 | 0/943 | 0.59 | 0/1269 |
| 11 | 1P | 0.51 | 0/1152 | 0.78 | 2/1533 (0.1%) |
| 11 | 2P | 0.43 | 0/1152 | 0.73 | 2/1533 (0.1%) |
| 12 | 1Q | 0.51 | 0/1143 | 0.69 | 0/1527 |
| 12 | 2Q | 0.41 | 0/1143 | 0.57 | 0/1527 |
| 13 | 1R | 0.57 | 0/982 | 0.77 | 0/1312 |
| 13 | 2R | 0.41 | 0/982 | 0.63 | 0/1312 |
| 14 | 1S | 0.45 | 0/883 | 0.69 | 0/1176 |
| 14 | 2S | 0.39 | 0/880 | 0.61 | 0/1172 |
| 15 | 1T | 0.48 | 0/1105 | 0.71 | 0/1477 |
| 15 | 2T | 0.39 | 0/1097 | 0.61 | 0/1468 |
| 16 | 1U | 0.57 | 0/977 | 0.73 | 0/1301 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|----------------|-------------|----------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 16 | 2U | 0.41 | 0/977 | 0.60 | 0/1301 |
| 17 | 1V | 0.52 | 0/782 | 0.71 | 0/1049 |
| 17 | 2V | 0.38 | 0/782 | 0.63 | 0/1049 |
| 18 | 1W | 0.57 | 0/897 | 0.70 | 0/1205 |
| 18 | 2W | 0.45 | 0/897 | 0.58 | 0/1205 |
| 19 | 1X | 0.56 | 0/764 | 0.76 | 2/1025 (0.2%) |
| 19 | 2X | 0.42 | 0/764 | 0.68 | 2/1025 (0.2%) |
| 20 | 1Y | 0.45 | 0/819 | 0.70 | 0/1095 |
| 20 | 2Y | 0.40 | 0/819 | 0.65 | 0/1095 |
| 21 | 1Z | 0.45 | 0/1267 | 0.66 | 0/1717 |
| 21 | 2Z | 0.38 | 0/1299 | 0.61 | 0/1763 |
| 22 | 10 | 0.52 | 0/662 | 0.73 | 0/881 |
| 22 | 20 | 0.40 | 0/662 | 0.67 | 0/881 |
| 23 | 11 | 0.53 | 0/762 | 0.63 | 0/1014 |
| 23 | 21 | 0.42 | 0/762 | 0.56 | 0/1014 |
| 24 | 12 | 0.53 | 0/590 | 0.66 | 0/781 |
| 24 | 22 | 0.37 | 0/590 | 0.60 | 0/781 |
| 25 | 13 | 0.53 | 0/474 | 0.70 | 0/635 |
| 25 | 23 | 0.38 | 0/469 | 0.67 | 0/630 |
| 26 | 14 | 0.48 | 0/565 | 0.70 | 0/761 |
| 26 | 24 | 0.40 | 0/545 | 0.71 | 0/737 |
| 27 | 15 | 0.55 | 0/469 | 0.76 | 0/635 |
| 27 | 25 | 0.42 | 0/469 | 0.62 | 0/635 |
| 28 | 16 | 0.50 | 0/460 | 0.64 | 0/613 |
| 28 | 26 | 0.44 | 0/456 | 0.60 | 0/608 |
| 29 | 17 | 0.60 | 0/426 | 0.76 | 0/561 |
| 29 | 27 | 0.54 | 0/426 | 0.71 | 0/561 |
| 30 | 18 | 0.49 | 0/525 | 0.72 | 0/691 |
| 30 | 28 | 0.45 | 0/525 | 0.63 | 0/691 |
| 31 | 19 | 0.53 | 0/310 | 0.81 | 1/407 (0.2%) |
| 31 | 29 | 0.38 | 0/310 | 0.65 | 0/407 |
| 32 | 1a | 0.40 | 0/35795 | 0.60 | 3/55864 (0.0%) |
| 32 | 2a | 0.37 | 1/35886 (0.0%) | 0.57 | 3/56005 (0.0%) |
| 33 | 1b | 0.37 | 0/1881 | 0.66 | 0/2542 |
| 33 | 2b | 0.41 | 0/1860 | 0.60 | 0/2518 |
| 34 | 1c | 0.39 | 0/1572 | 0.61 | 0/2126 |
| 34 | 2c | 0.38 | 0/1566 | 0.57 | 1/2119 (0.0%) |
| 35 | 1d | 0.37 | 0/1685 | 0.61 | 0/2262 |
| 35 | 2d | 0.37 | 0/1704 | 0.59 | 0/2284 |
| 36 | 1e | 0.40 | 0/1145 | 0.62 | 0/1543 |
| 36 | 2e | 0.40 | 0/1149 | 0.59 | 0/1548 |
| 37 | 1f | 0.39 | 0/823 | 0.56 | 0/1115 |
| 37 | 2f | 0.39 | 0/829 | 0.59 | 0/1123 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|-----------------|-------------|------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 38 | 1g | 0.36 | 0/1250 | 0.59 | 0/1679 |
| 38 | 2g | 0.38 | 0/1254 | 0.58 | 0/1683 |
| 39 | 1h | 0.36 | 0/1108 | 0.57 | 0/1494 |
| 39 | 2h | 0.33 | 0/1108 | 0.55 | 0/1494 |
| 40 | 1i | 0.36 | 0/1002 | 0.61 | 1/1346 (0.1%) |
| 40 | 2i | 0.38 | 0/997 | 0.59 | 0/1343 |
| 41 | 1j | 0.43 | 0/722 | 0.62 | 0/982 |
| 41 | 2j | 0.40 | 0/727 | 0.68 | 1/988 (0.1%) |
| 42 | 1k | 0.39 | 0/844 | 0.59 | 0/1145 |
| 42 | 2k | 0.39 | 0/848 | 0.60 | 0/1149 |
| 43 | 1l | 0.43 | 0/937 | 0.62 | 0/1260 |
| 43 | 2l | 0.39 | 0/937 | 0.60 | 0/1260 |
| 44 | 1m | 0.41 | 0/990 | 0.68 | 0/1327 |
| 44 | 2m | 0.37 | 0/961 | 0.62 | 0/1291 |
| 45 | 1n | 0.39 | 0/501 | 0.60 | 0/664 |
| 45 | 2n | 0.38 | 0/501 | 0.63 | 0/664 |
| 46 | 1o | 0.39 | 0/739 | 0.53 | 0/985 |
| 46 | 2o | 0.38 | 0/739 | 0.52 | 0/985 |
| 47 | 1p | 0.39 | 0/697 | 0.62 | 0/939 |
| 47 | 2p | 0.35 | 0/693 | 0.62 | 0/935 |
| 48 | 1q | 0.40 | 0/836 | 0.56 | 0/1117 |
| 48 | 2q | 0.37 | 0/836 | 0.57 | 0/1117 |
| 49 | 1r | 0.39 | 0/560 | 0.60 | 0/746 |
| 49 | 2r | 0.39 | 0/560 | 0.56 | 0/746 |
| 50 | 1s | 0.36 | 0/667 | 0.66 | 0/900 |
| 50 | 2s | 0.39 | 0/661 | 0.72 | 2/893 (0.2%) |
| 51 | 1t | 0.39 | 0/730 | 0.69 | 0/965 |
| 51 | 2t | 0.40 | 0/729 | 0.60 | 0/965 |
| 52 | 1u | 0.34 | 0/203 | 0.54 | 0/266 |
| 52 | 2u | 0.35 | 0/203 | 0.53 | 0/266 |
| 53 | 1v | 0.46 | 0/310 | 0.60 | 0/480 |
| 53 | 2v | 0.43 | 0/310 | 0.52 | 0/480 |
| 54 | 1w | 0.49 | 2/1603 (0.1%) | 0.63 | 0/2492 |
| 54 | 2w | 0.46 | 1/1531 (0.1%) | 0.60 | 0/2379 |
| 55 | 1x | 0.48 | 0/1723 | 0.62 | 0/2684 |
| 55 | 2x | 0.40 | 0/1723 | 0.58 | 0/2684 |
| 56 | 1y | 0.58 | 2/1606 (0.1%) | 0.56 | 0/2497 |
| 56 | 2y | 0.60 | 2/1583 (0.1%) | 0.60 | 0/2459 |
| 57 | 1z | 0.40 | 0/128 | 0.82 | 0/163 |
| 57 | 2z | 0.37 | 0/128 | 0.77 | 0/163 |
| All | All | 0.45 | 8/316935 (0.0%) | 0.64 | 39/474426 (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 |
|-----|-------|---------------------|---------------------|
| 15 | 1T | 0 | 1 |
| 21 | 1Z | 0 | 1 |
| 26 | 14 | 0 | 1 |
| 26 | 24 | 0 | 1 |
| 33 | 1b | 0 | 1 |
| 40 | 2i | 0 | 1 |
| 44 | 2m | 0 | 1 |
| 47 | 1p | 0 | 1 |
| All | All | 0 | 8 |

All (8) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 56 | 2y | 46 | G7M | O3'-P | 6.51 | 1.62 | 1.56 |
| 56 | 2y | 8 | 4SU | O3'-P | 6.11 | 1.62 | 1.56 |
| 54 | 1w | 46 | G7M | O3'-P | 5.87 | 1.62 | 1.56 |
| 56 | 1y | 8 | 4SU | O3'-P | 5.47 | 1.61 | 1.56 |
| 32 | 2a | 1498 | UR3 | O3'-P | 5.45 | 1.61 | 1.56 |
| 54 | 1w | 8 | 4SU | O3'-P | 5.36 | 1.61 | 1.56 |
| 56 | 1y | 46 | G7M | O3'-P | 5.23 | 1.61 | 1.56 |
| 54 | 2w | 46 | G7M | O3'-P | 5.17 | 1.61 | 1.56 |

All (39) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | 1A | 1992 | G | C2'-C3'-O3' | 9.78 | 124.16 | 109.50 |
| 11 | 1P | 35 | HIS | CA-C-N | -7.85 | 106.55 | 121.54 |
| 11 | 1P | 35 | HIS | C-N-CA | -7.85 | 106.55 | 121.54 |
| 1 | 2A | 1992 | G | C2'-C3'-O3' | 7.07 | 120.10 | 109.50 |
| 32 | 2a | 1272 | G | N1-C2-N2 | -7.00 | 95.19 | 116.20 |
| 5 | 1F | 89 | VAL | CA-C-N | -6.88 | 110.95 | 123.34 |
| 5 | 1F | 89 | VAL | C-N-CA | -6.88 | 110.95 | 123.34 |
| 32 | 1a | 266 | G | C2'-C3'-O3' | 6.46 | 119.19 | 109.50 |
| 41 | 2j | 82 | ILE | N-CA-C | -6.08 | 105.04 | 112.76 |
| 11 | 2P | 35 | HIS | CA-C-N | -6.08 | 109.93 | 121.54 |
| 11 | 2P | 35 | HIS | C-N-CA | -6.08 | 109.93 | 121.54 |
| 1 | 1A | 1992 | G | P-O3'-C3' | 6.08 | 129.31 | 120.20 |
| 1 | 1A | 2689 | U | C2'-C3'-O3' | 5.98 | 118.47 | 109.50 |
| 1 | 2A | 2689 | U | P-O3'-C3' | 5.93 | 129.10 | 120.20 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 19 | 2X | 94 | GLY | CA-C-N | 5.77 | 132.09 | 121.70 |
| 19 | 2X | 94 | GLY | C-N-CA | 5.77 | 132.09 | 121.70 |
| 1 | 2A | 1653 | G | C2'-C3'-O3' | 5.69 | 118.03 | 109.50 |
| 5 | 2F | 21 | ALA | CA-C-N | 5.66 | 131.89 | 121.70 |
| 5 | 2F | 21 | ALA | C-N-CA | 5.66 | 131.89 | 121.70 |
| 32 | 2a | 1263 | C | N1-C2-O2 | 5.63 | 135.78 | 118.90 |
| 1 | 1A | 512 | G | O4'-C1'-N9 | 5.59 | 116.58 | 108.20 |
| 1 | 2A | 1210 | A | C4'-C3'-O3' | 5.56 | 117.74 | 109.40 |
| 1 | 1A | 2629 | A | P-O3'-C3' | 5.41 | 128.32 | 120.20 |
| 1 | 2A | 1368 | G | O5'-P-OP2 | -5.38 | 91.86 | 108.00 |
| 32 | 1a | 913 | A | P-O3'-C3' | 5.35 | 128.22 | 120.20 |
| 1 | 1A | 2689 | U | P-O3'-C3' | 5.29 | 128.14 | 120.20 |
| 34 | 2c | 126 | ARG | N-CA-C | -5.28 | 107.38 | 112.97 |
| 31 | 19 | 10 | ILE | N-CA-C | -5.27 | 107.69 | 112.96 |
| 32 | 2a | 1272 | G | N3-C2-N2 | 5.22 | 135.57 | 119.90 |
| 1 | 2A | 2689 | U | C4'-C3'-O3' | 5.22 | 117.23 | 109.40 |
| 32 | 1a | 913 | A | C2'-C3'-O3' | 5.20 | 117.30 | 109.50 |
| 40 | 1i | 125 | TYR | CA-CB-CG | 5.20 | 123.25 | 113.90 |
| 1 | 1A | 1128 | A | C5'-C4'-C3' | 5.19 | 122.99 | 115.20 |
| 1 | 1A | 2629 | A | C2'-C3'-O3' | 5.15 | 117.23 | 109.50 |
| 50 | 2s | 28 | LYS | CA-C-N | 5.15 | 130.97 | 121.70 |
| 50 | 2s | 28 | LYS | C-N-CA | 5.15 | 130.97 | 121.70 |
| 19 | 1X | 94 | GLY | CA-C-N | 5.12 | 130.91 | 121.70 |
| 19 | 1X | 94 | GLY | C-N-CA | 5.12 | 130.91 | 121.70 |
| 1 | 1A | 818 | G | O3'-P-O5' | 5.09 | 111.64 | 104.00 |

There are no chirality outliers.

All (8) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 26 | 14 | 67 | TYR | Peptide |
| 15 | 1T | 128 | GLU | Peptide |
| 21 | 1Z | 136 | PHE | Peptide |
| 33 | 1b | 122 | PHE | Peptide |
| 47 | 1p | 4 | ILE | Peptide |
| 26 | 24 | 67 | TYR | Peptide |
| 40 | 2i | 20 | ARG | Peptide |
| 44 | 2m | 105 | THR | Peptide |

5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | 1A | 61852 | 0 | 31193 | 646 | 0 |
| 1 | 2A | 60322 | 0 | 30427 | 689 | 0 |
| 2 | 1B | 2577 | 0 | 1305 | 23 | 0 |
| 2 | 2B | 2575 | 0 | 1303 | 45 | 0 |
| 3 | 1D | 2136 | 0 | 2218 | 51 | 0 |
| 3 | 2D | 2136 | 0 | 2218 | 43 | 0 |
| 4 | 1E | 1559 | 0 | 1618 | 35 | 0 |
| 4 | 2E | 1559 | 0 | 1618 | 43 | 0 |
| 5 | 1F | 1584 | 0 | 1625 | 40 | 0 |
| 5 | 2F | 1580 | 0 | 1619 | 52 | 0 |
| 6 | 1G | 1423 | 0 | 1436 | 44 | 0 |
| 6 | 2G | 1428 | 0 | 1438 | 59 | 0 |
| 7 | 1H | 1330 | 0 | 1407 | 29 | 0 |
| 7 | 2H | 1330 | 0 | 1407 | 46 | 0 |
| 8 | 1I | 1097 | 0 | 1140 | 37 | 1 |
| 8 | 2I | 1064 | 0 | 1082 | 44 | 0 |
| 9 | 1N | 1117 | 0 | 1184 | 15 | 0 |
| 9 | 2N | 1117 | 0 | 1184 | 19 | 0 |
| 10 | 1O | 933 | 0 | 996 | 23 | 0 |
| 10 | 2O | 933 | 0 | 996 | 22 | 0 |
| 11 | 1P | 1135 | 0 | 1212 | 33 | 0 |
| 11 | 2P | 1135 | 0 | 1212 | 45 | 0 |
| 12 | 1Q | 1122 | 0 | 1179 | 17 | 0 |
| 12 | 2Q | 1122 | 0 | 1179 | 48 | 0 |
| 13 | 1R | 968 | 0 | 1033 | 19 | 0 |
| 13 | 2R | 968 | 0 | 1033 | 20 | 0 |
| 14 | 1S | 873 | 0 | 927 | 22 | 0 |
| 14 | 2S | 870 | 0 | 923 | 29 | 0 |
| 15 | 1T | 1091 | 0 | 1151 | 24 | 0 |
| 15 | 2T | 1083 | 0 | 1136 | 24 | 0 |
| 16 | 1U | 959 | 0 | 1019 | 16 | 0 |
| 16 | 2U | 959 | 0 | 1019 | 18 | 0 |
| 17 | 1V | 771 | 0 | 830 | 14 | 0 |
| 17 | 2V | 771 | 0 | 830 | 15 | 0 |
| 18 | 1W | 886 | 0 | 940 | 15 | 0 |
| 18 | 2W | 886 | 0 | 940 | 13 | 0 |
| 19 | 1X | 750 | 0 | 814 | 16 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 19 | 2X | 750 | 0 | 814 | 20 | 0 |
| 20 | 1Y | 806 | 0 | 881 | 13 | 0 |
| 20 | 2Y | 806 | 0 | 881 | 23 | 0 |
| 21 | 1Z | 1240 | 0 | 1240 | 34 | 0 |
| 21 | 2Z | 1271 | 0 | 1273 | 62 | 0 |
| 22 | 10 | 653 | 0 | 674 | 7 | 0 |
| 22 | 20 | 653 | 0 | 674 | 14 | 0 |
| 23 | 11 | 755 | 0 | 826 | 19 | 0 |
| 23 | 21 | 755 | 0 | 826 | 23 | 0 |
| 24 | 12 | 588 | 0 | 643 | 14 | 0 |
| 24 | 22 | 588 | 0 | 643 | 16 | 0 |
| 25 | 13 | 469 | 0 | 518 | 14 | 0 |
| 25 | 23 | 464 | 0 | 514 | 19 | 0 |
| 26 | 14 | 552 | 0 | 533 | 32 | 0 |
| 26 | 24 | 532 | 0 | 503 | 36 | 0 |
| 27 | 15 | 455 | 0 | 465 | 7 | 0 |
| 27 | 25 | 455 | 0 | 465 | 7 | 0 |
| 28 | 16 | 453 | 0 | 473 | 9 | 0 |
| 28 | 26 | 449 | 0 | 469 | 11 | 0 |
| 29 | 17 | 418 | 0 | 467 | 7 | 0 |
| 29 | 27 | 418 | 0 | 467 | 9 | 0 |
| 30 | 18 | 517 | 0 | 582 | 12 | 0 |
| 30 | 28 | 517 | 0 | 582 | 12 | 0 |
| 31 | 19 | 307 | 0 | 335 | 3 | 0 |
| 31 | 29 | 307 | 0 | 335 | 4 | 0 |
| 32 | 1a | 32246 | 0 | 16295 | 471 | 0 |
| 32 | 2a | 32327 | 0 | 16338 | 523 | 1 |
| 33 | 1b | 1846 | 0 | 1867 | 87 | 0 |
| 33 | 2b | 1825 | 0 | 1828 | 91 | 0 |
| 34 | 1c | 1548 | 0 | 1535 | 42 | 0 |
| 34 | 2c | 1542 | 0 | 1517 | 57 | 0 |
| 35 | 1d | 1655 | 0 | 1672 | 59 | 0 |
| 35 | 2d | 1674 | 0 | 1714 | 53 | 0 |
| 36 | 1e | 1129 | 0 | 1185 | 42 | 0 |
| 36 | 2e | 1133 | 0 | 1191 | 47 | 0 |
| 37 | 1f | 810 | 0 | 804 | 16 | 0 |
| 37 | 2f | 816 | 0 | 808 | 31 | 0 |
| 38 | 1g | 1231 | 0 | 1238 | 31 | 0 |
| 38 | 2g | 1235 | 0 | 1249 | 45 | 0 |
| 39 | 1h | 1088 | 0 | 1126 | 31 | 0 |
| 39 | 2h | 1088 | 0 | 1126 | 27 | 0 |
| 40 | 1i | 983 | 0 | 986 | 52 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 40 | 2i | 978 | 0 | 966 | 37 | 0 |
| 41 | 1j | 709 | 0 | 650 | 36 | 0 |
| 41 | 2j | 714 | 0 | 672 | 45 | 0 |
| 42 | 1k | 829 | 0 | 825 | 21 | 0 |
| 42 | 2k | 833 | 0 | 836 | 28 | 0 |
| 43 | 1l | 932 | 0 | 981 | 14 | 0 |
| 43 | 2l | 932 | 0 | 980 | 20 | 0 |
| 44 | 1m | 979 | 0 | 1028 | 38 | 0 |
| 44 | 2m | 950 | 0 | 988 | 41 | 0 |
| 45 | 1n | 492 | 0 | 529 | 14 | 0 |
| 45 | 2n | 492 | 0 | 529 | 24 | 0 |
| 46 | 1o | 728 | 0 | 760 | 22 | 0 |
| 46 | 2o | 728 | 0 | 760 | 20 | 0 |
| 47 | 1p | 681 | 0 | 697 | 35 | 0 |
| 47 | 2p | 677 | 0 | 686 | 29 | 0 |
| 48 | 1q | 823 | 0 | 891 | 17 | 0 |
| 48 | 2q | 823 | 0 | 891 | 16 | 0 |
| 49 | 1r | 555 | 0 | 618 | 11 | 0 |
| 49 | 2r | 555 | 0 | 618 | 15 | 0 |
| 50 | 1s | 652 | 0 | 662 | 34 | 0 |
| 50 | 2s | 646 | 0 | 644 | 28 | 0 |
| 51 | 1t | 728 | 0 | 798 | 23 | 0 |
| 51 | 2t | 727 | 0 | 796 | 24 | 0 |
| 52 | 1u | 199 | 0 | 208 | 10 | 0 |
| 52 | 2u | 199 | 0 | 208 | 9 | 0 |
| 53 | 1v | 277 | 0 | 140 | 5 | 0 |
| 53 | 2v | 277 | 0 | 140 | 2 | 0 |
| 54 | 1w | 1623 | 0 | 839 | 21 | 0 |
| 54 | 2w | 1555 | 0 | 798 | 23 | 0 |
| 55 | 1x | 1656 | 0 | 848 | 15 | 0 |
| 55 | 2x | 1656 | 0 | 849 | 12 | 0 |
| 56 | 1y | 1585 | 0 | 803 | 36 | 0 |
| 56 | 2y | 1565 | 0 | 794 | 38 | 0 |
| 57 | 1z | 127 | 0 | 139 | 7 | 0 |
| 57 | 2z | 127 | 0 | 140 | 4 | 0 |
| 58 | 10 | 9 | 0 | 0 | 0 | 0 |
| 58 | 11 | 6 | 0 | 0 | 0 | 0 |
| 58 | 12 | 2 | 0 | 0 | 0 | 0 |
| 58 | 13 | 3 | 0 | 0 | 0 | 0 |
| 58 | 15 | 9 | 0 | 0 | 0 | 0 |
| 58 | 16 | 2 | 0 | 0 | 0 | 0 |
| 58 | 17 | 3 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 58 | 18 | 5 | 0 | 0 | 0 | 0 |
| 58 | 19 | 1 | 0 | 0 | 0 | 0 |
| 58 | 1A | 1105 | 0 | 0 | 0 | 0 |
| 58 | 1B | 37 | 0 | 0 | 0 | 0 |
| 58 | 1D | 12 | 0 | 0 | 0 | 0 |
| 58 | 1E | 14 | 0 | 0 | 0 | 0 |
| 58 | 1F | 13 | 0 | 0 | 0 | 0 |
| 58 | 1G | 5 | 0 | 0 | 0 | 0 |
| 58 | 1I | 1 | 0 | 0 | 0 | 0 |
| 58 | 1N | 7 | 0 | 0 | 0 | 0 |
| 58 | 1O | 5 | 0 | 0 | 0 | 0 |
| 58 | 1P | 4 | 0 | 0 | 0 | 0 |
| 58 | 1Q | 7 | 0 | 0 | 0 | 0 |
| 58 | 1R | 4 | 0 | 0 | 0 | 0 |
| 58 | 1S | 3 | 0 | 0 | 0 | 0 |
| 58 | 1T | 3 | 0 | 0 | 0 | 0 |
| 58 | 1U | 11 | 0 | 0 | 0 | 0 |
| 58 | 1V | 7 | 0 | 0 | 0 | 0 |
| 58 | 1W | 8 | 0 | 0 | 0 | 0 |
| 58 | 1X | 6 | 0 | 0 | 0 | 0 |
| 58 | 1Y | 3 | 0 | 0 | 0 | 0 |
| 58 | 1Z | 3 | 0 | 0 | 0 | 0 |
| 58 | 1a | 218 | 0 | 0 | 0 | 0 |
| 58 | 1b | 1 | 0 | 0 | 0 | 0 |
| 58 | 1d | 1 | 0 | 0 | 0 | 0 |
| 58 | 1e | 2 | 0 | 0 | 0 | 0 |
| 58 | 1f | 2 | 0 | 0 | 0 | 0 |
| 58 | 1h | 1 | 0 | 0 | 0 | 0 |
| 58 | 1l | 2 | 0 | 0 | 0 | 0 |
| 58 | 1m | 1 | 0 | 0 | 0 | 0 |
| 58 | 1n | 1 | 0 | 0 | 0 | 0 |
| 58 | 1p | 1 | 0 | 0 | 0 | 0 |
| 58 | 1s | 1 | 0 | 0 | 0 | 0 |
| 58 | 1t | 1 | 0 | 0 | 0 | 0 |
| 58 | 1v | 2 | 0 | 0 | 0 | 0 |
| 58 | 1w | 8 | 0 | 0 | 0 | 0 |
| 58 | 1x | 13 | 0 | 0 | 0 | 0 |
| 58 | 1y | 1 | 0 | 0 | 0 | 0 |
| 58 | 21 | 1 | 0 | 0 | 0 | 0 |
| 58 | 23 | 1 | 0 | 0 | 0 | 0 |
| 58 | 25 | 4 | 0 | 0 | 0 | 0 |
| 58 | 26 | 1 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 58 | 27 | 3 | 0 | 0 | 0 | 0 |
| 58 | 28 | 4 | 0 | 0 | 0 | 0 |
| 58 | 29 | 1 | 0 | 0 | 0 | 0 |
| 58 | 2A | 883 | 0 | 0 | 0 | 0 |
| 58 | 2B | 19 | 0 | 0 | 0 | 0 |
| 58 | 2D | 7 | 0 | 0 | 0 | 0 |
| 58 | 2E | 11 | 0 | 0 | 0 | 0 |
| 58 | 2F | 9 | 0 | 0 | 0 | 0 |
| 58 | 2G | 1 | 0 | 0 | 0 | 0 |
| 58 | 2N | 1 | 0 | 0 | 0 | 0 |
| 58 | 2O | 1 | 0 | 0 | 0 | 0 |
| 58 | 2Q | 3 | 0 | 0 | 0 | 0 |
| 58 | 2R | 3 | 0 | 0 | 0 | 0 |
| 58 | 2S | 1 | 0 | 0 | 0 | 0 |
| 58 | 2T | 3 | 0 | 0 | 0 | 0 |
| 58 | 2U | 2 | 0 | 0 | 0 | 0 |
| 58 | 2V | 2 | 0 | 0 | 0 | 0 |
| 58 | 2W | 2 | 0 | 0 | 0 | 0 |
| 58 | 2X | 1 | 0 | 0 | 0 | 0 |
| 58 | 2Z | 1 | 0 | 0 | 0 | 0 |
| 58 | 2a | 242 | 0 | 0 | 0 | 0 |
| 58 | 2d | 1 | 0 | 0 | 0 | 0 |
| 58 | 2e | 1 | 0 | 0 | 0 | 0 |
| 58 | 2f | 2 | 0 | 0 | 0 | 0 |
| 58 | 2g | 1 | 0 | 0 | 0 | 0 |
| 58 | 2i | 1 | 0 | 0 | 0 | 0 |
| 58 | 2j | 1 | 0 | 0 | 0 | 0 |
| 58 | 2l | 5 | 0 | 0 | 0 | 0 |
| 58 | 2p | 1 | 0 | 0 | 0 | 0 |
| 58 | 2q | 2 | 0 | 0 | 0 | 0 |
| 58 | 2r | 1 | 0 | 0 | 0 | 0 |
| 58 | 2t | 1 | 0 | 0 | 0 | 0 |
| 58 | 2v | 3 | 0 | 0 | 0 | 0 |
| 58 | 2w | 12 | 0 | 0 | 0 | 0 |
| 58 | 2x | 5 | 0 | 0 | 0 | 0 |
| 58 | 2y | 6 | 0 | 0 | 0 | 0 |
| 59 | 1A | 1 | 0 | 0 | 0 | 0 |
| 59 | 2x | 1 | 0 | 0 | 0 | 0 |
| 60 | 14 | 1 | 0 | 0 | 0 | 0 |
| 60 | 15 | 1 | 0 | 0 | 0 | 0 |
| 60 | 16 | 1 | 0 | 0 | 0 | 0 |
| 60 | 19 | 1 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 60 | 1Y | 1 | 0 | 0 | 0 | 0 |
| 60 | 1n | 1 | 0 | 0 | 0 | 0 |
| 60 | 24 | 1 | 0 | 0 | 0 | 0 |
| 60 | 25 | 1 | 0 | 0 | 0 | 0 |
| 60 | 26 | 1 | 0 | 0 | 0 | 0 |
| 60 | 29 | 1 | 0 | 0 | 0 | 0 |
| 60 | 2Y | 1 | 0 | 0 | 0 | 0 |
| 60 | 2n | 1 | 0 | 0 | 0 | 0 |
| 61 | 1d | 8 | 0 | 0 | 2 | 0 |
| 61 | 2d | 8 | 0 | 0 | 0 | 0 |
| 62 | 10 | 13 | 0 | 0 | 1 | 0 |
| 62 | 11 | 11 | 0 | 0 | 0 | 0 |
| 62 | 12 | 4 | 0 | 0 | 0 | 0 |
| 62 | 13 | 5 | 0 | 0 | 0 | 0 |
| 62 | 14 | 1 | 0 | 0 | 0 | 0 |
| 62 | 15 | 5 | 0 | 0 | 0 | 0 |
| 62 | 16 | 4 | 0 | 0 | 0 | 0 |
| 62 | 17 | 7 | 0 | 0 | 1 | 0 |
| 62 | 18 | 9 | 0 | 0 | 1 | 0 |
| 62 | 1A | 2019 | 0 | 0 | 73 | 0 |
| 62 | 1B | 63 | 0 | 0 | 2 | 0 |
| 62 | 1D | 24 | 0 | 0 | 1 | 0 |
| 62 | 1E | 24 | 0 | 0 | 2 | 0 |
| 62 | 1F | 15 | 0 | 0 | 1 | 0 |
| 62 | 1G | 2 | 0 | 0 | 0 | 0 |
| 62 | 1H | 2 | 0 | 0 | 0 | 0 |
| 62 | 1I | 1 | 0 | 0 | 1 | 0 |
| 62 | 1N | 5 | 0 | 0 | 0 | 0 |
| 62 | 1O | 6 | 0 | 0 | 0 | 0 |
| 62 | 1P | 19 | 0 | 0 | 0 | 0 |
| 62 | 1Q | 8 | 0 | 0 | 0 | 0 |
| 62 | 1R | 12 | 0 | 0 | 2 | 0 |
| 62 | 1S | 5 | 0 | 0 | 0 | 0 |
| 62 | 1T | 9 | 0 | 0 | 1 | 0 |
| 62 | 1U | 15 | 0 | 0 | 1 | 0 |
| 62 | 1V | 8 | 0 | 0 | 0 | 0 |
| 62 | 1W | 9 | 0 | 0 | 1 | 0 |
| 62 | 1X | 4 | 0 | 0 | 0 | 0 |
| 62 | 1Y | 3 | 0 | 0 | 0 | 0 |
| 62 | 1Z | 1 | 0 | 0 | 0 | 0 |
| 62 | 1a | 388 | 0 | 0 | 28 | 0 |
| 62 | 1b | 1 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 62 | 1f | 1 | 0 | 0 | 0 | 0 |
| 62 | 1l | 8 | 0 | 0 | 0 | 0 |
| 62 | 1m | 2 | 0 | 0 | 0 | 0 |
| 62 | 1n | 1 | 0 | 0 | 0 | 0 |
| 62 | 1o | 1 | 0 | 0 | 0 | 0 |
| 62 | 1p | 1 | 0 | 0 | 0 | 0 |
| 62 | 1q | 2 | 0 | 0 | 0 | 0 |
| 62 | 1u | 1 | 0 | 0 | 1 | 0 |
| 62 | 1v | 6 | 0 | 0 | 0 | 0 |
| 62 | 1w | 20 | 0 | 0 | 1 | 0 |
| 62 | 1x | 15 | 0 | 0 | 0 | 0 |
| 62 | 1y | 2 | 0 | 0 | 0 | 0 |
| 62 | 1z | 1 | 0 | 0 | 0 | 0 |
| 62 | 20 | 3 | 0 | 0 | 0 | 0 |
| 62 | 21 | 13 | 0 | 0 | 1 | 0 |
| 62 | 23 | 1 | 0 | 0 | 0 | 0 |
| 62 | 25 | 1 | 0 | 0 | 0 | 0 |
| 62 | 27 | 5 | 0 | 0 | 0 | 0 |
| 62 | 28 | 4 | 0 | 0 | 1 | 0 |
| 62 | 29 | 1 | 0 | 0 | 0 | 0 |
| 62 | 2A | 1153 | 0 | 0 | 74 | 0 |
| 62 | 2B | 23 | 0 | 0 | 2 | 0 |
| 62 | 2D | 24 | 0 | 0 | 0 | 0 |
| 62 | 2E | 14 | 0 | 0 | 0 | 0 |
| 62 | 2F | 13 | 0 | 0 | 0 | 0 |
| 62 | 2I | 2 | 0 | 0 | 0 | 0 |
| 62 | 2N | 3 | 0 | 0 | 0 | 0 |
| 62 | 2O | 3 | 0 | 0 | 0 | 0 |
| 62 | 2P | 14 | 0 | 0 | 2 | 0 |
| 62 | 2Q | 3 | 0 | 0 | 0 | 0 |
| 62 | 2R | 3 | 0 | 0 | 0 | 0 |
| 62 | 2T | 4 | 0 | 0 | 0 | 0 |
| 62 | 2U | 2 | 0 | 0 | 0 | 0 |
| 62 | 2W | 2 | 0 | 0 | 0 | 0 |
| 62 | 2X | 2 | 0 | 0 | 0 | 0 |
| 62 | 2Y | 1 | 0 | 0 | 0 | 0 |
| 62 | 2Z | 1 | 0 | 0 | 0 | 0 |
| 62 | 2a | 283 | 0 | 0 | 20 | 0 |
| 62 | 2c | 2 | 0 | 0 | 0 | 0 |
| 62 | 2d | 2 | 0 | 0 | 0 | 0 |
| 62 | 2e | 1 | 0 | 0 | 0 | 0 |
| 62 | 2j | 3 | 0 | 0 | 1 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 62 | 2l | 6 | 0 | 0 | 1 | 0 |
| 62 | 2p | 1 | 0 | 0 | 0 | 0 |
| 62 | 2r | 1 | 0 | 0 | 0 | 0 |
| 62 | 2t | 1 | 0 | 0 | 0 | 0 |
| 62 | 2v | 2 | 0 | 0 | 0 | 0 |
| 62 | 2w | 10 | 0 | 0 | 0 | 0 |
| 62 | 2x | 6 | 0 | 0 | 0 | 0 |
| 62 | 2y | 9 | 0 | 0 | 0 | 0 |
| All | All | 300583 | 0 | 197064 | 4696 | 1 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (4696) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:1A:1082:U:H3 | 1:1A:1086:A:N6 | 1.31 | 1.29 |
| 1:1A:2136:C:N4 | 1:1A:2155:G:H1 | 1.49 | 1.08 |
| 1:1A:1054:A:N6 | 1:1A:1105:U:H3 | 1.55 | 1.04 |
| 1:2A:1604:C:OP2 | 62:2A:3903:HOH:O | 1.77 | 1.03 |
| 1:1A:1798:U:H5' | 3:1D:259:THR:HG22 | 1.40 | 1.03 |
| 1:1A:2427:C:OP1 | 62:1A:4203:HOH:O | 1.77 | 1.03 |
| 1:1A:1014:U:OP2 | 62:1A:4204:HOH:O | 1.77 | 1.02 |
| 1:1A:1082:U:O4 | 1:1A:1086:A:N1 | 1.95 | 1.00 |
| 1:2A:1603:A:OP1 | 62:2A:3903:HOH:O | 1.79 | 0.98 |
| 1:1A:631:A:OP1 | 11:1P:65:ARG:NH1 | 1.96 | 0.97 |
| 1:2A:2136:C:HO2' | 1:2A:2137:C:H6 | 1.04 | 0.97 |
| 2:2B:7:G:H21 | 14:2S:38:GLN:HE22 | 1.09 | 0.97 |
| 44:2m:13:LYS:HA | 44:2m:44:ARG:HH11 | 1.28 | 0.96 |
| 19:1X:31:HIS:HD2 | 19:1X:33:LYS:H | 1.15 | 0.95 |
| 1:2A:2807:G:N1 | 1:2A:2893:G:O6 | 2.00 | 0.94 |
| 1:2A:2319:G:H22 | 14:2S:3:ARG:HH11 | 1.12 | 0.94 |
| 18:2W:1:MET:HE3 | 18:2W:62:HIS:HB3 | 1.51 | 0.93 |
| 1:1A:2099:U:H3 | 1:1A:2190:G:H1 | 0.97 | 0.93 |
| 10:2O:48:PRO:HB3 | 32:2a:1422:G:H5'' | 1.49 | 0.92 |
| 10:1O:48:PRO:HB3 | 32:1a:1422:G:H5'' | 1.49 | 0.91 |
| 1:1A:301:G:OP2 | 20:1Y:84:ARG:NH2 | 2.04 | 0.90 |
| 1:1A:2136:C:N3 | 1:1A:2155:G:N2 | 2.20 | 0.90 |
| 32:1a:677:U:H3 | 32:1a:713:G:H22 | 1.18 | 0.89 |
| 32:1a:1004:A:N6 | 32:1a:1037:C:N3 | 2.19 | 0.89 |
| 33:1b:33:TYR:HB2 | 33:1b:43:ASP:HB2 | 1.53 | 0.89 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 32:1a:1318:A:H5'' | 50:1s:3:ARG:HH12 | 1.36 | 0.89 |
| 1:1A:1065:U:O2 | 1:1A:1073:A:N6 | 2.04 | 0.89 |
| 1:2A:1798:U:H5' | 3:2D:259:THR:HG22 | 1.54 | 0.89 |
| 32:2a:1224:G:OP1 | 62:2a:1902:HOH:O | 1.90 | 0.89 |
| 40:1i:48:GLU:HA | 40:1i:51:ARG:HD3 | 1.54 | 0.88 |
| 1:2A:2134:A:H62 | 1:2A:2157:G:H4' | 1.38 | 0.88 |
| 1:2A:994:C:OP1 | 16:2U:53:ARG:NH2 | 2.07 | 0.88 |
| 1:1A:1670:C:OP2 | 62:1A:4205:HOH:O | 1.91 | 0.88 |
| 1:1A:2100:G:H1 | 1:1A:2189:U:H3 | 1.18 | 0.88 |
| 1:2A:1254:A:OP2 | 62:2A:3904:HOH:O | 1.91 | 0.88 |
| 12:1Q:12:GLN:HE21 | 12:1Q:73:PRO:HD2 | 1.37 | 0.88 |
| 54:1w:75:C:O3' | 54:1w:76:F3N:P | 2.32 | 0.87 |
| 40:2i:128:ARG:NH2 | 55:2x:33:U:OP2 | 2.07 | 0.87 |
| 1:2A:2133:G:O2' | 1:2A:2157:G:N2 | 2.07 | 0.86 |
| 2:2B:103:G:H21 | 21:2Z:73:GLN:HE22 | 1.19 | 0.86 |
| 1:2A:1812:A:OP2 | 62:2A:3906:HOH:O | 1.93 | 0.86 |
| 1:2A:2615:U:OP1 | 62:2A:3905:HOH:O | 1.93 | 0.86 |
| 34:2c:47:LEU:HB2 | 34:2c:52:LEU:HD22 | 1.56 | 0.86 |
| 40:2i:16:ARG:HB2 | 40:2i:64:THR:HG23 | 1.57 | 0.86 |
| 1:1A:1013:C:OP2 | 62:1A:4204:HOH:O | 1.93 | 0.85 |
| 1:1A:1054:A:H61 | 1:1A:1105:U:H3 | 0.88 | 0.85 |
| 34:1c:6:HIS:HD2 | 34:1c:8:ILE:H | 1.20 | 0.85 |
| 1:1A:2102:U:H3 | 1:1A:2187:G:H1 | 1.21 | 0.85 |
| 46:2o:54:ARG:HG2 | 46:2o:58:MET:HE2 | 1.59 | 0.85 |
| 32:1a:405:U:O4 | 35:1d:2:GLY:N | 2.10 | 0.85 |
| 1:2A:2206:G:H3' | 1:2A:2207:G:C8 | 2.11 | 0.84 |
| 39:1h:10:LEU:HD22 | 39:1h:83:ILE:HD11 | 1.59 | 0.84 |
| 33:2b:112:VAL:HG22 | 33:2b:149:LEU:HD13 | 1.59 | 0.84 |
| 6:1G:77:ILE:HD12 | 6:1G:82:LEU:HD12 | 1.59 | 0.84 |
| 1:1A:1082:U:N3 | 1:1A:1086:A:N6 | 2.07 | 0.84 |
| 32:2a:448:A:OP2 | 32:2a:485:G:N2 | 2.09 | 0.84 |
| 1:1A:2550:G:OP1 | 62:1A:4205:HOH:O | 1.96 | 0.84 |
| 22:20:10:THR:HG22 | 22:20:12:ASN:H | 1.42 | 0.84 |
| 1:1A:2702:U:OP2 | 62:1A:4207:HOH:O | 1.95 | 0.83 |
| 56:2y:14:A:H61 | 56:2y:21:A:H2 | 1.26 | 0.83 |
| 1:1A:2277:G:OP2 | 22:10:10:THR:HG21 | 1.78 | 0.83 |
| 57:1z:3:LYS:HE2 | 57:1z:17:ARG:HG3 | 1.60 | 0.83 |
| 4:2E:47:VAL:HG11 | 4:2E:86:PRO:HD2 | 1.61 | 0.83 |
| 1:2A:2839:G:H5' | 13:2R:46:GLY:HA2 | 1.60 | 0.83 |
| 1:1A:1036:G:O6 | 62:1A:4206:HOH:O | 1.95 | 0.83 |
| 1:2A:2677:G:N3 | 62:2A:3928:HOH:O | 2.10 | 0.83 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:1A:826:U:OP1 | 62:1A:4203:HOH:O | 1.96 | 0.83 |
| 32:2a:1181:G:O2' | 32:2a:1182:G:N7 | 2.11 | 0.83 |
| 7:2H:124:GLU:HB2 | 7:2H:132:ARG:HB3 | 1.60 | 0.82 |
| 32:1a:342:C:N4 | 32:1a:347:G:O6 | 2.11 | 0.82 |
| 1:2A:1225:G:H4' | 17:2V:84:LYS:HG2 | 1.61 | 0.82 |
| 42:2k:48:ILE:O | 42:2k:50:TYR:N | 2.13 | 0.82 |
| 46:1o:16:ALA:HB1 | 46:1o:21:ASP:HB3 | 1.60 | 0.82 |
| 1:1A:1176:G:N2 | 1:1A:1178:C:OP2 | 2.12 | 0.82 |
| 46:2o:16:ALA:HB1 | 46:2o:21:ASP:HB3 | 1.61 | 0.82 |
| 14:1S:25:ARG:NH1 | 14:1S:42:ASP:OD1 | 2.13 | 0.82 |
| 5:1F:185:ASP:OD1 | 5:1F:188:ARG:NH1 | 2.13 | 0.82 |
| 32:1a:700:G:N7 | 62:1a:1915:HOH:O | 2.13 | 0.82 |
| 11:1P:126:VAL:HG12 | 11:1P:148:LEU:HD22 | 1.61 | 0.81 |
| 1:1A:1647:G:OP1 | 62:1A:4208:HOH:O | 1.96 | 0.81 |
| 1:1A:2206:G:H3' | 1:1A:2207:G:C8 | 2.14 | 0.81 |
| 1:2A:2100:G:H1 | 1:2A:2189:U:H3 | 1.24 | 0.81 |
| 33:2b:111:ARG:HH11 | 33:2b:111:ARG:HA | 1.45 | 0.81 |
| 42:1k:15:ALA:HB1 | 42:1k:78:GLN:HB2 | 1.62 | 0.81 |
| 32:1a:1499:A:OP2 | 62:1a:1903:HOH:O | 1.98 | 0.81 |
| 57:1z:4:SER:O | 57:1z:14:GLY:HA3 | 1.81 | 0.81 |
| 21:2Z:93:ASP:HA | 21:2Z:131:ARG:HH12 | 1.43 | 0.81 |
| 1:2A:1204:A:H2 | 1:2A:1241:A:H62 | 1.26 | 0.81 |
| 13:2R:97:VAL:HG22 | 13:2R:114:VAL:HG13 | 1.63 | 0.80 |
| 3:1D:147:LEU:HD13 | 3:1D:155:LEU:HD11 | 1.61 | 0.80 |
| 35:2d:15:GLU:OE2 | 35:2d:66:ARG:NH1 | 2.15 | 0.80 |
| 32:1a:542:G:OP1 | 35:1d:10:ARG:NH2 | 2.15 | 0.80 |
| 12:2Q:110:THR:HG22 | 12:2Q:112:GLU:H | 1.46 | 0.80 |
| 52:1u:5:ASP:OD2 | 62:1u:101:HOH:O | 1.97 | 0.80 |
| 1:1A:847:U:OP2 | 62:1A:4211:HOH:O | 1.99 | 0.80 |
| 32:1a:1025:U:O2 | 32:1a:1036:G:O6 | 2.00 | 0.80 |
| 1:2A:2808:U:O2 | 1:2A:2892:A:N6 | 2.15 | 0.80 |
| 32:2a:677:U:H3 | 32:2a:713:G:H22 | 1.27 | 0.80 |
| 33:2b:185:ILE:HG22 | 33:2b:199:TYR:HB2 | 1.62 | 0.80 |
| 44:2m:15:VAL:HG13 | 44:2m:45:VAL:HG12 | 1.64 | 0.80 |
| 32:1a:545:C:OP1 | 35:1d:61:LYS:NZ | 2.15 | 0.80 |
| 32:2a:1086:U:H3 | 32:2a:1099:G:H22 | 1.29 | 0.80 |
| 47:2p:53:VAL:HG13 | 47:2p:79:VAL:HG22 | 1.64 | 0.80 |
| 1:1A:2575:C:OP2 | 62:1A:4209:HOH:O | 1.99 | 0.79 |
| 1:2A:1689:A:H62 | 1:2A:1698:A:H2 | 1.25 | 0.79 |
| 1:1A:1047:G:H2' | 1:1A:1110:G:H22 | 1.47 | 0.79 |
| 1:1A:2646:C:OP2 | 1:1A:2732:G:O2' | 1.98 | 0.79 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:2D:38:LYS:NZ | 3:2D:39:LYS:O | 2.16 | 0.79 |
| 32:2a:157:G:H1 | 32:2a:164:U:H3 | 1.29 | 0.79 |
| 1:1A:2124:G:H1 | 1:1A:2174:C:H42 | 1.28 | 0.79 |
| 32:1a:664:G:H22 | 32:1a:741:G:H1 | 1.30 | 0.79 |
| 35:1d:76:ARG:NH1 | 35:1d:80:GLU:OE2 | 2.16 | 0.78 |
| 1:2A:2062:A:OP1 | 62:2A:3910:HOH:O | 2.02 | 0.78 |
| 8:2I:59:ALA:HA | 8:2I:62:LYS:HG2 | 1.63 | 0.78 |
| 1:2A:2079:U:OP1 | 23:21:21:ARG:NH2 | 2.13 | 0.78 |
| 5:2F:180:GLY:O | 5:2F:182:ASN:ND2 | 2.15 | 0.78 |
| 1:2A:1021:A:H62 | 1:2A:1141:U:H3 | 1.31 | 0.78 |
| 1:2A:1647:G:OP1 | 62:2A:3912:HOH:O | 2.02 | 0.78 |
| 33:2b:54:THR:HG22 | 33:2b:199:TYR:HB3 | 1.66 | 0.78 |
| 1:1A:1896:G:N7 | 62:1A:4236:HOH:O | 2.16 | 0.78 |
| 1:2A:1024:G:OP2 | 62:2A:3911:HOH:O | 2.02 | 0.78 |
| 37:1f:2:ARG:HD2 | 37:1f:69:GLU:HB3 | 1.65 | 0.78 |
| 1:2A:890:A:N6 | 1:2A:893:C:O2 | 2.17 | 0.78 |
| 32:1a:1136:U:H5'' | 32:1a:1137:C:C4 | 2.19 | 0.78 |
| 32:1a:1189:C:OP1 | 41:1j:51:ARG:NH2 | 2.17 | 0.78 |
| 1:2A:752:A:H3' | 29:27:1:MET:HE1 | 1.66 | 0.78 |
| 1:2A:783:A:OP2 | 62:2A:3907:HOH:O | 1.99 | 0.78 |
| 1:2A:2448:A:OP1 | 62:2A:3914:HOH:O | 2.02 | 0.78 |
| 6:2G:115:ARG:NH1 | 6:2G:137:GLU:OE2 | 2.17 | 0.78 |
| 32:1a:944:G:OP1 | 62:1a:1904:HOH:O | 2.02 | 0.77 |
| 32:1a:1505:G:OP2 | 62:1a:1903:HOH:O | 2.01 | 0.77 |
| 1:1A:2784:C:H1' | 4:1E:37:ARG:HH12 | 1.49 | 0.77 |
| 1:2A:792:G:O6 | 62:2A:3913:HOH:O | 2.02 | 0.77 |
| 1:2A:1203:G:O6 | 62:2A:3908:HOH:O | 2.01 | 0.77 |
| 1:2A:963:U:OP2 | 62:2A:3909:HOH:O | 2.01 | 0.77 |
| 32:2a:544:G:OP1 | 35:2d:59:ARG:NH2 | 2.18 | 0.77 |
| 1:1A:1039:G:H1 | 1:1A:1116:C:H42 | 1.33 | 0.77 |
| 51:1t:86:ARG:O | 51:1t:90:GLN:NE2 | 2.17 | 0.77 |
| 1:2A:1341:U:OP2 | 1:2A:1394:U:O2' | 2.01 | 0.77 |
| 10:1O:98:VAL:HG21 | 10:1O:114:ILE:HG23 | 1.64 | 0.77 |
| 15:2T:109:GLU:HG2 | 15:2T:112:ARG:HH22 | 1.49 | 0.77 |
| 1:1A:1669:A:OP2 | 62:1A:4205:HOH:O | 2.02 | 0.77 |
| 51:1t:10:LEU:HB3 | 51:1t:12:ALA:H | 1.50 | 0.77 |
| 21:2Z:171:ILE:HD12 | 21:2Z:172:ALA:H | 1.49 | 0.77 |
| 23:21:50:ARG:HG2 | 23:21:59:THR:HG22 | 1.67 | 0.77 |
| 32:1a:975:A:H4' | 32:1a:976:G:H5'' | 1.67 | 0.76 |
| 4:2E:28:ALA:HB3 | 4:2E:93:VAL:HG12 | 1.65 | 0.76 |
| 21:2Z:106:GLY:HA3 | 21:2Z:141:VAL:HB | 1.66 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 32:2a:1272:G:N2 | 32:2a:1273:G:C5 | 2.53 | 0.76 |
| 56:1y:19:G:N2 | 56:1y:56:C:N3 | 2.34 | 0.76 |
| 1:2A:2063:C:OP1 | 62:2A:3915:HOH:O | 2.03 | 0.76 |
| 1:2A:2453:A:N7 | 62:2A:3947:HOH:O | 2.19 | 0.76 |
| 1:1A:654:A:OP2 | 62:1A:4213:HOH:O | 2.04 | 0.76 |
| 33:1b:185:ILE:HG22 | 33:1b:199:TYR:HB2 | 1.68 | 0.76 |
| 35:1d:187:ARG:HH22 | 35:1d:190:ASP:HB2 | 1.49 | 0.76 |
| 32:1a:1004:A:H5' | 32:1a:1024:G:H1 | 1.51 | 0.76 |
| 1:2A:1670:C:OP1 | 62:2A:3916:HOH:O | 2.03 | 0.76 |
| 32:1a:1108:G:O6 | 62:1a:1906:HOH:O | 2.03 | 0.76 |
| 56:1y:8:4SU:H4' | 56:1y:48:C:H4' | 1.66 | 0.76 |
| 32:2a:656:C:O2' | 46:2o:28:GLN:OE1 | 2.02 | 0.76 |
| 32:1a:159:G:N2 | 32:1a:162:A:OP2 | 2.18 | 0.76 |
| 50:2s:28:LYS:HB3 | 50:2s:29:ARG:HA | 1.66 | 0.76 |
| 1:2A:845:G:OP2 | 1:2A:845:G:N2 | 2.18 | 0.76 |
| 32:1a:1224:G:OP1 | 62:1a:1905:HOH:O | 2.02 | 0.75 |
| 40:1i:50:LEU:HD13 | 40:1i:56:LEU:HA | 1.68 | 0.75 |
| 1:1A:1055:G:H1 | 1:1A:1104:C:H42 | 1.34 | 0.75 |
| 32:2a:1314:C:OP2 | 50:2s:4:SER:OG | 2.02 | 0.75 |
| 38:2g:73:MET:HE2 | 38:2g:90:GLU:HG3 | 1.68 | 0.75 |
| 13:1R:97:VAL:HG22 | 13:1R:114:VAL:HG13 | 1.68 | 0.75 |
| 32:1a:933:G:O6 | 38:1g:3:ARG:NH2 | 2.20 | 0.75 |
| 5:2F:53:THR:HG23 | 5:2F:55:GLY:H | 1.51 | 0.75 |
| 32:1a:224:C:OP1 | 51:1t:74:LYS:NZ | 2.15 | 0.75 |
| 40:1i:16:ARG:HB2 | 40:1i:64:THR:HG22 | 1.69 | 0.75 |
| 1:1A:248:G:OP1 | 62:1A:4212:HOH:O | 2.02 | 0.75 |
| 32:1a:953:G:H5' | 32:1a:965:A:H61 | 1.52 | 0.75 |
| 32:2a:1058:G:OP1 | 34:2c:199:LYS:NZ | 2.19 | 0.75 |
| 32:1a:376:G:O3' | 47:1p:5:ARG:HD2 | 1.86 | 0.75 |
| 32:1a:1521:G:N3 | 62:1a:1923:HOH:O | 2.20 | 0.75 |
| 40:1i:51:ARG:HG2 | 40:1i:56:LEU:HD21 | 1.68 | 0.75 |
| 24:12:65:ASN:OD1 | 24:12:69:ARG:NH1 | 2.20 | 0.75 |
| 32:2a:1189:C:OP1 | 41:2j:51:ARG:NH2 | 2.18 | 0.75 |
| 1:2A:1604:C:OP1 | 62:2A:3917:HOH:O | 2.05 | 0.75 |
| 1:2A:1648:C:OP1 | 62:2A:3912:HOH:O | 2.04 | 0.75 |
| 33:2b:8:LYS:NZ | 33:2b:9:GLU:OE1 | 2.19 | 0.75 |
| 32:2a:1272:G:N2 | 32:2a:1273:G:N7 | 2.34 | 0.74 |
| 32:1a:1149:C:P | 40:1i:9:ARG:HH21 | 2.10 | 0.74 |
| 32:1a:1334:G:OP2 | 62:1a:1907:HOH:O | 2.04 | 0.74 |
| 50:1s:50:ALA:HB1 | 50:1s:57:HIS:HB3 | 1.69 | 0.74 |
| 1:2A:2110:G:OP1 | 1:2A:2118:U:N3 | 2.20 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 32:2a:1002:G:N3 | 32:2a:1003:G:H1' | 2.03 | 0.74 |
| 50:2s:15:LEU:HA | 50:2s:18:LYS:HD2 | 1.70 | 0.74 |
| 1:1A:1184:G:H5' | 25:13:29:ARG:HH21 | 1.51 | 0.74 |
| 35:1d:187:ARG:NH2 | 35:1d:193:ASP:OD2 | 2.19 | 0.74 |
| 1:2A:1395:A:OP1 | 62:2A:3903:HOH:O | 2.05 | 0.74 |
| 1:1A:307:G:N7 | 62:1A:4248:HOH:O | 2.21 | 0.74 |
| 39:2h:64:LYS:HG2 | 39:2h:79:VAL:HG21 | 1.70 | 0.74 |
| 1:1A:110:G:N7 | 62:1A:4246:HOH:O | 2.20 | 0.74 |
| 1:2A:72:U:OP1 | 62:2A:3918:HOH:O | 2.05 | 0.74 |
| 1:2A:948:G:OP1 | 62:2A:3909:HOH:O | 2.04 | 0.74 |
| 32:2a:903:G:OP1 | 62:2a:1903:HOH:O | 2.05 | 0.74 |
| 32:2a:1191:A:H5'' | 34:2c:4:LYS:HE3 | 1.70 | 0.74 |
| 41:2j:16:LEU:HD13 | 41:2j:70:ARG:HG2 | 1.70 | 0.74 |
| 41:2j:46:ARG:NH2 | 41:2j:64:GLU:OE1 | 2.21 | 0.74 |
| 1:1A:1023:U:OP2 | 62:1A:4210:HOH:O | 2.05 | 0.74 |
| 32:1a:166:G:H2' | 32:1a:167:G:H8 | 1.53 | 0.74 |
| 33:2b:69:LEU:HB3 | 33:2b:162:ILE:HG22 | 1.69 | 0.74 |
| 1:1A:1890:A:OP2 | 62:1A:4214:HOH:O | 2.05 | 0.74 |
| 29:17:46:VAL:HG22 | 29:17:48:LYS:HD2 | 1.68 | 0.74 |
| 6:2G:111:LEU:HD21 | 6:2G:120:LEU:HD21 | 1.70 | 0.74 |
| 7:2H:70:THR:O | 7:2H:74:ASN:ND2 | 2.21 | 0.74 |
| 1:2A:1394:U:OP1 | 62:2A:3917:HOH:O | 2.05 | 0.74 |
| 1:2A:2819:G:N7 | 62:2A:3949:HOH:O | 2.19 | 0.74 |
| 34:2c:179:ARG:NH1 | 34:2c:206:GLU:OE1 | 2.16 | 0.74 |
| 1:1A:2821:A:OP2 | 62:1R:301:HOH:O | 2.04 | 0.73 |
| 1:2A:931:G:O2' | 25:23:24:LYS:NZ | 2.20 | 0.73 |
| 32:1a:1381:U:H1' | 38:1g:79:ARG:HG2 | 1.70 | 0.73 |
| 1:2A:1971:A:OP1 | 62:2A:3919:HOH:O | 2.05 | 0.73 |
| 11:2P:121:LYS:O | 11:2P:123:LEU:N | 2.21 | 0.73 |
| 25:23:39:ASP:OD2 | 25:23:44:ARG:NH1 | 2.21 | 0.73 |
| 1:1A:1970:A:OP1 | 62:1A:4215:HOH:O | 2.06 | 0.73 |
| 20:1Y:102:CYS:SG | 20:1Y:103:GLY:N | 2.55 | 0.73 |
| 34:2c:36:ASP:HA | 34:2c:39:ILE:HD12 | 1.69 | 0.73 |
| 1:2A:781:A:OP1 | 62:2A:3922:HOH:O | 2.06 | 0.73 |
| 1:2A:2582:G:OP2 | 62:2A:3920:HOH:O | 2.06 | 0.73 |
| 18:2W:34:ASN:OD1 | 18:2W:37:ARG:NH2 | 2.22 | 0.73 |
| 32:2a:596:C:OP2 | 62:2a:1904:HOH:O | 2.06 | 0.73 |
| 32:1a:504:C:OP1 | 62:1a:1908:HOH:O | 2.05 | 0.73 |
| 1:2A:2072:G:O6 | 62:2A:3924:HOH:O | 2.07 | 0.73 |
| 11:2P:118:GLY:O | 11:2P:137:LYS:NZ | 2.21 | 0.73 |
| 32:2a:1151:A:HO2' | 32:2a:1152:A:H8 | 1.34 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 32:1a:1518:MA6:H93 | 32:1a:1519:MA6:H92 | 1.71 | 0.73 |
| 39:1h:64:LYS:HG2 | 39:1h:79:VAL:HG21 | 1.69 | 0.73 |
| 32:2a:1280:A:H5' | 41:2j:40:LEU:HD22 | 1.71 | 0.73 |
| 1:1A:1702:G:N7 | 62:1A:4255:HOH:O | 2.22 | 0.73 |
| 1:2A:1237:A:OP1 | 62:2A:3921:HOH:O | 2.06 | 0.73 |
| 32:2a:504:C:OP1 | 62:2a:1905:HOH:O | 2.07 | 0.73 |
| 41:2j:49:VAL:HG23 | 45:2n:41:ARG:HB2 | 1.69 | 0.73 |
| 1:1A:2136:C:H42 | 1:1A:2155:G:H1 | 0.76 | 0.73 |
| 33:2b:162:ILE:HD11 | 33:2b:177:ALA:HB2 | 1.68 | 0.73 |
| 1:1A:1622:G:OP2 | 62:1A:4216:HOH:O | 2.06 | 0.72 |
| 2:1B:99:G:OP2 | 62:1B:301:HOH:O | 2.07 | 0.72 |
| 41:2j:78:ASN:O | 41:2j:80:LYS:N | 2.22 | 0.72 |
| 33:2b:16:HIS:HB3 | 33:2b:210:SER:HB2 | 1.70 | 0.72 |
| 1:2A:141:A:H8 | 1:2A:1408:C:HO2' | 1.35 | 0.72 |
| 12:2Q:78:PRO:HG2 | 12:2Q:81:VAL:HG11 | 1.69 | 0.72 |
| 1:2A:570:G:O6 | 62:2A:3914:HOH:O | 2.06 | 0.72 |
| 1:2A:690:G:O6 | 62:2A:3925:HOH:O | 2.07 | 0.72 |
| 1:2A:2805:G:H2' | 1:2A:2807:G:C8 | 2.23 | 0.72 |
| 44:2m:23:TYR:HB3 | 44:2m:67:GLU:HA | 1.71 | 0.72 |
| 1:2A:1345:C:OP2 | 62:2A:3926:HOH:O | 2.08 | 0.72 |
| 1:1A:1183:G:O2' | 25:13:29:ARG:NH2 | 2.23 | 0.72 |
| 26:14:46:GLN:O | 26:14:48:ARG:N | 2.22 | 0.72 |
| 47:1p:53:VAL:HG13 | 47:1p:79:VAL:HG22 | 1.71 | 0.72 |
| 17:2V:40:LEU:HB2 | 17:2V:46:VAL:HB | 1.69 | 0.72 |
| 49:2r:32:ARG:HA | 49:2r:69:THR:HG21 | 1.72 | 0.72 |
| 1:2A:1762:A:N1 | 62:2A:3959:HOH:O | 2.22 | 0.72 |
| 8:1I:92:VAL:HG13 | 8:1I:120:ILE:HB | 1.70 | 0.72 |
| 21:2Z:52:SER:OG | 21:2Z:53:ILE:N | 2.23 | 0.72 |
| 26:24:53:GLU:HG2 | 26:24:55:ARG:H | 1.55 | 0.72 |
| 1:1A:2630:G:O6 | 1:1A:2788:C:N4 | 2.19 | 0.72 |
| 50:1s:12:ASP:OD2 | 50:1s:35:SER:OG | 2.08 | 0.72 |
| 21:2Z:28:MET:HE1 | 21:2Z:61:LEU:HD21 | 1.70 | 0.72 |
| 32:2a:1020:U:H2' | 32:2a:1021:G:C8 | 2.25 | 0.72 |
| 35:2d:20:TYR:HD1 | 35:2d:26:CYS:HB3 | 1.54 | 0.72 |
| 4:1E:29:GLY:HA3 | 62:1E:402:HOH:O | 1.90 | 0.71 |
| 32:1a:539:A:OP2 | 43:1l:115:LYS:NZ | 2.23 | 0.71 |
| 1:2A:2551:C:OP1 | 62:2A:3923:HOH:O | 2.06 | 0.71 |
| 37:1f:6:VAL:HG22 | 37:1f:90:VAL:HG22 | 1.73 | 0.71 |
| 1:1A:744:G:OP1 | 62:1A:4219:HOH:O | 2.08 | 0.71 |
| 1:1A:1288:U:OP1 | 62:1A:4218:HOH:O | 2.08 | 0.71 |
| 35:1d:112:VAL:HG23 | 35:1d:116:GLN:HE22 | 1.55 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 12:2Q:111:GLU:OE2 | 12:2Q:133:ARG:NH2 | 2.22 | 0.71 |
| 33:2b:74:LYS:O | 33:2b:78:GLN:HG2 | 1.90 | 0.71 |
| 33:2b:121:LEU:HA | 33:2b:125:PRO:HG2 | 1.72 | 0.71 |
| 1:1A:615:G:OP2 | 5:1F:43:LYS:NZ | 2.23 | 0.71 |
| 24:12:41:ILE:HG13 | 24:12:43:GLN:HG3 | 1.73 | 0.71 |
| 32:1a:1009:G:O6 | 32:1a:1020:U:O2 | 2.09 | 0.71 |
| 32:2a:1347:G:N2 | 32:2a:1373:G:H2' | 2.05 | 0.71 |
| 1:1A:1948:G:O6 | 62:1A:4217:HOH:O | 2.08 | 0.71 |
| 32:2a:1020:U:H2' | 32:2a:1021:G:H8 | 1.55 | 0.71 |
| 10:1O:63:VAL:HG12 | 10:1O:106:LEU:HD11 | 1.72 | 0.71 |
| 32:1a:316:G:O2' | 62:1a:1910:HOH:O | 2.09 | 0.71 |
| 26:24:46:GLN:C | 26:24:48:ARG:H | 1.99 | 0.71 |
| 37:2f:8:ILE:HD13 | 37:2f:26:ILE:HD13 | 1.73 | 0.71 |
| 32:1a:903:G:OP1 | 62:1a:1911:HOH:O | 2.09 | 0.71 |
| 35:2d:187:ARG:NH1 | 35:2d:190:ASP:OD1 | 2.24 | 0.71 |
| 4:1E:7:VAL:HG23 | 4:1E:51:PHE:HE2 | 1.55 | 0.70 |
| 18:1W:92:ARG:NH1 | 62:1W:301:HOH:O | 2.24 | 0.70 |
| 32:2a:189(F):U:O2 | 48:2q:63:ARG:NH2 | 2.24 | 0.70 |
| 32:2a:1301:U:O2' | 32:2a:1302:U:H5' | 1.91 | 0.70 |
| 1:2A:1264:G:OP1 | 27:25:19:ARG:NH2 | 2.24 | 0.70 |
| 48:2q:95:TYR:HA | 48:2q:98:LEU:HD12 | 1.73 | 0.70 |
| 32:2a:1053:G:H4' | 32:2a:1054:C:H3' | 1.72 | 0.70 |
| 47:2p:1:MET:HE3 | 47:2p:3:LYS:HD3 | 1.73 | 0.70 |
| 26:14:16:CYS:SG | 26:14:17:GLY:N | 2.64 | 0.70 |
| 1:2A:2611:U:C4 | 27:25:3:LYS:HG2 | 2.26 | 0.70 |
| 33:2b:197:VAL:HB | 33:2b:200:ILE:HG13 | 1.73 | 0.70 |
| 38:1g:78:ARG:HG3 | 38:1g:79:ARG:H | 1.55 | 0.70 |
| 1:1A:1041:C:H42 | 1:1A:1114:G:H1 | 1.40 | 0.70 |
| 32:1a:1414:U:O4 | 62:1a:1912:HOH:O | 2.09 | 0.70 |
| 1:2A:2327:A:H2' | 1:2A:2328:A:C8 | 2.25 | 0.70 |
| 1:2A:218:A:OP2 | 62:2A:3927:HOH:O | 2.09 | 0.70 |
| 2:2B:28:C:N4 | 2:2B:56:G:O6 | 2.18 | 0.70 |
| 2:2B:54:G:OP2 | 62:2B:301:HOH:O | 2.10 | 0.70 |
| 35:2d:150:GLU:HA | 35:2d:153:ARG:HD2 | 1.71 | 0.70 |
| 39:2h:51:VAL:HG11 | 39:2h:60:ARG:HH12 | 1.54 | 0.70 |
| 1:1A:11:G:H2' | 1:1A:12:U:H5' | 1.74 | 0.70 |
| 1:2A:2171:A:N3 | 1:2A:2172:U:N3 | 2.39 | 0.70 |
| 1:2A:2218:U:O2 | 23:21:52:ARG:NH1 | 2.25 | 0.70 |
| 1:2A:10:G:H1' | 1:2A:2801(A):A:H62 | 1.57 | 0.70 |
| 32:2a:548:G:OP1 | 62:2a:1906:HOH:O | 2.10 | 0.70 |
| 32:2a:1095:U:H5'' | 32:2a:1109:C:O2 | 1.92 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 32:1a:324:G:N7 | 62:1a:1931:HOH:O | 2.25 | 0.69 |
| 32:1a:1356:G:H2' | 32:1a:1357:A:C8 | 2.27 | 0.69 |
| 1:2A:607:U:OP1 | 5:2F:102:PRO:HA | 1.92 | 0.69 |
| 32:2a:266:G:H5'' | 32:2a:268:C:H41 | 1.57 | 0.69 |
| 36:2e:36:ASP:O | 36:2e:38:GLN:N | 2.25 | 0.69 |
| 3:1D:39:LYS:NZ | 3:1D:57:GLY:O | 2.24 | 0.69 |
| 32:1a:1178:G:OP2 | 40:1i:97:LYS:NZ | 2.25 | 0.69 |
| 1:2A:271(L):U:H5' | 8:2I:50:ARG:HH11 | 1.57 | 0.69 |
| 6:2G:38:VAL:HG22 | 6:2G:93:THR:HG23 | 1.74 | 0.69 |
| 14:2S:3:ARG:NH2 | 14:2S:4:LEU:O | 2.25 | 0.69 |
| 56:1y:26:A:H61 | 56:1y:44:G:H1 | 1.40 | 0.69 |
| 1:2A:2445:G:OP1 | 5:2F:74:ARG:NH2 | 2.25 | 0.69 |
| 1:2A:2130:U:H2' | 1:2A:2158:A:H61 | 1.57 | 0.69 |
| 7:2H:70:THR:HG22 | 7:2H:74:ASN:HD21 | 1.55 | 0.69 |
| 11:2P:38:GLN:O | 11:2P:39:LYS:HB3 | 1.92 | 0.69 |
| 14:2S:48:LEU:HD23 | 14:2S:82:ILE:HD11 | 1.73 | 0.69 |
| 32:2a:612:C:O2 | 32:2a:629:G:N2 | 2.25 | 0.69 |
| 1:1A:1332:G:OP1 | 62:1A:4221:HOH:O | 2.10 | 0.69 |
| 32:2a:603:U:H2' | 32:2a:604:G:H8 | 1.57 | 0.69 |
| 42:2k:19:ALA:HB3 | 42:2k:82:VAL:HG22 | 1.72 | 0.69 |
| 32:1a:53:A:OP2 | 62:1a:1913:HOH:O | 2.09 | 0.69 |
| 1:1A:299:A:OP2 | 62:1A:4220:HOH:O | 2.09 | 0.69 |
| 32:1a:1086:U:H3 | 32:1a:1099:G:H22 | 1.41 | 0.69 |
| 40:1i:50:LEU:HD23 | 40:1i:81:ILE:HD11 | 1.75 | 0.69 |
| 43:1l:32:PHE:HB3 | 43:1l:84:LEU:HD11 | 1.74 | 0.69 |
| 1:1A:2596:U:OP1 | 62:1A:4223:HOH:O | 2.11 | 0.69 |
| 32:1a:1495:U:OP1 | 62:1a:1914:HOH:O | 2.11 | 0.69 |
| 2:2B:9:G:H1 | 2:2B:112:U:H3 | 1.40 | 0.69 |
| 32:1a:1305:G:N2 | 32:1a:1331:G:H1' | 2.08 | 0.69 |
| 1:2A:1530:C:O2' | 1:2A:1531:C:O5' | 2.10 | 0.69 |
| 1:2A:2751:G:H8 | 7:2H:2:SER:HA | 1.57 | 0.69 |
| 1:1A:1176:G:H1' | 1:1A:1177:A:H5'' | 1.75 | 0.68 |
| 40:1i:128:ARG:NH2 | 55:1x:33:U:OP2 | 2.26 | 0.68 |
| 8:2I:92:VAL:HG13 | 8:2I:120:ILE:HB | 1.75 | 0.68 |
| 10:2O:2:ILE:HB | 10:2O:33:ALA:HB3 | 1.75 | 0.68 |
| 21:2Z:153:SER:HB2 | 21:2Z:167:PRO:HB3 | 1.75 | 0.68 |
| 32:2a:1271:G:C2 | 32:2a:1272:G:N7 | 2.61 | 0.68 |
| 7:1H:40:GLU:OE2 | 7:1H:61:HIS:NE2 | 2.24 | 0.68 |
| 56:1y:5:G:H1' | 56:1y:69:G:N2 | 2.08 | 0.68 |
| 5:2F:21:ALA:HB3 | 5:2F:22:ALA:HA | 1.76 | 0.68 |
| 25:23:59:VAL:HG12 | 25:23:60:GLU:H | 1.59 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 21:1Z:163:LEU:HD23 | 21:1Z:167:PRO:HG3 | 1.74 | 0.68 |
| 1:2A:832:G:OP1 | 62:2A:3929:HOH:O | 2.10 | 0.68 |
| 17:2V:1:MET:HE2 | 17:2V:43:GLU:HB2 | 1.74 | 0.68 |
| 19:2X:46:ALA:HB1 | 24:22:33:MET:HE1 | 1.75 | 0.68 |
| 1:1A:1420:U:O2' | 1:1A:1421:G:OP1 | 2.11 | 0.68 |
| 1:1A:1587:A:H2' | 1:1A:1588:C:C6 | 2.29 | 0.68 |
| 34:1c:52:LEU:HD12 | 34:1c:53:ALA:H | 1.59 | 0.68 |
| 1:2A:639:U:H2' | 1:2A:640:C:C6 | 2.28 | 0.68 |
| 1:2A:880:G:H22 | 1:2A:898:C:H1' | 1.58 | 0.68 |
| 1:2A:2242:G:OP1 | 62:2A:3930:HOH:O | 2.10 | 0.68 |
| 35:2d:119:GLN:HG3 | 35:2d:123:HIS:HD2 | 1.58 | 0.68 |
| 6:2G:161:THR:HG22 | 6:2G:163:ALA:H | 1.58 | 0.68 |
| 1:1A:1175:U:OP1 | 1:1A:1177:A:N6 | 2.27 | 0.68 |
| 26:14:55:ARG:N | 26:14:56:VAL:HA | 2.09 | 0.68 |
| 1:2A:2577:A:H5'' | 1:2A:2578:G:H5' | 1.76 | 0.68 |
| 8:2I:110:ASP:N | 8:2I:130:TYR:OH | 2.19 | 0.68 |
| 2:1B:23:G:O6 | 62:1B:302:HOH:O | 2.09 | 0.67 |
| 1:2A:962:G:OP1 | 62:2A:3909:HOH:O | 2.11 | 0.67 |
| 12:2Q:35:VAL:HG22 | 12:2Q:102:VAL:HG22 | 1.76 | 0.67 |
| 32:2a:165:C:H2' | 32:2a:166:G:H8 | 1.59 | 0.67 |
| 32:2a:501:C:OP1 | 43:2l:117:ARG:NH2 | 2.24 | 0.67 |
| 51:2t:33:ILE:O | 51:2t:37:SER:OG | 2.11 | 0.67 |
| 1:1A:2196:C:OP2 | 62:1A:4224:HOH:O | 2.12 | 0.67 |
| 32:2a:560:U:H5' | 32:2a:566:G:N2 | 2.09 | 0.67 |
| 54:2w:13:C:O2' | 54:2w:14:A:O5' | 2.11 | 0.67 |
| 1:1A:2155:G:H2' | 1:1A:2155:G:N3 | 2.10 | 0.67 |
| 21:1Z:40:ASP:HB3 | 21:1Z:43:GLU:HB2 | 1.76 | 0.67 |
| 1:2A:1023:U:OP2 | 62:2A:3911:HOH:O | 2.10 | 0.67 |
| 31:29:25:VAL:HB | 31:29:34:GLN:HB2 | 1.74 | 0.67 |
| 32:2a:134:A:H61 | 47:2p:25:ARG:HH12 | 1.39 | 0.67 |
| 32:2a:624:C:H2' | 32:2a:625:G:H8 | 1.60 | 0.67 |
| 1:1A:400:G:N7 | 62:1A:4277:HOH:O | 2.27 | 0.67 |
| 34:1c:35:GLU:CD | 34:1c:59:ARG:HH22 | 2.01 | 0.67 |
| 1:2A:2107:C:H42 | 1:2A:2182:G:H1 | 1.41 | 0.67 |
| 33:2b:133:LYS:HA | 33:2b:136:VAL:HG22 | 1.75 | 0.67 |
| 1:1A:1062:G:H1 | 1:1A:1077:A:H61 | 1.40 | 0.67 |
| 50:1s:27:GLU:N | 50:1s:27:GLU:OE1 | 2.28 | 0.67 |
| 21:2Z:92:SER:O | 21:2Z:130:PRO:HG3 | 1.95 | 0.67 |
| 1:1A:668:G:N7 | 62:1A:4287:HOH:O | 2.28 | 0.67 |
| 16:1U:81:HIS:CE1 | 16:1U:85:LYS:HD2 | 2.30 | 0.67 |
| 56:1y:18:G:O2' | 56:1y:57:G:O6 | 2.13 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:2A:563:G:OP2 | 62:2A:3931:HOH:O | 2.10 | 0.67 |
| 34:2c:37:GLN:NE2 | 45:2n:52:GLN:OE1 | 2.28 | 0.67 |
| 34:2c:127:ARG:NH2 | 34:2c:192:THR:OG1 | 2.27 | 0.67 |
| 56:2y:9:A:O2' | 56:2y:11:C:N4 | 2.24 | 0.67 |
| 33:1b:18:GLY:HA3 | 33:1b:42:ILE:HG13 | 1.77 | 0.67 |
| 37:2f:30:LEU:HD23 | 37:2f:75:LEU:HD11 | 1.75 | 0.67 |
| 32:1a:1123:A:O2' | 41:1j:37:PRO:O | 2.12 | 0.67 |
| 1:2A:131:G:OP1 | 62:2A:3932:HOH:O | 2.13 | 0.67 |
| 1:2A:881:G:C2 | 1:2A:882:G:H1' | 2.30 | 0.67 |
| 3:2D:12:SER:HB3 | 3:2D:208:LYS:HB3 | 1.77 | 0.67 |
| 21:2Z:154:ASP:N | 21:2Z:154:ASP:OD1 | 2.27 | 0.67 |
| 26:24:45:GLY:C | 26:24:47:GLN:H | 2.03 | 0.67 |
| 11:1P:39:LYS:HB2 | 11:1P:45:LEU:HG | 1.76 | 0.67 |
| 46:1o:55:GLY:HA2 | 46:1o:58:MET:HE3 | 1.77 | 0.67 |
| 2:2B:8:U:OP1 | 14:2S:11:LYS:NZ | 2.27 | 0.67 |
| 5:2F:116:ASP:OD2 | 11:2P:1:MET:N | 2.27 | 0.67 |
| 32:2a:1035:A:H2' | 32:2a:1036:G:H8 | 1.60 | 0.67 |
| 1:1A:654:A:N7 | 62:1A:4286:HOH:O | 2.28 | 0.66 |
| 1:1A:1060:U:H3 | 1:1A:1088:A:H8 | 1.42 | 0.66 |
| 1:1A:1783:A:N7 | 62:1A:4279:HOH:O | 2.27 | 0.66 |
| 32:2a:1010:G:H2' | 32:2a:1011:G:H8 | 1.60 | 0.66 |
| 1:1A:1062:G:H2' | 1:1A:1063:G:H8 | 1.60 | 0.66 |
| 1:1A:1452:A:OP2 | 62:1A:4228:HOH:O | 2.13 | 0.66 |
| 1:1A:2759:G:N7 | 62:1A:4288:HOH:O | 2.28 | 0.66 |
| 40:1i:26:VAL:HG13 | 40:1i:61:ALA:HB3 | 1.77 | 0.66 |
| 1:2A:1278:A:OP1 | 13:2R:36:THR:HG23 | 1.95 | 0.66 |
| 4:2E:1:MET:HE3 | 4:2E:199:ARG:HD2 | 1.76 | 0.66 |
| 7:2H:27:LYS:HG2 | 7:2H:32:GLU:HB3 | 1.76 | 0.66 |
| 42:2k:67:ASP:HA | 42:2k:70:LYS:HE3 | 1.77 | 0.66 |
| 1:1A:1069:A:H1' | 1:1A:1096:A:H4' | 1.77 | 0.66 |
| 38:1g:54:THR:O | 38:1g:56:GLN:N | 2.29 | 0.66 |
| 1:2A:2788:C:OP1 | 4:2E:61:ARG:NH2 | 2.29 | 0.66 |
| 14:2S:83:LYS:HE3 | 14:2S:84:GLN:HG3 | 1.77 | 0.66 |
| 33:2b:58:ILE:HA | 33:2b:61:LEU:HB3 | 1.78 | 0.66 |
| 44:1m:3:ARG:HD2 | 44:1m:9:ILE:HG12 | 1.78 | 0.66 |
| 1:2A:2646:C:OP2 | 1:2A:2732:G:O2' | 2.13 | 0.66 |
| 32:1a:1004:A:H5' | 32:1a:1024:G:N1 | 2.11 | 0.66 |
| 20:2Y:44:ILE:HA | 20:2Y:63:LYS:O | 1.94 | 0.66 |
| 33:2b:171:ALA:O | 33:2b:175:ARG:N | 2.28 | 0.66 |
| 41:2j:38:ILE:HD11 | 41:2j:71:LEU:HD23 | 1.76 | 0.66 |
| 15:1T:29:ARG:HG3 | 15:1T:46:GLU:HB2 | 1.78 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:2A:882:G:H1 | 1:2A:894:C:H42 | 1.43 | 0.66 |
| 21:2Z:54:HIS:CD2 | 21:2Z:101:PRO:HG3 | 2.31 | 0.66 |
| 1:1A:2518:A:OP1 | 62:1A:4232:HOH:O | 2.14 | 0.66 |
| 39:1h:34:GLU:OE1 | 39:1h:37:ARG:NH1 | 2.28 | 0.66 |
| 1:2A:621:A:OP2 | 11:2P:108:LYS:NZ | 2.27 | 0.66 |
| 1:2A:2470:G:OP1 | 12:2Q:56:ARG:NH2 | 2.28 | 0.66 |
| 30:28:62:LEU:HB3 | 30:28:65:GLU:HG2 | 1.78 | 0.66 |
| 32:2a:405:U:O4 | 35:2d:2:GLY:N | 2.29 | 0.66 |
| 32:2a:1327:C:OP2 | 52:2u:12:LYS:NZ | 2.25 | 0.66 |
| 1:1A:1024:G:OP2 | 62:1A:4210:HOH:O | 2.11 | 0.66 |
| 1:1A:2467:C:OP2 | 62:1A:4231:HOH:O | 2.14 | 0.66 |
| 32:1a:216:G:H2' | 32:1a:217:C:C6 | 2.31 | 0.66 |
| 1:2A:2805:G:H2' | 1:2A:2807:G:H8 | 1.60 | 0.66 |
| 11:2P:35:HIS:O | 62:2P:202:HOH:O | 2.14 | 0.66 |
| 16:2U:49:HIS:HA | 16:2U:52:ARG:HB2 | 1.77 | 0.66 |
| 32:2a:1256:A:H61 | 32:2a:1278:U:H1' | 1.61 | 0.66 |
| 38:1g:74:GLU:HG2 | 38:1g:91:VAL:HG22 | 1.77 | 0.66 |
| 1:2A:679:C:OP1 | 62:2A:3930:HOH:O | 2.14 | 0.66 |
| 34:2c:53:ALA:HB2 | 34:2c:115:LEU:HD21 | 1.78 | 0.66 |
| 1:1A:2128:C:H42 | 1:1A:2160:G:H1 | 1.43 | 0.65 |
| 3:1D:95:LEU:HD11 | 3:1D:105:ILE:HD13 | 1.78 | 0.65 |
| 4:1E:12:THR:HG22 | 4:1E:13:ARG:H | 1.60 | 0.65 |
| 32:1a:165:C:H2' | 32:1a:166:G:C8 | 2.31 | 0.65 |
| 32:1a:1136:U:H5'' | 32:1a:1137:C:N4 | 2.10 | 0.65 |
| 1:2A:277:C:H4' | 1:2A:278:A:OP2 | 1.96 | 0.65 |
| 1:2A:1271:G:OP2 | 62:2A:3912:HOH:O | 2.12 | 0.65 |
| 34:2c:148:GLY:HA3 | 34:2c:172:ARG:O | 1.96 | 0.65 |
| 1:1A:1139:G:OP2 | 9:1N:70:LYS:NZ | 2.28 | 0.65 |
| 32:1a:975:A:H5' | 32:1a:975:A:H8 | 1.61 | 0.65 |
| 36:1e:85:GLY:O | 36:1e:87:SER:N | 2.29 | 0.65 |
| 10:2O:63:VAL:HG23 | 10:2O:64:ARG:HG3 | 1.77 | 0.65 |
| 50:2s:49:ILE:HG22 | 50:2s:62:ILE:HD11 | 1.77 | 0.65 |
| 1:1A:1077:A:H2' | 1:1A:1078:U:H4' | 1.78 | 0.65 |
| 12:2Q:12:GLN:HE21 | 12:2Q:73:PRO:HD2 | 1.60 | 0.65 |
| 21:2Z:7:ALA:HB2 | 21:2Z:59:LEU:HB3 | 1.78 | 0.65 |
| 30:28:30:ARG:O | 62:28:201:HOH:O | 2.14 | 0.65 |
| 1:1A:1453:U:OP1 | 13:1R:77:ARG:HD3 | 1.95 | 0.65 |
| 1:1A:2190:G:H2' | 1:1A:2191:G:O4' | 1.97 | 0.65 |
| 1:2A:1365:A:O2' | 23:21:11:ARG:NH1 | 2.27 | 0.65 |
| 13:2R:51:LEU:HD22 | 13:2R:66:VAL:HG13 | 1.78 | 0.65 |
| 32:2a:1279:A:O2' | 32:2a:1281:U:OP2 | 2.14 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 33:2b:78:GLN:HE22 | 33:2b:95:GLN:NE2 | 1.94 | 0.65 |
| 37:2f:67:MET:HE1 | 37:2f:75:LEU:HD22 | 1.76 | 0.65 |
| 1:1A:636:G:OP1 | 11:1P:132:LYS:NZ | 2.26 | 0.65 |
| 7:2H:126:PRO:HG2 | 7:2H:130:ARG:HH21 | 1.61 | 0.65 |
| 1:1A:621:A:OP2 | 11:1P:108:LYS:NZ | 2.28 | 0.65 |
| 33:1b:88:ALA:HB2 | 33:1b:219:VAL:HG13 | 1.76 | 0.65 |
| 39:1h:29:SER:HB3 | 39:1h:32:LYS:HG3 | 1.76 | 0.65 |
| 1:2A:1297:C:OP1 | 62:2A:3933:HOH:O | 2.14 | 0.65 |
| 4:1E:77:ILE:HD12 | 4:1E:195:LEU:HD13 | 1.76 | 0.65 |
| 54:1w:1:G:H2' | 54:1w:2:C:C6 | 2.32 | 0.65 |
| 1:2A:248:G:OP1 | 62:2A:3934:HOH:O | 2.15 | 0.65 |
| 5:2F:108:LYS:HG2 | 5:2F:112:MET:HE2 | 1.78 | 0.65 |
| 1:2A:301:G:OP2 | 20:2Y:84:ARG:NH2 | 2.29 | 0.65 |
| 17:2V:33:VAL:HG23 | 17:2V:59:ALA:HB3 | 1.79 | 0.65 |
| 21:2Z:146:ILE:HG12 | 21:2Z:174:VAL:HG13 | 1.79 | 0.65 |
| 32:2a:396:G:O2' | 32:2a:398:C:OP1 | 2.08 | 0.65 |
| 32:2a:603:U:H2' | 32:2a:604:G:C8 | 2.31 | 0.65 |
| 33:2b:16:HIS:O | 33:2b:18:GLY:N | 2.30 | 0.65 |
| 50:2s:27:GLU:OE1 | 50:2s:28:LYS:NZ | 2.28 | 0.65 |
| 44:1m:17:VAL:O | 44:1m:20:THR:OG1 | 2.14 | 0.65 |
| 1:2A:2306:C:N4 | 6:2G:42:GLY:O | 2.30 | 0.65 |
| 1:2A:2758:A:C2 | 1:2A:2759:G:H1' | 2.31 | 0.65 |
| 11:2P:36:LYS:O | 62:2P:201:HOH:O | 2.13 | 0.65 |
| 38:1g:20:ASP:HB3 | 38:1g:23:VAL:HB | 1.80 | 0.65 |
| 25:23:40:THR:HG22 | 25:23:42:ALA:H | 1.61 | 0.65 |
| 32:2a:1095:U:OP2 | 62:2a:1909:HOH:O | 2.15 | 0.65 |
| 1:1A:759:G:OP2 | 62:1A:4230:HOH:O | 2.14 | 0.64 |
| 32:2a:742:G:OP2 | 46:2o:35:ARG:NH2 | 2.30 | 0.64 |
| 33:2b:18:GLY:HA2 | 33:2b:42:ILE:HG13 | 1.79 | 0.64 |
| 1:1A:604:G:OP2 | 11:1P:90:ARG:NH1 | 2.29 | 0.64 |
| 1:1A:2592:G:OP1 | 62:1A:4234:HOH:O | 2.15 | 0.64 |
| 32:2a:1305:G:N2 | 32:2a:1331:G:H1' | 2.12 | 0.64 |
| 38:1g:28:ASN:HD21 | 38:1g:36:LYS:HZ3 | 1.46 | 0.64 |
| 46:1o:25:THR:HG21 | 46:1o:70:LEU:HB2 | 1.77 | 0.64 |
| 32:2a:920:U:H2' | 32:2a:921:U:H6 | 1.63 | 0.64 |
| 32:2a:1060:C:H2' | 32:2a:1061:G:H8 | 1.61 | 0.64 |
| 34:2c:7:PRO:O | 34:2c:11:ARG:NH1 | 2.28 | 0.64 |
| 32:1a:955:U:O2' | 50:1s:83:HIS:HD2 | 1.80 | 0.64 |
| 35:1d:23:GLY:HA3 | 35:1d:112:VAL:HG12 | 1.79 | 0.64 |
| 39:1h:113:SER:HB2 | 39:1h:134:ILE:HD11 | 1.79 | 0.64 |
| 1:2A:1495:A:H2' | 1:2A:1496:A:C8 | 2.32 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:2A:1803:A:O2' | 3:2D:259:THR:HG21 | 1.97 | 0.64 |
| 32:2a:1161:C:H2' | 32:2a:1162:C:C6 | 2.33 | 0.64 |
| 33:2b:33:TYR:HB2 | 33:2b:43:ASP:HB2 | 1.78 | 0.64 |
| 36:2e:11:ILE:HG21 | 36:2e:31:LEU:HD23 | 1.79 | 0.64 |
| 44:2m:48:LEU:HD23 | 44:2m:53:VAL:HG12 | 1.77 | 0.64 |
| 1:1A:2069:G:OP2 | 62:1A:4233:HOH:O | 2.15 | 0.64 |
| 2:1B:75:G:H22 | 21:1Z:73:GLN:HE22 | 1.44 | 0.64 |
| 12:1Q:89:ASN:HB2 | 55:1x:1:C:N3 | 2.12 | 0.64 |
| 6:2G:109:VAL:HG11 | 26:24:14:ILE:HG21 | 1.79 | 0.64 |
| 32:2a:533:A:OP1 | 62:2a:1908:HOH:O | 2.14 | 0.64 |
| 32:2a:779:C:H2' | 32:2a:780:A:O4' | 1.98 | 0.64 |
| 44:2m:82:MET:HE2 | 44:2m:92:HIS:HB3 | 1.78 | 0.64 |
| 56:2y:26:A:N1 | 56:2y:44:G:O6 | 2.30 | 0.64 |
| 6:1G:79:ASN:OD1 | 6:1G:79:ASN:N | 2.31 | 0.64 |
| 6:1G:137:GLU:HG2 | 6:1G:152:LEU:HD22 | 1.80 | 0.64 |
| 32:1a:165:C:H2' | 32:1a:166:G:H8 | 1.63 | 0.64 |
| 20:2Y:102:CYS:SG | 20:2Y:103:GLY:N | 2.68 | 0.64 |
| 37:2f:76:ALA:HB1 | 37:2f:80:ARG:NH2 | 2.13 | 0.64 |
| 1:1A:2291:U:H2' | 1:1A:2292:C:C6 | 2.33 | 0.64 |
| 32:2a:460:G:N2 | 32:2a:471:G:N7 | 2.45 | 0.64 |
| 32:2a:1161:C:H2' | 32:2a:1162:C:H6 | 1.62 | 0.64 |
| 32:2a:1238:A:H2 | 32:2a:1241:G:N3 | 1.96 | 0.64 |
| 1:1A:615:G:OP1 | 5:1F:40:GLN:NE2 | 2.29 | 0.64 |
| 32:1a:572:A:OP1 | 62:1a:1917:HOH:O | 2.15 | 0.64 |
| 44:1m:23:TYR:HB3 | 44:1m:67:GLU:HA | 1.80 | 0.64 |
| 32:2a:134:A:H61 | 47:2p:25:ARG:NH1 | 1.95 | 0.64 |
| 37:2f:91:VAL:HG11 | 49:2r:72:ARG:NH1 | 2.12 | 0.64 |
| 1:1A:568:U:H5' | 1:1A:945:A:N6 | 2.13 | 0.64 |
| 32:1a:174:C:H2' | 32:1a:175:C:H6 | 1.62 | 0.64 |
| 8:2I:130:TYR:HE2 | 8:2I:132:PRO:HB3 | 1.62 | 0.64 |
| 12:2Q:32:TYR:OH | 12:2Q:111:GLU:OE2 | 2.15 | 0.64 |
| 32:2a:1003:G:N7 | 32:2a:1035:A:N6 | 2.46 | 0.64 |
| 32:1a:1027:C:C2 | 32:1a:1034:G:N2 | 2.66 | 0.64 |
| 54:2w:75:C:O3' | 54:2w:76:F3N:P | 2.56 | 0.64 |
| 3:1D:2:ALA:N | 3:1D:200:ASP:OD2 | 2.31 | 0.63 |
| 6:1G:110:ALA:HB1 | 6:1G:140:ILE:HG23 | 1.80 | 0.63 |
| 32:1a:948:C:OP1 | 44:1m:109:THR:OG1 | 2.16 | 0.63 |
| 34:1c:6:HIS:CD2 | 34:1c:8:ILE:H | 2.10 | 0.63 |
| 32:2a:8:A:H5' | 36:2e:101:ILE:HG22 | 1.79 | 0.63 |
| 36:2e:40:ARG:NH1 | 36:2e:68:GLU:HA | 2.13 | 0.63 |
| 26:24:50:VAL:HB | 44:2m:65:LYS:HB3 | 1.80 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 33:2b:189:ASP:N | 33:2b:189:ASP:OD1 | 2.31 | 0.63 |
| 1:1A:2126:A:N7 | 1:1A:2163:C:H1' | 2.13 | 0.63 |
| 1:1A:2690:C:OP1 | 13:1R:17:ARG:NH2 | 2.32 | 0.63 |
| 32:1a:376:G:H5'' | 47:1p:5:ARG:CG | 2.28 | 0.63 |
| 33:1b:165:VAL:HG13 | 33:1b:166:ASP:H | 1.63 | 0.63 |
| 1:2A:819:A:OP2 | 1:2A:1187:G:N2 | 2.19 | 0.63 |
| 1:2A:2183:C:H2' | 1:2A:2184:G:H8 | 1.64 | 0.63 |
| 32:1a:1005:A:OP2 | 32:1a:1006:C:N4 | 2.32 | 0.63 |
| 1:2A:1800:C:OP2 | 3:2D:183:ARG:NH2 | 2.31 | 0.63 |
| 21:2Z:40:ASP:OD2 | 21:2Z:43:GLU:N | 2.29 | 0.63 |
| 32:2a:558:G:OP1 | 62:2a:1911:HOH:O | 2.15 | 0.63 |
| 45:2n:53:LEU:HB3 | 45:2n:56:VAL:HB | 1.81 | 0.63 |
| 1:1A:1025:G:C4 | 1:1A:1135:C:H1' | 2.33 | 0.63 |
| 1:1A:1632:A:OP2 | 62:1A:4235:HOH:O | 2.15 | 0.63 |
| 32:1a:78:G:O6 | 32:1a:92:C:N4 | 2.32 | 0.63 |
| 33:1b:82:ARG:NH1 | 33:1b:86:GLU:OE2 | 2.32 | 0.63 |
| 37:1f:78:GLU:HA | 37:1f:81:ILE:HG13 | 1.81 | 0.63 |
| 50:1s:28:LYS:HB3 | 50:1s:47:HIS:HD2 | 1.63 | 0.63 |
| 19:2X:94:GLY:H | 19:2X:95:LEU:HB2 | 1.62 | 0.63 |
| 1:1A:2206:G:H3' | 1:1A:2207:G:N7 | 2.13 | 0.63 |
| 34:2c:101:LEU:HD22 | 34:2c:102:ASN:H | 1.63 | 0.63 |
| 1:1A:1859:A:N6 | 1:1A:1883:G:O2' | 2.32 | 0.63 |
| 44:1m:3:ARG:HG3 | 44:1m:4:ILE:H | 1.63 | 0.63 |
| 32:2a:1286:A:C8 | 32:2a:1287:A:H4' | 2.34 | 0.63 |
| 35:2d:173:TRP:CD2 | 35:2d:189:PRO:HB3 | 2.34 | 0.63 |
| 10:1O:68:GLU:HB3 | 10:1O:78:ARG:HB2 | 1.81 | 0.63 |
| 32:1a:118:U:O4 | 62:1a:1916:HOH:O | 2.14 | 0.63 |
| 24:22:46:GLN:O | 24:22:49:LYS:HG3 | 1.99 | 0.63 |
| 33:2b:230:VAL:HG13 | 33:2b:232:PRO:HD2 | 1.80 | 0.63 |
| 5:1F:184:TYR:CE2 | 5:1F:188:ARG:HD2 | 2.32 | 0.63 |
| 1:2A:2110:G:H3' | 1:2A:2111:C:H5' | 1.81 | 0.63 |
| 1:1A:602:G:O2' | 1:1A:655:A:N6 | 2.31 | 0.62 |
| 1:1A:1223:G:N2 | 1:1A:1226:A:OP2 | 2.29 | 0.62 |
| 32:1a:1129:C:O2 | 32:1a:1130:A:N6 | 2.29 | 0.62 |
| 1:2A:1325:G:OP1 | 1:2A:1647:G:O2' | 2.12 | 0.62 |
| 1:2A:2299:G:H2' | 1:2A:2300:G:H8 | 1.64 | 0.62 |
| 32:2a:1442:G:H2' | 32:2a:1442:G:N3 | 2.14 | 0.62 |
| 36:1e:50:GLU:HB2 | 36:1e:53:LEU:HD13 | 1.81 | 0.62 |
| 5:2F:184:TYR:CE2 | 5:2F:188:ARG:HD2 | 2.34 | 0.62 |
| 32:2a:1129:C:H2' | 32:2a:1139:G:N7 | 2.14 | 0.62 |
| 51:2t:72:LEU:HD23 | 51:2t:77:ALA:HB2 | 1.81 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:1P:38:GLN:O | 11:1P:39:LYS:HB3 | 1.99 | 0.62 |
| 32:1a:96:U:H2' | 32:1a:97:G:C8 | 2.34 | 0.62 |
| 32:1a:1414:U:H3 | 32:1a:1486:G:H1 | 1.46 | 0.62 |
| 49:1r:73:ALA:HB3 | 49:1r:79:LEU:HD12 | 1.80 | 0.62 |
| 7:2H:56:SER:HB3 | 7:2H:61:HIS:ND1 | 2.14 | 0.62 |
| 32:2a:509:A:N3 | 32:2a:543:C:O2' | 2.28 | 0.62 |
| 32:2a:1312:G:H5' | 50:2s:5:LEU:HD11 | 1.81 | 0.62 |
| 35:2d:8:VAL:HG22 | 35:2d:21:LEU:HD13 | 1.81 | 0.62 |
| 44:2m:40:ASN:ND2 | 44:2m:41:PRO:HD2 | 2.14 | 0.62 |
| 1:1A:2572:A:C8 | 4:1E:144:ARG:HD3 | 2.34 | 0.62 |
| 32:1a:749:C:H2' | 32:1a:750:G:H8 | 1.65 | 0.62 |
| 1:2A:1434:A:H61 | 1:2A:1558:A:H62 | 1.47 | 0.62 |
| 32:2a:618:C:O2 | 32:2a:622:A:N6 | 2.33 | 0.62 |
| 42:2k:81:ASP:OD1 | 42:2k:107:SER:OG | 2.16 | 0.62 |
| 1:1A:1803:A:O2' | 3:1D:259:THR:HG21 | 1.98 | 0.62 |
| 32:1a:1435:G:H2' | 32:1a:1436:U:C6 | 2.35 | 0.62 |
| 17:2V:43:GLU:OE1 | 17:2V:43:GLU:N | 2.32 | 0.62 |
| 56:2y:61:C:H2' | 56:2y:62:C:C6 | 2.34 | 0.62 |
| 1:1A:607:U:OP1 | 5:1F:102:PRO:HA | 2.00 | 0.62 |
| 1:1A:2124:G:H1 | 1:1A:2174:C:N4 | 1.97 | 0.62 |
| 5:1F:32:LEU:HD11 | 5:1F:105:VAL:HG13 | 1.80 | 0.62 |
| 45:1n:3:ARG:HD2 | 45:1n:7:ILE:HD11 | 1.82 | 0.62 |
| 1:2A:1489:U:HO2' | 1:2A:1490:A:H8 | 1.48 | 0.62 |
| 26:24:45:GLY:O | 26:24:47:GLN:N | 2.31 | 0.62 |
| 32:2a:952:U:H2' | 32:2a:953:G:H8 | 1.63 | 0.62 |
| 32:2a:1226:C:H2' | 44:2m:103:THR:HB | 1.81 | 0.62 |
| 39:2h:41:ARG:NH2 | 39:2h:123:GLU:OE2 | 2.32 | 0.62 |
| 32:1a:1027:C:N4 | 32:1a:1034:G:H1 | 1.97 | 0.62 |
| 33:1b:170:GLU:O | 33:1b:174:VAL:HG23 | 2.00 | 0.62 |
| 46:1o:70:LEU:HD11 | 46:1o:77:ARG:HB2 | 1.82 | 0.62 |
| 32:2a:1053:G:N7 | 32:2a:1200:C:H5' | 2.15 | 0.62 |
| 32:2a:1518:MA6:H93 | 32:2a:1519:MA6:H92 | 1.81 | 0.62 |
| 40:2i:28:VAL:HG12 | 40:2i:63:ILE:HB | 1.81 | 0.62 |
| 11:1P:98:GLU:O | 11:1P:101:VAL:HG12 | 2.00 | 0.62 |
| 19:1X:94:GLY:H | 19:1X:95:LEU:HB2 | 1.65 | 0.62 |
| 32:1a:161:A:H2' | 32:1a:162:A:C8 | 2.35 | 0.62 |
| 32:1a:1183:A:O2' | 32:1a:1184:G:OP1 | 2.18 | 0.62 |
| 1:2A:2115:G:O2' | 1:2A:2117:A:N7 | 2.27 | 0.62 |
| 12:2Q:111:GLU:O | 12:2Q:115:MET:HG2 | 2.00 | 0.62 |
| 32:2a:1286:A:H8 | 32:2a:1287:A:H4' | 1.64 | 0.62 |
| 34:2c:150:LYS:HB3 | 34:2c:201:TYR:HB2 | 1.81 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 39:2h:119:LEU:HB3 | 39:2h:123:GLU:HB2 | 1.81 | 0.62 |
| 8:1I:40:THR:O | 8:1I:44:LEU:HB2 | 1.99 | 0.62 |
| 33:2b:16:HIS:HB2 | 33:2b:204:ASN:HB3 | 1.81 | 0.62 |
| 35:2d:199:ASN:HB3 | 35:2d:202:LEU:HD12 | 1.82 | 0.62 |
| 10:1O:2:ILE:HD12 | 10:1O:6:THR:HG21 | 1.82 | 0.62 |
| 1:2A:1153:C:OP1 | 16:2U:92:ARG:NH2 | 2.32 | 0.62 |
| 14:2S:38:GLN:NE2 | 14:2S:47:THR:OG1 | 2.32 | 0.62 |
| 32:2a:448:A:P | 32:2a:485:G:H22 | 2.22 | 0.62 |
| 32:2a:1259:C:O2' | 32:2a:1283:G:N2 | 2.26 | 0.62 |
| 50:2s:64:GLU:OE2 | 50:2s:65:ASN:ND2 | 2.33 | 0.62 |
| 21:1Z:59:LEU:HB3 | 21:1Z:61:LEU:HD21 | 1.82 | 0.61 |
| 1:2A:2592:G:OP1 | 62:2A:3936:HOH:O | 2.16 | 0.61 |
| 36:2e:147:ASP:OD1 | 36:2e:147:ASP:N | 2.23 | 0.61 |
| 48:2q:56:VAL:HG12 | 48:2q:77:VAL:HB | 1.82 | 0.61 |
| 1:1A:2115:G:H21 | 1:1A:2117:A:H62 | 1.47 | 0.61 |
| 1:1A:2629:A:O2' | 1:1A:2630:G:OP2 | 2.18 | 0.61 |
| 1:2A:1019:U:HO2' | 1:2A:1021:A:H2 | 1.47 | 0.61 |
| 1:2A:2815:C:H2' | 1:2A:2816:C:H6 | 1.63 | 0.61 |
| 8:2I:57:ARG:HA | 8:2I:61:ARG:HH21 | 1.62 | 0.61 |
| 15:2T:24:PRO:HA | 15:2T:49:VAL:HG12 | 1.81 | 0.61 |
| 16:2U:79:PHE:CZ | 16:2U:83:LEU:HD11 | 2.35 | 0.61 |
| 33:2b:12:GLU:HB2 | 33:2b:213:LEU:HD21 | 1.82 | 0.61 |
| 1:1A:639:U:H2' | 1:1A:640:C:C6 | 2.35 | 0.61 |
| 1:1A:1359:A:H2' | 1:1A:1360:A:H5' | 1.82 | 0.61 |
| 42:1k:89:ALA:O | 42:1k:91:ARG:N | 2.27 | 0.61 |
| 26:24:26:SER:OG | 26:24:27:THR:N | 2.33 | 0.61 |
| 33:2b:8:LYS:HA | 33:2b:217:ARG:HH11 | 1.64 | 0.61 |
| 38:2g:15:ASP:OD1 | 38:2g:20:ASP:N | 2.32 | 0.61 |
| 47:2p:28:ARG:NH1 | 47:2p:29:ASP:OD1 | 2.34 | 0.61 |
| 54:2w:72:C:H2' | 54:2w:73:A:C8 | 2.35 | 0.61 |
| 39:1h:4:ASP:OD2 | 39:1h:85:ARG:NE | 2.30 | 0.61 |
| 40:1i:9:ARG:HG2 | 40:1i:14:VAL:HG12 | 1.83 | 0.61 |
| 32:2a:597:G:OP2 | 62:2a:1904:HOH:O | 2.16 | 0.61 |
| 32:2a:1194:U:H4' | 36:2e:22:GLY:HA2 | 1.82 | 0.61 |
| 32:1a:222:U:H2' | 32:1a:223:U:C6 | 2.35 | 0.61 |
| 3:2D:60:ARG:NH1 | 3:2D:86:PRO:O | 2.33 | 0.61 |
| 1:1A:1815:A:OP2 | 3:1D:54:ARG:NH2 | 2.32 | 0.61 |
| 2:1B:75:G:H22 | 21:1Z:73:GLN:NE2 | 1.98 | 0.61 |
| 32:1a:1531:A:H8 | 32:1a:1531:A:O5' | 1.83 | 0.61 |
| 47:1p:4:ILE:HG12 | 47:1p:21:VAL:HG22 | 1.81 | 0.61 |
| 13:2R:56:LYS:NZ | 13:2R:90:ARG:O | 2.33 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 43:2l:57:LYS:HE3 | 43:2l:65:GLU:OE2 | 2.01 | 0.61 |
| 12:1Q:77:LYS:NZ | 12:1Q:84:GLY:O | 2.30 | 0.61 |
| 33:1b:109:SER:O | 33:1b:112:VAL:HG22 | 2.00 | 0.61 |
| 1:2A:1627:G:OP1 | 62:2A:3935:HOH:O | 2.15 | 0.61 |
| 14:2S:67:ARG:HH12 | 14:2S:103:GLU:HB3 | 1.65 | 0.61 |
| 37:2f:95:GLU:O | 49:2r:32:ARG:NH1 | 2.33 | 0.61 |
| 1:1A:1140:C:OP2 | 9:1N:66:LYS:NZ | 2.30 | 0.61 |
| 1:1A:2306:C:O2 | 62:1A:4222:HOH:O | 2.11 | 0.61 |
| 33:1b:20:GLU:HG2 | 33:1b:23:ARG:HH11 | 1.66 | 0.61 |
| 1:2A:1430:C:H2' | 1:2A:1431:U:C6 | 2.36 | 0.61 |
| 1:2A:2557:G:H2' | 1:2A:2558:C:C6 | 2.36 | 0.61 |
| 21:2Z:53:ILE:HG22 | 21:2Z:71:VAL:HG23 | 1.83 | 0.61 |
| 24:22:35:LEU:HD12 | 24:22:53:LEU:HD12 | 1.82 | 0.61 |
| 32:2a:67:C:H2' | 32:2a:68:G:C8 | 2.36 | 0.61 |
| 41:2j:44:VAL:HG11 | 41:2j:46:ARG:HH22 | 1.66 | 0.61 |
| 51:2t:9:ASN:OD1 | 51:2t:9:ASN:N | 2.34 | 0.61 |
| 3:1D:37:LEU:HD22 | 3:1D:87:ASN:ND2 | 2.15 | 0.61 |
| 12:1Q:89:ASN:HB2 | 55:1x:1:C:C4 | 2.36 | 0.61 |
| 1:2A:2163:C:OP1 | 1:2A:2165:G:N2 | 2.34 | 0.61 |
| 32:2a:148:G:H2' | 32:2a:149:A:H8 | 1.65 | 0.61 |
| 34:2c:117:ALA:HB2 | 34:2c:200:ALA:HB2 | 1.83 | 0.61 |
| 1:1A:2784:C:H1' | 4:1E:37:ARG:NH1 | 2.15 | 0.61 |
| 32:1a:342:C:N3 | 32:1a:347:G:N1 | 2.48 | 0.61 |
| 40:1i:16:ARG:HH11 | 40:1i:64:THR:HG21 | 1.65 | 0.61 |
| 1:2A:1183:G:H5'' | 25:23:30:ARG:HH21 | 1.66 | 0.61 |
| 33:2b:82:ARG:HB3 | 33:2b:94:ASN:ND2 | 2.15 | 0.61 |
| 43:2l:53:ARG:HG3 | 43:2l:93:LEU:HD21 | 1.82 | 0.61 |
| 8:1I:93:THR:O | 8:1I:97:ILE:HG13 | 2.00 | 0.60 |
| 32:1a:1060:C:C5 | 34:1c:2:GLY:HA3 | 2.36 | 0.60 |
| 33:1b:83:MET:O | 33:1b:85:ALA:N | 2.34 | 0.60 |
| 33:1b:197:VAL:HB | 33:1b:200:ILE:HG13 | 1.84 | 0.60 |
| 1:2A:2080:G:OP1 | 23:21:35:THR:HG21 | 2.00 | 0.60 |
| 6:2G:5:VAL:HG22 | 6:2G:8:LYS:H | 1.66 | 0.60 |
| 6:2G:101:ILE:HD13 | 26:24:25:TYR:HB2 | 1.83 | 0.60 |
| 21:2Z:54:HIS:HD2 | 21:2Z:101:PRO:HG3 | 1.65 | 0.60 |
| 56:1y:20:U:H1' | 56:1y:21:A:H4' | 1.83 | 0.60 |
| 6:2G:16:ARG:HH21 | 6:2G:31:VAL:HG11 | 1.66 | 0.60 |
| 32:2a:187:C:O2' | 51:2t:89:ARG:NH2 | 2.34 | 0.60 |
| 32:2a:1060:C:O2' | 41:2j:56:HIS:ND1 | 2.31 | 0.60 |
| 42:2k:54:ARG:NH2 | 56:2y:39:PSU:O2' | 2.34 | 0.60 |
| 1:1A:2315:G:H2' | 1:1A:2316:C:C6 | 2.36 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:1I:109:ILE:HD12 | 8:1I:130:TYR:CZ | 2.36 | 0.60 |
| 32:1a:1202:G:O2' | 45:1n:29:ARG:HG3 | 2.01 | 0.60 |
| 35:1d:60:GLU:HG3 | 35:1d:202:LEU:HD12 | 1.82 | 0.60 |
| 36:1e:77:PRO:HD2 | 36:1e:142:LEU:HD13 | 1.83 | 0.60 |
| 38:1g:34:GLY:O | 38:1g:36:LYS:N | 2.34 | 0.60 |
| 32:2a:1104:G:H4' | 33:2b:111:ARG:HH21 | 1.66 | 0.60 |
| 56:2y:8:4SU:H1' | 56:2y:48:C:H1' | 1.83 | 0.60 |
| 33:1b:87:ARG:NH1 | 33:1b:233:SER:OG | 2.34 | 0.60 |
| 32:2a:289:G:OP2 | 62:2a:1910:HOH:O | 2.15 | 0.60 |
| 36:2e:10:MET:HE2 | 36:2e:55:VAL:HG21 | 1.84 | 0.60 |
| 48:2q:58:GLU:OE2 | 48:2q:75:ARG:NH2 | 2.35 | 0.60 |
| 32:1a:1025:U:C2 | 32:1a:1036:G:O6 | 2.55 | 0.60 |
| 35:1d:107:ARG:HH21 | 35:1d:194:LEU:HD21 | 1.66 | 0.60 |
| 35:1d:112:VAL:H | 35:1d:116:GLN:NE2 | 1.98 | 0.60 |
| 1:2A:922:U:H2' | 1:2A:923:C:C6 | 2.37 | 0.60 |
| 5:2F:40:GLN:NE2 | 5:2F:182:ASN:HB2 | 2.16 | 0.60 |
| 32:2a:64:G:H4' | 32:2a:65:U:H3' | 1.84 | 0.60 |
| 3:1D:38:LYS:NZ | 3:1D:39:LYS:O | 2.34 | 0.60 |
| 7:1H:164:TYR:HB2 | 7:1H:167:GLU:HB2 | 1.83 | 0.60 |
| 50:1s:28:LYS:HB3 | 50:1s:47:HIS:CD2 | 2.37 | 0.60 |
| 8:2I:110:ASP:H | 8:2I:130:TYR:HH | 1.47 | 0.60 |
| 32:2a:1005:A:H3' | 32:2a:1006:C:C6 | 2.36 | 0.60 |
| 32:2a:1072:G:H2' | 32:2a:1073:U:C6 | 2.37 | 0.60 |
| 1:1A:191:A:H2' | 1:1A:192:C:C6 | 2.37 | 0.60 |
| 1:1A:1187:G:H5'' | 17:1V:81:TYR:CE1 | 2.36 | 0.60 |
| 7:1H:149:ARG:NH1 | 7:1H:167:GLU:OE2 | 2.33 | 0.60 |
| 38:1g:28:ASN:HD21 | 38:1g:36:LYS:NZ | 1.99 | 0.60 |
| 1:2A:83:G:H1 | 1:2A:102:G:HO2' | 1.48 | 0.60 |
| 1:2A:2114:A:H2 | 1:2A:2171:A:H61 | 1.48 | 0.60 |
| 5:2F:185:ASP:OD1 | 5:2F:188:ARG:NH1 | 2.33 | 0.60 |
| 21:2Z:15:PRO:HB2 | 21:2Z:19:ARG:NH2 | 2.16 | 0.60 |
| 21:2Z:93:ASP:HA | 21:2Z:131:ARG:NH1 | 2.16 | 0.60 |
| 32:1a:1343:G:H1' | 40:1i:121:ARG:NH1 | 2.16 | 0.60 |
| 44:1m:40:ASN:O | 44:1m:43:THR:OG1 | 2.19 | 0.60 |
| 1:2A:141:A:H8 | 1:2A:1408:C:O2' | 1.85 | 0.60 |
| 6:2G:63:ILE:HD11 | 6:2G:144:ILE:HG12 | 1.84 | 0.60 |
| 6:2G:120:LEU:N | 6:2G:179:PRO:O | 2.32 | 0.60 |
| 32:2a:750:G:N3 | 46:2o:23:GLY:HA3 | 2.17 | 0.60 |
| 32:2a:1016:A:H2' | 32:2a:1017:G:O4' | 2.02 | 0.60 |
| 32:2a:1150:U:H4' | 41:2j:41:PRO:HG3 | 1.84 | 0.60 |
| 36:2e:144:THR:OG1 | 36:2e:147:ASP:OD1 | 2.12 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 32:1a:258:G:H2' | 32:1a:259:G:H8 | 1.67 | 0.60 |
| 21:2Z:124:ILE:HD11 | 21:2Z:165:VAL:HG21 | 1.83 | 0.60 |
| 32:2a:1060:C:H5'' | 41:2j:51:ARG:HB3 | 1.84 | 0.60 |
| 32:1a:1047:G:H5'' | 45:1n:4:LYS:HD3 | 1.83 | 0.60 |
| 33:1b:174:VAL:HG13 | 33:1b:184:VAL:HG11 | 1.84 | 0.60 |
| 12:2Q:82:ARG:NH2 | 22:20:4:LYS:HG3 | 2.17 | 0.60 |
| 32:2a:1329:A:OP2 | 52:2u:7:ARG:NH2 | 2.35 | 0.60 |
| 38:2g:54:THR:O | 38:2g:56:GLN:N | 2.33 | 0.60 |
| 1:1A:423:A:N7 | 62:1A:4300:HOH:O | 2.31 | 0.59 |
| 1:1A:1846:G:H5'' | 1:1A:1847:A:OP2 | 2.02 | 0.59 |
| 12:1Q:111:GLU:OE2 | 12:1Q:133:ARG:NH2 | 2.35 | 0.59 |
| 19:1X:31:HIS:CD2 | 19:1X:33:LYS:H | 2.06 | 0.59 |
| 32:1a:160:A:H8 | 32:1a:160:A:OP1 | 1.84 | 0.59 |
| 32:1a:1191:A:OP1 | 34:1c:4:LYS:NZ | 2.23 | 0.59 |
| 32:1a:1314:C:OP2 | 50:1s:4:SER:OG | 2.13 | 0.59 |
| 1:2A:2135:A:N1 | 1:2A:2156:G:O2' | 2.25 | 0.59 |
| 46:2o:71:GLN:HB2 | 46:2o:78:TYR:CD1 | 2.37 | 0.59 |
| 50:2s:33:THR:HG23 | 50:2s:35:SER:H | 1.67 | 0.59 |
| 1:1A:1062:G:O5' | 1:1A:1070:A:O2' | 2.17 | 0.59 |
| 1:1A:2243:U:OP1 | 62:1A:4237:HOH:O | 2.17 | 0.59 |
| 1:1A:2820:A:O2' | 1:1A:2821:A:OP1 | 2.19 | 0.59 |
| 2:1B:105:A:OP1 | 21:1Z:72:ARG:NH1 | 2.35 | 0.59 |
| 5:1F:185:ASP:HA | 5:1F:188:ARG:HD3 | 1.83 | 0.59 |
| 35:1d:172:PRO:O | 35:1d:174:LEU:N | 2.34 | 0.59 |
| 56:1y:40:C:H2' | 56:1y:41:C:C6 | 2.37 | 0.59 |
| 21:2Z:4:ARG:NH2 | 21:2Z:60:GLU:OE2 | 2.27 | 0.59 |
| 32:2a:1348:U:H4' | 40:2i:120:ARG:HD2 | 1.84 | 0.59 |
| 41:2j:44:VAL:HG22 | 41:2j:66:ARG:HG2 | 1.83 | 0.59 |
| 55:2x:15:G:H2' | 55:2x:59:A:N1 | 2.18 | 0.59 |
| 1:1A:1047:G:H2' | 1:1A:1110:G:N2 | 2.15 | 0.59 |
| 12:1Q:103:MET:HE1 | 12:1Q:125:LEU:HD13 | 1.85 | 0.59 |
| 26:14:61:ARG:NH1 | 50:1s:42:PRO:HD3 | 2.16 | 0.59 |
| 1:2A:271(H):G:H2' | 1:2A:271(I):G:H8 | 1.67 | 0.59 |
| 21:2Z:51:ALA:O | 21:2Z:52:SER:HB3 | 2.02 | 0.59 |
| 32:2a:920:U:H2' | 32:2a:921:U:C6 | 2.37 | 0.59 |
| 1:1A:530:G:N1 | 1:1A:2023:G:OP1 | 2.31 | 0.59 |
| 32:1a:473:G:H2' | 32:1a:474:G:H8 | 1.67 | 0.59 |
| 33:1b:105:PHE:C | 33:1b:107:THR:H | 2.11 | 0.59 |
| 1:2A:2318:G:H21 | 14:2S:3:ARG:HD3 | 1.67 | 0.59 |
| 1:2A:2496:C:OP2 | 12:2Q:82:ARG:HD3 | 2.03 | 0.59 |
| 26:24:60:GLN:O | 26:24:62:ARG:N | 2.36 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 62:2a:2070:HOH:O | 45:2n:3:ARG:HG2 | 2.02 | 0.59 |
| 40:2i:50:LEU:HD13 | 40:2i:56:LEU:HA | 1.83 | 0.59 |
| 56:2y:58:A:O2' | 56:2y:60:U:OP2 | 2.20 | 0.59 |
| 1:1A:1354:A:H4' | 3:1D:38:LYS:HE2 | 1.83 | 0.59 |
| 1:2A:265:A:C8 | 1:2A:266:G:H1' | 2.37 | 0.59 |
| 1:2A:1188:U:H4' | 17:2V:79:VAL:HG22 | 1.85 | 0.59 |
| 2:2B:94:C:H2' | 2:2B:95:C:C6 | 2.38 | 0.59 |
| 32:2a:1002:G:C2 | 32:2a:1003:G:H1' | 2.37 | 0.59 |
| 1:1A:2439:A:N6 | 55:1x:76:31H:OP1 | 2.36 | 0.59 |
| 26:14:61:ARG:HH11 | 50:1s:42:PRO:HD3 | 1.68 | 0.59 |
| 33:1b:189:ASP:OD1 | 33:1b:189:ASP:N | 2.36 | 0.59 |
| 43:2l:97:ARG:O | 62:2l:301:HOH:O | 2.17 | 0.59 |
| 1:1A:247:G:H4' | 1:1A:386:G:C5 | 2.37 | 0.59 |
| 1:1A:651:G:OP1 | 30:18:19:SER:OG | 2.12 | 0.59 |
| 6:1G:126:ASP:HB3 | 6:1G:128:ARG:H | 1.67 | 0.59 |
| 8:1I:75:LEU:HD22 | 8:1I:105:HIS:CD2 | 2.38 | 0.59 |
| 21:1Z:136:PHE:O | 21:1Z:137:ILE:HG13 | 2.01 | 0.59 |
| 47:1p:45:THR:OG1 | 47:1p:47:ASP:OD1 | 2.21 | 0.59 |
| 1:2A:890:A:H2' | 1:2A:892:G:H8 | 1.67 | 0.59 |
| 1:2A:2035:G:OP1 | 62:2A:3941:HOH:O | 2.17 | 0.59 |
| 32:2a:1004:A:N6 | 32:2a:1037:C:H1' | 2.17 | 0.59 |
| 38:2g:27:ILE:HD13 | 38:2g:40:ALA:HA | 1.84 | 0.59 |
| 47:2p:19:ILE:N | 47:2p:37:GLY:O | 2.32 | 0.59 |
| 1:1A:184:C:H2' | 1:1A:185:U:C6 | 2.37 | 0.59 |
| 1:1A:796:C:H2' | 1:1A:797:C:C6 | 2.38 | 0.59 |
| 34:1c:124:ILE:HG22 | 34:1c:130:VAL:HG22 | 1.84 | 0.59 |
| 35:1d:119:GLN:HG2 | 35:1d:123:HIS:CD2 | 2.38 | 0.59 |
| 46:1o:17:ARG:HH11 | 46:1o:17:ARG:HG3 | 1.66 | 0.59 |
| 53:1v:23:A:H4' | 53:1v:24:A:O5' | 2.02 | 0.59 |
| 56:1y:67:C:H2' | 56:1y:68:C:C6 | 2.38 | 0.59 |
| 34:2c:18:TRP:HE3 | 34:2c:18:TRP:H | 1.51 | 0.59 |
| 56:2y:63:G:H2' | 56:2y:64:A:C8 | 2.37 | 0.59 |
| 20:1Y:14:LEU:HB2 | 20:1Y:75:ILE:HD11 | 1.83 | 0.59 |
| 1:2A:184:C:H2' | 1:2A:185:U:C6 | 2.38 | 0.59 |
| 3:2D:25:THR:HG21 | 3:2D:113:VAL:HG21 | 1.85 | 0.59 |
| 19:2X:53:LYS:HB3 | 19:2X:82:GLN:HB3 | 1.85 | 0.59 |
| 21:2Z:100:VAL:HG21 | 21:2Z:134:PRO:HG2 | 1.83 | 0.59 |
| 32:2a:1149:C:H2' | 32:2a:1150:U:C6 | 2.38 | 0.59 |
| 1:1A:363(A):A:H2' | 1:1A:363(B):G:H8 | 1.68 | 0.59 |
| 1:1A:1048:A:N1 | 1:1A:1112:G:O2' | 2.26 | 0.59 |
| 1:1A:1671:U:O4 | 62:1A:4205:HOH:O | 2.13 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:2A:1025:G:O2' | 62:2A:3911:HOH:O | 2.02 | 0.59 |
| 1:2A:1591:G:H2' | 1:2A:1592:C:C6 | 2.37 | 0.59 |
| 32:2a:1087:G:N2 | 32:2a:1099:G:H1' | 2.17 | 0.59 |
| 1:1A:1062:G:H2' | 1:1A:1063:G:C8 | 2.38 | 0.58 |
| 1:1A:1074:G:C2 | 1:1A:1075:C:H1' | 2.38 | 0.58 |
| 13:2R:36:THR:HG22 | 13:2R:37:THR:H | 1.68 | 0.58 |
| 14:2S:105:ALA:HB1 | 14:2S:110:LEU:HD23 | 1.84 | 0.58 |
| 32:2a:1427:U:H2' | 32:2a:1428:A:H8 | 1.67 | 0.58 |
| 1:1A:271(E):U:H2' | 1:1A:271(F):C:C6 | 2.37 | 0.58 |
| 32:1a:1125:U:H4' | 41:1j:5:ARG:NH2 | 2.17 | 0.58 |
| 32:2a:1178:G:N2 | 32:2a:1180:A:H3' | 2.17 | 0.58 |
| 1:1A:1937:A:H1' | 1:1A:1939:5MU:H72 | 1.86 | 0.58 |
| 6:1G:18:GLU:OE2 | 6:1G:22:ARG:NH1 | 2.34 | 0.58 |
| 32:1a:166:G:H2' | 32:1a:167:G:C8 | 2.36 | 0.58 |
| 41:1j:57:LYS:HE2 | 41:1j:60:ARG:NH2 | 2.18 | 0.58 |
| 56:1y:36:A:H2' | 56:1y:37:MIA:O4' | 2.03 | 0.58 |
| 32:2a:112:G:HO2' | 32:2a:354:G:HO2' | 1.50 | 0.58 |
| 32:2a:1004:A:C8 | 32:2a:1005:A:H4' | 2.38 | 0.58 |
| 32:2a:1456:G:O6 | 51:2t:54:LYS:NZ | 2.27 | 0.58 |
| 41:2j:81:THR:C | 41:2j:83:GLU:N | 2.61 | 0.58 |
| 1:1A:994:C:OP1 | 16:1U:53:ARG:NH2 | 2.36 | 0.58 |
| 15:1T:98:LYS:NZ | 62:1T:301:HOH:O | 2.18 | 0.58 |
| 30:18:63:PRO:HG2 | 30:18:64:TYR:CE2 | 2.38 | 0.58 |
| 32:1a:757:U:H2' | 32:1a:758:G:O4' | 2.03 | 0.58 |
| 32:1a:1323:G:H2' | 32:1a:1324:A:C8 | 2.39 | 0.58 |
| 40:1i:42:ARG:NH1 | 40:1i:71:SER:OG | 2.37 | 0.58 |
| 44:1m:126:LYS:HZ3 | 44:1m:126:LYS:HB2 | 1.69 | 0.58 |
| 3:2D:133:LEU:HD12 | 3:2D:189:CYS:HB2 | 1.85 | 0.58 |
| 32:2a:945:G:C2 | 32:2a:946:A:C8 | 2.90 | 0.58 |
| 33:2b:67:THR:N | 33:2b:160:ASP:OD2 | 2.35 | 0.58 |
| 1:1A:1062:G:H8 | 1:1A:1070:A:H4' | 1.68 | 0.58 |
| 1:1A:1171:G:OP2 | 1:1A:1174:A:N6 | 2.37 | 0.58 |
| 1:1A:2182:G:H2' | 1:1A:2183:C:C6 | 2.38 | 0.58 |
| 1:2A:1314:C:H6 | 1:2A:1314:C:H5' | 1.68 | 0.58 |
| 1:2A:2567:G:H2' | 1:2A:2568:C:C6 | 2.38 | 0.58 |
| 39:2h:51:VAL:HG21 | 39:2h:60:ARG:HH11 | 1.69 | 0.58 |
| 1:1A:264:C:O2' | 1:1A:265:A:H2' | 2.03 | 0.58 |
| 3:1D:180:GLY:HA3 | 3:1D:275:LYS:HG2 | 1.85 | 0.58 |
| 3:1D:183:ARG:HG3 | 3:1D:270:ILE:HD13 | 1.85 | 0.58 |
| 32:1a:448:A:OP2 | 32:1a:485:G:N1 | 2.29 | 0.58 |
| 32:1a:452:A:H4' | 47:1p:72:ARG:NH1 | 2.19 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 41:1j:35:SER:HB3 | 41:1j:73:ASP:HB2 | 1.85 | 0.58 |
| 45:1n:23:ARG:NH1 | 45:1n:30:ALA:HB2 | 2.18 | 0.58 |
| 50:1s:20:LEU:HD23 | 50:1s:23:ASN:HD22 | 1.67 | 0.58 |
| 56:1y:56:C:H2' | 56:1y:57:G:C8 | 2.38 | 0.58 |
| 32:2a:1427:U:H2' | 32:2a:1428:A:C8 | 2.37 | 0.58 |
| 1:1A:1778:U:H2' | 1:1A:1784:A:N6 | 2.18 | 0.58 |
| 1:2A:2114:A:H2 | 1:2A:2171:A:N6 | 2.01 | 0.58 |
| 1:2A:2758:A:OP2 | 62:2A:3943:HOH:O | 2.17 | 0.58 |
| 21:2Z:55:HIS:CE1 | 21:2Z:135:GLU:HB2 | 2.39 | 0.58 |
| 32:2a:946:A:H2' | 32:2a:947:G:C8 | 2.39 | 0.58 |
| 32:2a:1033:G:H2' | 32:2a:1034:G:H8 | 1.68 | 0.58 |
| 42:2k:54:ARG:HH21 | 56:2y:39:PSU:H4' | 1.68 | 0.58 |
| 1:1A:443:A:H1' | 1:1A:1201:C:O4' | 2.04 | 0.58 |
| 32:1a:159:G:O2' | 32:1a:161:A:N7 | 2.25 | 0.58 |
| 32:1a:512:U:H2' | 32:1a:513:C:C6 | 2.39 | 0.58 |
| 33:1b:218:ALA:O | 33:1b:222:ILE:HG13 | 2.04 | 0.58 |
| 39:1h:86:ILE:HD12 | 39:1h:133:LEU:HD22 | 1.85 | 0.58 |
| 1:2A:271(H):G:H2' | 1:2A:271(I):G:C8 | 2.38 | 0.58 |
| 1:2A:1019:U:H3 | 1:2A:1142(A):A:H62 | 1.50 | 0.58 |
| 1:2A:1283:G:O2' | 1:2A:1285:G:N7 | 2.35 | 0.58 |
| 1:2A:1405:U:H2' | 1:2A:1406:U:C6 | 2.39 | 0.58 |
| 50:2s:36:ARG:HD2 | 50:2s:52:TYR:O | 2.04 | 0.58 |
| 1:1A:2788:C:OP1 | 4:1E:61:ARG:NH2 | 2.37 | 0.58 |
| 4:1E:3:GLY:HA3 | 4:1E:81:ILE:HD12 | 1.84 | 0.58 |
| 8:1I:92:VAL:HG11 | 8:1I:144:VAL:HG11 | 1.86 | 0.58 |
| 17:1V:1:MET:HE3 | 17:1V:43:GLU:HB2 | 1.86 | 0.58 |
| 25:13:39:ASP:OD2 | 25:13:44:ARG:NH1 | 2.37 | 0.58 |
| 56:1y:19:G:N1 | 56:1y:56:C:N4 | 2.52 | 0.58 |
| 1:2A:568:U:H5' | 1:2A:945:A:N1 | 2.18 | 0.58 |
| 1:2A:1568:G:N7 | 62:2A:3994:HOH:O | 2.32 | 0.58 |
| 1:2A:2319:G:N2 | 14:2S:3:ARG:HD2 | 2.19 | 0.58 |
| 9:2N:71:ILE:HG21 | 9:2N:84:LYS:HB3 | 1.85 | 0.58 |
| 14:2S:10:ARG:NE | 14:2S:91:PRO:O | 2.28 | 0.58 |
| 32:2a:1005:A:H5'' | 32:2a:1006:C:C5 | 2.38 | 0.58 |
| 1:1A:2135:A:N6 | 1:1A:2156:G:O2' | 2.36 | 0.58 |
| 6:2G:114:ILE:HA | 6:2G:140:ILE:HD11 | 1.85 | 0.58 |
| 10:2O:49:ARG:NH1 | 32:2a:1422:G:O3' | 2.37 | 0.58 |
| 41:2j:8:LEU:HB3 | 41:2j:96:ILE:HG23 | 1.85 | 0.58 |
| 8:1I:72:LEU:C | 8:1I:74:ASN:H | 2.12 | 0.57 |
| 28:16:18:ARG:HD2 | 28:16:42:TRP:CD1 | 2.39 | 0.57 |
| 33:1b:77:ALA:HB2 | 33:1b:211:ILE:HD13 | 1.85 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:2A:2206:G:H3' | 1:2A:2207:G:N7 | 2.19 | 0.57 |
| 1:2A:2467:C:H4' | 12:2Q:123:HIS:CD2 | 2.39 | 0.57 |
| 3:2D:132:PRO:HD3 | 3:2D:190:TYR:CZ | 2.39 | 0.57 |
| 24:22:3:LEU:O | 24:22:7:ARG:HG3 | 2.03 | 0.57 |
| 25:23:5:LYS:HB3 | 25:23:57:GLU:HG2 | 1.86 | 0.57 |
| 35:1d:57:ARG:HD3 | 35:1d:205:GLU:HB3 | 1.87 | 0.57 |
| 39:1h:21:LYS:O | 39:1h:65:TYR:OH | 2.21 | 0.57 |
| 12:2Q:89:ASN:HB2 | 55:2x:1:C:C4 | 2.39 | 0.57 |
| 32:2a:692:U:O2' | 32:2a:694:A:N7 | 2.27 | 0.57 |
| 1:1A:1381:G:N7 | 62:1A:4308:HOH:O | 2.32 | 0.57 |
| 8:1I:38:LEU:HD23 | 8:1I:38:LEU:H | 1.70 | 0.57 |
| 1:2A:2105:C:H2' | 1:2A:2106:G:H8 | 1.69 | 0.57 |
| 4:2E:178:GLU:CD | 4:2E:178:GLU:H | 2.11 | 0.57 |
| 4:2E:183:LEU:HD11 | 15:2T:10:VAL:HG11 | 1.86 | 0.57 |
| 13:2R:72:ASP:O | 13:2R:76:VAL:HG23 | 2.03 | 0.57 |
| 32:2a:1005:A:O2' | 32:2a:1036:G:N2 | 2.36 | 0.57 |
| 32:2a:1280:A:O2' | 32:2a:1281:U:H5' | 2.04 | 0.57 |
| 5:1F:123:LEU:HD13 | 5:1F:192:LEU:HD13 | 1.87 | 0.57 |
| 32:1a:45:U:H2' | 32:1a:46:G:C8 | 2.39 | 0.57 |
| 32:1a:149:A:H2' | 32:1a:150:C:C6 | 2.40 | 0.57 |
| 32:1a:767:A:H2' | 32:1a:768:A:O4' | 2.04 | 0.57 |
| 32:1a:1068:G:H8 | 32:1a:1068:G:OP2 | 1.87 | 0.57 |
| 32:1a:1080:A:H5' | 36:1e:14:ARG:HH21 | 1.69 | 0.57 |
| 32:1a:1241:G:H2' | 32:1a:1242:C:H6 | 1.69 | 0.57 |
| 11:2P:39:LYS:HB2 | 11:2P:45:LEU:HG | 1.86 | 0.57 |
| 32:2a:1062:U:H2' | 32:2a:1063:C:C6 | 2.40 | 0.57 |
| 32:2a:1316:G:H22 | 32:2a:1319:A:H5'' | 1.69 | 0.57 |
| 50:2s:18:LYS:O | 50:2s:22:LEU:HB2 | 2.05 | 0.57 |
| 2:1B:66:A:H61 | 2:1B:108:U:H2' | 1.69 | 0.57 |
| 32:1a:1318:A:H5'' | 50:1s:3:ARG:NH1 | 2.15 | 0.57 |
| 33:1b:167:PRO:HG3 | 33:1b:188:ALA:HB2 | 1.86 | 0.57 |
| 56:1y:19:G:H4' | 56:1y:57:G:H22 | 1.69 | 0.57 |
| 1:2A:375:C:H2' | 1:2A:376:C:C6 | 2.39 | 0.57 |
| 1:2A:528:A:O2' | 1:2A:529:A:H5' | 2.03 | 0.57 |
| 7:2H:149:ARG:NH1 | 7:2H:167:GLU:OE2 | 2.37 | 0.57 |
| 21:2Z:19:ARG:NH1 | 21:2Z:84:GLU:O | 2.38 | 0.57 |
| 32:2a:1026:G:O6 | 32:2a:1036:G:N2 | 2.37 | 0.57 |
| 32:2a:1119:C:H2' | 32:2a:1120:G:C8 | 2.39 | 0.57 |
| 1:1A:1278:A:OP1 | 13:1R:36:THR:HG23 | 2.05 | 0.57 |
| 1:1A:2115:G:N2 | 1:1A:2117:A:N7 | 2.53 | 0.57 |
| 51:1t:43:LEU:O | 51:1t:47:GLY:N | 2.38 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 14:2S:66:ALA:O | 14:2S:69:VAL:HG12 | 2.05 | 0.57 |
| 3:1D:26:LYS:HE2 | 3:1D:28:GLU:O | 2.05 | 0.57 |
| 21:1Z:48:PHE:CE1 | 21:1Z:52:SER:HA | 2.40 | 0.57 |
| 1:2A:492:A:H2' | 1:2A:493:G:O4' | 2.05 | 0.57 |
| 26:24:41:PRO:HG3 | 26:24:49:PHE:CE1 | 2.40 | 0.57 |
| 33:2b:83:MET:O | 33:2b:87:ARG:N | 2.36 | 0.57 |
| 37:2f:91:VAL:HG11 | 49:2r:72:ARG:HH12 | 1.67 | 0.57 |
| 39:2h:51:VAL:HG11 | 39:2h:60:ARG:NH1 | 2.20 | 0.57 |
| 40:2i:9:ARG:HG2 | 40:2i:14:VAL:HA | 1.86 | 0.57 |
| 3:1D:108:PRO:HB3 | 3:1D:143:HIS:CE1 | 2.39 | 0.57 |
| 32:1a:1027:C:N3 | 32:1a:1034:G:N2 | 2.53 | 0.57 |
| 36:1e:81:GLU:HG2 | 36:1e:90:VAL:HG22 | 1.87 | 0.57 |
| 40:1i:79:LEU:HG | 40:1i:83:ARG:HD2 | 1.87 | 0.57 |
| 1:2A:363:G:H2' | 1:2A:363(A):A:H8 | 1.69 | 0.57 |
| 40:2i:85:LEU:HD12 | 40:2i:92:TYR:CE2 | 2.40 | 0.57 |
| 44:2m:38:GLY:O | 44:2m:55:ARG:NH1 | 2.38 | 0.57 |
| 1:1A:572:A:OP2 | 17:1V:78:LYS:NZ | 2.38 | 0.57 |
| 13:1R:104:ARG:HG3 | 13:1R:111:LEU:HD21 | 1.85 | 0.57 |
| 18:1W:13:SER:HB3 | 18:1W:16:LYS:HG3 | 1.86 | 0.57 |
| 26:14:43:TYR:O | 26:14:45:GLY:N | 2.38 | 0.57 |
| 32:1a:445:G:H2' | 32:1a:446:G:O4' | 2.04 | 0.57 |
| 32:1a:1152:A:H5'' | 41:1j:13:HIS:ND1 | 2.20 | 0.57 |
| 33:1b:66:GLY:O | 33:1b:90:MET:HE1 | 2.05 | 0.57 |
| 40:2i:100:GLY:O | 40:2i:103:THR:HG22 | 2.05 | 0.57 |
| 1:1A:481:G:OP2 | 20:1Y:47:LYS:NZ | 2.38 | 0.57 |
| 32:1a:673:G:H5' | 37:1f:87:ARG:CZ | 2.34 | 0.57 |
| 1:2A:106:C:H1' | 20:2Y:1:MET:HE2 | 1.86 | 0.57 |
| 1:2A:2815:C:H2' | 1:2A:2816:C:C6 | 2.40 | 0.57 |
| 47:2p:28:ARG:HG2 | 47:2p:29:ASP:OD1 | 2.05 | 0.57 |
| 22:10:43:THR:O | 22:10:43:THR:HG23 | 2.03 | 0.56 |
| 32:1a:736:C:H2' | 32:1a:737:A:C8 | 2.39 | 0.56 |
| 32:1a:742:G:OP2 | 46:1o:35:ARG:NH2 | 2.37 | 0.56 |
| 1:2A:304:G:O6 | 62:2A:3938:HOH:O | 2.16 | 0.56 |
| 1:2A:1912:A:OP1 | 62:2A:3940:HOH:O | 2.17 | 0.56 |
| 1:2A:2524:G:O6 | 62:2A:3937:HOH:O | 2.16 | 0.56 |
| 2:2B:48:A:H4' | 14:2S:95:HIS:HD2 | 1.68 | 0.56 |
| 7:2H:33:LEU:HD21 | 7:2H:136:ILE:HB | 1.87 | 0.56 |
| 9:2N:94:HIS:HB3 | 9:2N:97:ARG:HG3 | 1.87 | 0.56 |
| 28:26:14:THR:OG1 | 28:26:48:VAL:O | 2.22 | 0.56 |
| 56:2y:51:U:H3 | 56:2y:63:G:H1 | 1.52 | 0.56 |
| 1:1A:1069:A:H2' | 1:1A:1073:A:N7 | 2.20 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 16:1U:108:GLU:O | 16:1U:112:ARG:HG2 | 2.05 | 0.56 |
| 32:1a:1241:G:H2' | 32:1a:1242:C:C6 | 2.40 | 0.56 |
| 36:1e:62:ALA:O | 36:1e:64:ARG:N | 2.38 | 0.56 |
| 41:1j:13:HIS:CD2 | 41:1j:14:LYS:H | 2.23 | 0.56 |
| 54:1w:20:U:OP1 | 54:1w:20:U:H4' | 2.04 | 0.56 |
| 1:2A:1204:A:H2 | 1:2A:1241:A:N6 | 2.02 | 0.56 |
| 1:2A:1866:C:H2' | 1:2A:1876:A:O4' | 2.05 | 0.56 |
| 16:2U:76:TYR:OH | 16:2U:92:ARG:NE | 2.34 | 0.56 |
| 35:2d:156:GLU:OE1 | 35:2d:159:ARG:NH2 | 2.38 | 0.56 |
| 54:2w:21:A:H5' | 54:2w:21:A:H8 | 1.69 | 0.56 |
| 1:1A:1093:G:N2 | 1:1A:1097:U:H6 | 2.04 | 0.56 |
| 1:1A:2156:G:H2' | 1:1A:2157:G:C2 | 2.40 | 0.56 |
| 1:1A:2315:G:H2' | 1:1A:2316:C:H6 | 1.70 | 0.56 |
| 1:1A:2747:G:O6 | 1:1A:2755:C:H5'' | 2.04 | 0.56 |
| 16:1U:69:CYS:HB3 | 16:1U:74:LEU:HD13 | 1.87 | 0.56 |
| 16:1U:76:TYR:CZ | 16:1U:80:ILE:HG13 | 2.41 | 0.56 |
| 32:1a:134:A:H61 | 47:1p:25:ARG:NH1 | 2.03 | 0.56 |
| 32:1a:473:G:H2' | 32:1a:474:G:C8 | 2.40 | 0.56 |
| 41:1j:38:ILE:HD11 | 41:1j:71:LEU:HD23 | 1.88 | 0.56 |
| 1:2A:1257:C:H4' | 5:2F:83:PHE:CD1 | 2.41 | 0.56 |
| 1:2A:1423:G:OP1 | 1:2A:1492:G:O2' | 2.23 | 0.56 |
| 1:2A:2134:A:H1' | 1:2A:2158:A:C6 | 2.41 | 0.56 |
| 2:2B:75:G:H5'' | 2:2B:75:G:H8 | 1.69 | 0.56 |
| 32:2a:457:C:H2' | 32:2a:458:C:C6 | 2.39 | 0.56 |
| 32:2a:1442:G:O2' | 32:2a:1442(A):G:H5' | 2.06 | 0.56 |
| 33:2b:155:LEU:HD21 | 33:2b:159:PRO:HD3 | 1.86 | 0.56 |
| 33:2b:178:ARG:NH2 | 39:2h:74:PRO:HB3 | 2.21 | 0.56 |
| 50:2s:28:LYS:HB3 | 50:2s:29:ARG:CA | 2.34 | 0.56 |
| 1:1A:528:A:O2' | 1:1A:529:A:H5' | 2.04 | 0.56 |
| 1:2A:271(E):U:H2' | 1:2A:271(F):C:C6 | 2.39 | 0.56 |
| 1:2A:1507:A:O2' | 1:2A:1508:A:O5' | 2.24 | 0.56 |
| 4:2E:101:ARG:CZ | 4:2E:171:GLU:HB2 | 2.36 | 0.56 |
| 8:2I:75:LEU:HD22 | 8:2I:105:HIS:HD2 | 1.68 | 0.56 |
| 32:2a:1305:G:H22 | 32:2a:1331:G:H1' | 1.69 | 0.56 |
| 41:2j:15:THR:OG1 | 41:2j:94:VAL:HG22 | 2.06 | 0.56 |
| 1:1A:2839:G:H5' | 13:1R:46:GLY:HA2 | 1.87 | 0.56 |
| 32:1a:381:C:H2' | 32:1a:382:A:O4' | 2.05 | 0.56 |
| 32:1a:983:A:H5' | 32:1a:984:C:OP2 | 2.05 | 0.56 |
| 32:1a:1305:G:H22 | 32:1a:1331:G:H1' | 1.70 | 0.56 |
| 34:1c:19:GLU:O | 34:1c:40:ARG:NH2 | 2.38 | 0.56 |
| 47:1p:22:THR:HA | 47:1p:33:ILE:HD12 | 1.86 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 56:1y:5:G:H1' | 56:1y:69:G:H22 | 1.70 | 0.56 |
| 14:2S:27:SER:HA | 14:2S:88:ASP:HB3 | 1.88 | 0.56 |
| 21:2Z:72:ARG:NH2 | 21:2Z:97:GLU:O | 2.38 | 0.56 |
| 32:2a:674:G:OP1 | 37:2f:87:ARG:NH2 | 2.37 | 0.56 |
| 32:2a:1095:U:H2' | 32:2a:1096:C:C6 | 2.41 | 0.56 |
| 34:2c:113:ALA:HB2 | 34:2c:202:ILE:HG13 | 1.86 | 0.56 |
| 56:2y:18:G:O6 | 56:2y:56:C:N4 | 2.39 | 0.56 |
| 1:1A:2612:C:OP2 | 27:15:2:ALA:N | 2.39 | 0.56 |
| 4:1E:2:LYS:HB2 | 4:1E:95:ILE:HD12 | 1.88 | 0.56 |
| 26:14:58:ARG:O | 26:14:61:ARG:N | 2.24 | 0.56 |
| 32:1a:70:G:H1 | 32:1a:99:U:H3 | 1.53 | 0.56 |
| 32:1a:110:C:H2' | 32:1a:111:G:O4' | 2.04 | 0.56 |
| 32:1a:174:C:H2' | 32:1a:175:C:C6 | 2.39 | 0.56 |
| 1:2A:1612:C:O2' | 29:27:5:TRP:O | 2.23 | 0.56 |
| 33:2b:19:HIS:CE1 | 33:2b:206:ASP:HB2 | 2.40 | 0.56 |
| 38:2g:103:TRP:CH2 | 38:2g:141:VAL:HG21 | 2.40 | 0.56 |
| 41:2j:74:ILE:HG22 | 62:2j:301:HOH:O | 2.04 | 0.56 |
| 1:1A:1045:A:OP1 | 1:1A:1045:A:H4' | 2.05 | 0.56 |
| 15:1T:102:ILE:HA | 15:1T:105:LEU:HD12 | 1.88 | 0.56 |
| 32:1a:436:C:H2' | 32:1a:437:U:H6 | 1.71 | 0.56 |
| 32:1a:953:G:H2' | 32:1a:954:G:O4' | 2.06 | 0.56 |
| 1:2A:883:G:O6 | 1:2A:893:C:O2' | 2.24 | 0.56 |
| 1:2A:1131:G:O6 | 1:2A:2040:C:H1' | 2.05 | 0.56 |
| 1:2A:2298:A:N6 | 1:2A:2318:G:C8 | 2.74 | 0.56 |
| 1:2A:2483:C:N3 | 12:2Q:124:LYS:NZ | 2.51 | 0.56 |
| 3:2D:168:ARG:HG2 | 3:2D:173:VAL:HG22 | 1.88 | 0.56 |
| 21:2Z:121:HIS:N | 21:2Z:171:ILE:O | 2.39 | 0.56 |
| 32:2a:160:A:H1' | 32:2a:344:A:N7 | 2.20 | 0.56 |
| 32:2a:619:U:C2 | 35:2d:135:LEU:HD21 | 2.41 | 0.56 |
| 32:2a:1176:A:H2' | 32:2a:1177:G:C8 | 2.41 | 0.56 |
| 44:2m:79:LYS:HG2 | 44:2m:83:ASP:OD2 | 2.05 | 0.56 |
| 1:1A:2156:G:OP2 | 1:1A:2156:G:H8 | 1.88 | 0.56 |
| 6:1G:111:LEU:HA | 6:1G:114:ILE:HD12 | 1.87 | 0.56 |
| 13:1R:28:LEU:HD23 | 13:1R:48:VAL:HG21 | 1.87 | 0.56 |
| 39:1h:42:GLU:HG2 | 39:1h:109:ILE:HG21 | 1.87 | 0.56 |
| 1:2A:299:A:N1 | 1:2A:322:A:O2' | 2.33 | 0.56 |
| 1:2A:304:G:H2' | 1:2A:305:U:C6 | 2.40 | 0.56 |
| 32:2a:826:C:O2 | 39:2h:15:ASN:ND2 | 2.38 | 0.56 |
| 32:2a:953:G:H5' | 32:2a:965:A:H61 | 1.71 | 0.56 |
| 32:2a:1260:C:O5' | 32:2a:1284:C:H4' | 2.06 | 0.56 |
| 54:2w:21:A:O2' | 54:2w:22:G:OP1 | 2.24 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:1A:1025:G:O2' | 62:1A:4210:HOH:O | 1.99 | 0.56 |
| 28:16:6:ARG:HD3 | 28:16:24:GLU:OE2 | 2.06 | 0.56 |
| 32:1a:958:A:C6 | 32:1a:959:A:N1 | 2.74 | 0.56 |
| 36:1e:85:GLY:C | 36:1e:87:SER:H | 2.13 | 0.56 |
| 1:2A:1354:A:H5'' | 3:2D:38:LYS:HD3 | 1.88 | 0.56 |
| 20:2Y:30:VAL:HG13 | 20:2Y:37:VAL:HG12 | 1.88 | 0.56 |
| 32:2a:1068:G:N7 | 32:2a:1094:G:O2' | 2.34 | 0.56 |
| 32:2a:1144:G:N2 | 32:2a:1146:A:H62 | 2.04 | 0.56 |
| 34:2c:136:GLN:O | 34:2c:140:ARG:HG3 | 2.05 | 0.56 |
| 1:1A:2732:G:H3' | 1:1A:2733:A:O4' | 2.06 | 0.56 |
| 4:1E:105:THR:OG1 | 4:1E:199:ARG:NH2 | 2.39 | 0.56 |
| 21:1Z:139:VAL:HG12 | 21:1Z:140:ASP:H | 1.71 | 0.56 |
| 25:13:23:LEU:HD13 | 25:13:50:VAL:HG11 | 1.87 | 0.56 |
| 28:16:19:ARG:NH1 | 28:16:52:VAL:HG21 | 2.21 | 0.56 |
| 32:1a:204:U:P | 32:1a:204:U:H3' | 2.46 | 0.56 |
| 1:2A:271(O):C:H2' | 1:2A:271(P):C:C6 | 2.41 | 0.56 |
| 1:2A:2472:G:H2' | 1:2A:2475:C:H42 | 1.71 | 0.56 |
| 3:2D:158:ALA:O | 3:2D:161:THR:OG1 | 2.23 | 0.56 |
| 21:2Z:144:LEU:H | 21:2Z:144:LEU:HD23 | 1.71 | 0.56 |
| 32:2a:562:C:H1' | 43:2l:15:ARG:HB3 | 1.88 | 0.56 |
| 32:1a:1179:A:H4' | 40:1i:103:THR:HA | 1.89 | 0.55 |
| 36:1e:12:LEU:HB3 | 36:1e:31:LEU:HB2 | 1.89 | 0.55 |
| 44:1m:102:ARG:HD3 | 44:1m:105:THR:HG23 | 1.88 | 0.55 |
| 1:2A:1790:C:H5'' | 1:2A:1791:A:OP1 | 2.06 | 0.55 |
| 1:2A:2439:A:H5' | 1:2A:2439:A:C8 | 2.41 | 0.55 |
| 32:2a:1067:A:N3 | 32:2a:1068:G:H1' | 2.21 | 0.55 |
| 32:2a:1158:C:H4' | 33:2b:133:LYS:HZ1 | 1.72 | 0.55 |
| 36:2e:60:TYR:CE1 | 36:2e:64:ARG:HD2 | 2.41 | 0.55 |
| 41:2j:63:PHE:HE2 | 45:2n:45:ARG:HA | 1.70 | 0.55 |
| 50:2s:40:ILE:HA | 50:2s:44:MET:SD | 2.46 | 0.55 |
| 1:1A:880:G:H8 | 1:1A:880:G:OP2 | 1.89 | 0.55 |
| 1:1A:1359:A:C2 | 1:1A:1372:U:O4 | 2.59 | 0.55 |
| 13:1R:34:ILE:HG13 | 13:1R:114:VAL:HG23 | 1.89 | 0.55 |
| 32:1a:250:A:H4' | 32:1a:251:G:O5' | 2.05 | 0.55 |
| 32:1a:1292:U:OP2 | 38:1g:41:ARG:NH2 | 2.38 | 0.55 |
| 33:1b:134:GLU:HA | 33:1b:137:ARG:NE | 2.21 | 0.55 |
| 50:1s:80:TYR:CZ | 50:1s:82:GLY:HA2 | 2.42 | 0.55 |
| 56:1y:67:C:H2' | 56:1y:68:C:H6 | 1.72 | 0.55 |
| 32:1a:1006:C:H2' | 32:1a:1007:C:C6 | 2.41 | 0.55 |
| 32:1a:1530:G:H2' | 32:1a:1531:A:C8 | 2.41 | 0.55 |
| 34:1c:71:ALA:HA | 34:1c:106:VAL:HG21 | 1.88 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:2A:530:G:O4' | 1:2A:530:G:N3 | 2.36 | 0.55 |
| 1:2A:601:C:OP1 | 5:2F:108:LYS:NZ | 2.36 | 0.55 |
| 1:2A:2431:U:OP2 | 62:2A:3945:HOH:O | 2.18 | 0.55 |
| 5:2F:20:LEU:HG | 5:2F:21:ALA:H | 1.70 | 0.55 |
| 32:2a:392:G:H2' | 32:2a:393:A:C8 | 2.41 | 0.55 |
| 32:2a:664:G:H22 | 32:2a:741:G:H1 | 1.53 | 0.55 |
| 32:2a:1525:G:OP1 | 42:2k:120:ARG:NH2 | 2.40 | 0.55 |
| 33:2b:91:PRO:HG3 | 33:2b:154:LEU:HB2 | 1.88 | 0.55 |
| 1:1A:808:G:OP1 | 62:1A:4241:HOH:O | 2.18 | 0.55 |
| 1:1A:2243:U:H2' | 1:1A:2244:U:C6 | 2.41 | 0.55 |
| 6:1G:114:ILE:HA | 6:1G:140:ILE:HD11 | 1.87 | 0.55 |
| 38:1g:89:MET:SD | 38:1g:155:ARG:HB2 | 2.47 | 0.55 |
| 44:1m:87:TYR:HA | 44:1m:90:LEU:HD12 | 1.88 | 0.55 |
| 1:2A:2316:C:O2' | 6:2G:128:ARG:NH2 | 2.39 | 0.55 |
| 11:2P:126:VAL:HG12 | 11:2P:148:LEU:HD22 | 1.88 | 0.55 |
| 32:2a:769:G:H4' | 32:2a:1513:A:H4' | 1.89 | 0.55 |
| 1:1A:652(D):C:H42 | 1:1A:652(U):G:H1 | 1.54 | 0.55 |
| 1:1A:1055:G:H1 | 1:1A:1104:C:N4 | 2.03 | 0.55 |
| 1:1A:1359:A:H2 | 1:1A:1372:U:O4 | 1.88 | 0.55 |
| 24:12:51:ARG:O | 24:12:55:ARG:HG3 | 2.07 | 0.55 |
| 56:1y:26:A:N6 | 56:1y:44:G:H1 | 2.04 | 0.55 |
| 26:24:34:GLU:HB2 | 44:2m:57:ARG:NH2 | 2.21 | 0.55 |
| 32:2a:130:A:O2' | 32:2a:131:C:O5' | 2.24 | 0.55 |
| 32:2a:419:C:OP1 | 32:2a:513:C:O2' | 2.24 | 0.55 |
| 32:2a:1228:C:P | 44:2m:108:ARG:HH22 | 2.30 | 0.55 |
| 10:1O:13:ASN:OD1 | 10:1O:97:ARG:N | 2.37 | 0.55 |
| 11:1P:63:PRO:HG2 | 30:18:25:MET:HB2 | 1.89 | 0.55 |
| 35:1d:196:LEU:HD23 | 35:1d:197:PRO:HD2 | 1.89 | 0.55 |
| 1:2A:93:G:H2' | 1:2A:94:C:C6 | 2.42 | 0.55 |
| 1:2A:839:U:H2' | 1:2A:840:C:C6 | 2.41 | 0.55 |
| 4:2E:141:ILE:HD12 | 4:2E:150:VAL:HG21 | 1.89 | 0.55 |
| 5:2F:40:GLN:HE22 | 5:2F:184:TYR:H | 1.52 | 0.55 |
| 5:2F:64:ILE:HG21 | 5:2F:78:ILE:HG23 | 1.87 | 0.55 |
| 8:2I:4:ILE:HG12 | 8:2I:18:VAL:HG22 | 1.88 | 0.55 |
| 10:2O:120:GLU:OE2 | 10:2O:122:LEU:HD21 | 2.06 | 0.55 |
| 32:2a:1330:U:H4' | 44:2m:23:TYR:CE1 | 2.42 | 0.55 |
| 36:2e:5:ASP:CG | 36:2e:6:PHE:H | 2.14 | 0.55 |
| 41:2j:40:LEU:HB2 | 41:2j:69:ASN:HB2 | 1.88 | 0.55 |
| 32:1a:731:G:OP1 | 32:1a:766:A:H1' | 2.05 | 0.55 |
| 1:2A:2299:G:H2' | 1:2A:2300:G:C8 | 2.42 | 0.55 |
| 6:2G:64:THR:HB | 6:2G:94:LEU:HD21 | 1.89 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 32:2a:222:U:H2' | 32:2a:223:U:C6 | 2.42 | 0.55 |
| 36:2e:60:TYR:O | 36:2e:64:ARG:HG3 | 2.06 | 0.55 |
| 44:2m:58:GLU:O | 44:2m:62:ASN:ND2 | 2.40 | 0.55 |
| 1:1A:363(C):G:H2' | 1:1A:363(D):G:C8 | 2.42 | 0.55 |
| 3:1D:12:SER:HB3 | 3:1D:208:LYS:HB3 | 1.88 | 0.55 |
| 32:1a:447:G:H2' | 32:1a:485:G:N2 | 2.22 | 0.55 |
| 32:1a:812:C:O2 | 62:1a:1920:HOH:O | 2.17 | 0.55 |
| 1:2A:1817:G:OP1 | 3:2D:88:ARG:NH2 | 2.37 | 0.55 |
| 10:2O:2:ILE:HD12 | 10:2O:6:THR:HG21 | 1.89 | 0.55 |
| 12:2Q:103:MET:HE1 | 12:2Q:125:LEU:HD13 | 1.89 | 0.55 |
| 33:2b:111:ARG:HA | 33:2b:111:ARG:NH1 | 2.18 | 0.55 |
| 34:1c:143:GLU:C | 34:1c:145:GLY:H | 2.15 | 0.55 |
| 1:2A:286:C:H2' | 1:2A:287:C:C6 | 2.42 | 0.55 |
| 1:2A:644:A:H4' | 1:2A:645:C:C4 | 2.42 | 0.55 |
| 1:2A:2291:U:H2' | 1:2A:2292:C:C6 | 2.42 | 0.55 |
| 32:2a:1288:A:N1 | 32:2a:1371:G:H1' | 2.22 | 0.55 |
| 1:1A:592:G:O6 | 62:1A:4242:HOH:O | 2.18 | 0.55 |
| 1:1A:1803:A:H4' | 3:1D:259:THR:HG23 | 1.88 | 0.55 |
| 39:1h:81:HIS:N | 39:1h:138:TRP:O | 2.40 | 0.55 |
| 40:1i:4:TYR:CE2 | 40:1i:88:TYR:HD1 | 2.25 | 0.55 |
| 47:1p:20:VAL:HG21 | 47:1p:32:TYR:CD2 | 2.41 | 0.55 |
| 1:2A:2712(A):A:OP2 | 62:2A:3944:HOH:O | 2.18 | 0.55 |
| 35:2d:47:ARG:HB2 | 35:2d:47:ARG:HH11 | 1.72 | 0.55 |
| 40:2i:88:TYR:HD2 | 40:2i:89:ASN:HB2 | 1.72 | 0.55 |
| 1:1A:668:G:OP2 | 62:1A:4239:HOH:O | 2.18 | 0.54 |
| 11:1P:81:GLN:NE2 | 11:1P:105:LEU:O | 2.41 | 0.54 |
| 21:1Z:8:TYR:HB2 | 21:1Z:38:TYR:CE2 | 2.42 | 0.54 |
| 51:1t:50:GLU:HG3 | 51:1t:100:ILE:HG23 | 1.89 | 0.54 |
| 1:2A:2143:C:H2' | 1:2A:2144:U:O4' | 2.07 | 0.54 |
| 32:2a:297:G:N2 | 32:2a:300:A:OP2 | 2.40 | 0.54 |
| 32:2a:1518:MA6:H93 | 32:2a:1519:MA6:C9 | 2.37 | 0.54 |
| 56:2y:9:A:H5' | 56:2y:46:G7M:N3 | 2.21 | 0.54 |
| 1:1A:1899:G:N3 | 1:1A:1899:G:H2' | 2.20 | 0.54 |
| 25:13:3:ARG:O | 25:13:59:VAL:HG22 | 2.07 | 0.54 |
| 32:1a:453:A:C5 | 32:1a:454:C:C4 | 2.95 | 0.54 |
| 32:1a:657:G:H2' | 32:1a:658:G:H8 | 1.72 | 0.54 |
| 40:1i:23:ASN:ND2 | 40:1i:23:ASN:H | 2.03 | 0.54 |
| 1:2A:1021:A:H8 | 1:2A:1022:G:H5'' | 1.73 | 0.54 |
| 1:2A:2167:U:H3' | 1:2A:2168:G:H21 | 1.72 | 0.54 |
| 32:2a:56:U:H2' | 32:2a:57:G:C8 | 2.42 | 0.54 |
| 32:2a:457:C:H2' | 32:2a:458:C:H6 | 1.70 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 32:2a:1381:U:H1' | 38:2g:79:ARG:CD | 2.37 | 0.54 |
| 33:2b:80:ILE:HD11 | 33:2b:212:GLN:HB2 | 1.88 | 0.54 |
| 1:1A:1075:C:H2' | 1:1A:1076:C:H5' | 1.89 | 0.54 |
| 32:1a:1066:C:O2' | 32:1a:1067:A:H5' | 2.06 | 0.54 |
| 32:1a:1152:A:OP1 | 41:1j:68:HIS:ND1 | 2.41 | 0.54 |
| 37:1f:21:LEU:O | 37:1f:25:ILE:HG13 | 2.07 | 0.54 |
| 1:2A:1011:G:OP1 | 16:2U:77:SER:OG | 2.17 | 0.54 |
| 1:2A:1755:A:OP2 | 15:2T:113:LYS:NZ | 2.40 | 0.54 |
| 33:2b:21:ARG:HA | 33:2b:39:ILE:HG13 | 1.88 | 0.54 |
| 37:2f:76:ALA:HB1 | 37:2f:80:ARG:HH22 | 1.72 | 0.54 |
| 38:2g:113:GLU:HG2 | 38:2g:119:ARG:HG2 | 1.90 | 0.54 |
| 50:2s:30:LEU:HD11 | 50:2s:50:ALA:HB2 | 1.89 | 0.54 |
| 20:1Y:35:TYR:CE2 | 20:1Y:69:ALA:HB3 | 2.42 | 0.54 |
| 24:12:13:ALA:HA | 24:12:16:LEU:HD12 | 1.89 | 0.54 |
| 32:1a:376:G:H5'' | 47:1p:5:ARG:HG2 | 1.88 | 0.54 |
| 1:2A:1639:U:H2' | 1:2A:1640:C:H5'' | 1.88 | 0.54 |
| 20:2Y:21:LYS:O | 20:2Y:21:LYS:HG2 | 2.08 | 0.54 |
| 32:2a:1035:A:H2' | 32:2a:1036:G:C8 | 2.41 | 0.54 |
| 39:2h:27:PRO:O | 39:2h:32:LYS:NZ | 2.40 | 0.54 |
| 40:2i:21:PRO:HA | 40:2i:59:PHE:HA | 1.89 | 0.54 |
| 2:1B:114:C:H4' | 14:1S:46:VAL:HG23 | 1.90 | 0.54 |
| 32:1a:127:G:HO2' | 48:1q:2:PRO:N | 2.05 | 0.54 |
| 32:1a:628:G:O6 | 62:1a:1919:HOH:O | 2.17 | 0.54 |
| 40:1i:32:ASP:OD1 | 40:1i:33:PHE:N | 2.40 | 0.54 |
| 1:2A:796:C:H2' | 1:2A:797:C:C6 | 2.42 | 0.54 |
| 1:2A:2366:A:H3' | 1:2A:2367:G:H8 | 1.73 | 0.54 |
| 4:2E:181:LEU:HD11 | 15:2T:6:LEU:HD22 | 1.88 | 0.54 |
| 12:2Q:77:LYS:NZ | 12:2Q:84:GLY:O | 2.40 | 0.54 |
| 34:2c:37:GLN:O | 34:2c:40:ARG:N | 2.41 | 0.54 |
| 36:2e:71:LEU:O | 36:2e:72:GLN:NE2 | 2.33 | 0.54 |
| 38:2g:32:ARG:HH22 | 38:2g:109:ASN:ND2 | 2.05 | 0.54 |
| 52:2u:6:ARG:HE | 52:2u:15:ARG:NH1 | 2.06 | 0.54 |
| 1:1A:1518:U:H2' | 1:1A:1519:G:O4' | 2.08 | 0.54 |
| 1:1A:1686:C:H2' | 1:1A:1687:G:O4' | 2.08 | 0.54 |
| 5:1F:155:LEU:HD11 | 5:1F:176:LEU:HD12 | 1.90 | 0.54 |
| 32:1a:7:G:H5' | 32:1a:298:A:O4' | 2.06 | 0.54 |
| 32:1a:98:G:H3' | 32:1a:99:U:H6 | 1.72 | 0.54 |
| 35:1d:184:LYS:HB3 | 35:1d:186:LEU:HD21 | 1.90 | 0.54 |
| 46:1o:87:ILE:HG22 | 46:1o:88:ARG:H | 1.73 | 0.54 |
| 1:2A:323:G:H2' | 5:2F:169:ASN:OD1 | 2.08 | 0.54 |
| 1:2A:652(A):A:H3' | 1:2A:652(B):A:H5'' | 1.89 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:2A:1664:A:H61 | 1:2A:1996:C:H42 | 1.55 | 0.54 |
| 1:2A:2130:U:H2' | 1:2A:2131:G:N2 | 2.23 | 0.54 |
| 1:2A:2155:G:N7 | 1:2A:2156:G:H1' | 2.23 | 0.54 |
| 32:2a:179:A:H2' | 32:2a:180:U:C6 | 2.43 | 0.54 |
| 32:2a:1108:G:H5' | 34:2c:176:HIS:CD2 | 2.43 | 0.54 |
| 32:2a:1151:A:O2' | 32:2a:1152:A:H8 | 1.90 | 0.54 |
| 54:2w:21:A:N6 | 54:2w:46:G7M:H2' | 2.23 | 0.54 |
| 32:1a:503:C:OP1 | 62:1a:1922:HOH:O | 2.19 | 0.54 |
| 35:1d:172:PRO:C | 35:1d:174:LEU:H | 2.16 | 0.54 |
| 50:1s:80:TYR:O | 50:1s:81:ARG:HG2 | 2.07 | 0.54 |
| 1:2A:1580:A:H8 | 1:2A:1580:A:OP2 | 1.91 | 0.54 |
| 3:2D:66:ASP:OD2 | 3:2D:103:ARG:NH1 | 2.41 | 0.54 |
| 21:2Z:171:ILE:CD1 | 21:2Z:172:ALA:H | 2.17 | 0.54 |
| 32:2a:1004:A:C6 | 32:2a:1037:C:H1' | 2.43 | 0.54 |
| 32:2a:1119:C:H2' | 32:2a:1120:G:H8 | 1.71 | 0.54 |
| 32:2a:1347:G:H22 | 32:2a:1373:G:H2' | 1.73 | 0.54 |
| 32:2a:1352:C:OP1 | 52:2u:3:LYS:NZ | 2.28 | 0.54 |
| 40:2i:45:ALA:O | 40:2i:48:GLU:HB2 | 2.08 | 0.54 |
| 1:1A:2327:A:H2' | 1:1A:2328:A:C8 | 2.43 | 0.54 |
| 1:1A:2350:C:OP2 | 62:1A:4243:HOH:O | 2.19 | 0.54 |
| 8:1I:134:PRO:C | 8:1I:136:VAL:H | 2.16 | 0.54 |
| 24:12:2:LYS:O | 24:12:6:VAL:HG23 | 2.08 | 0.54 |
| 32:1a:57:G:H2' | 32:1a:58:C:C6 | 2.43 | 0.54 |
| 41:1j:68:HIS:HB3 | 41:1j:70:ARG:HH12 | 1.73 | 0.54 |
| 42:1k:33:THR:OG1 | 42:1k:34:ASP:N | 2.37 | 0.54 |
| 1:2A:631:A:H2' | 1:2A:632:A:O4' | 2.08 | 0.54 |
| 1:2A:1653:G:H3' | 13:2R:2:ARG:HD3 | 1.90 | 0.54 |
| 1:2A:2637:U:OP1 | 4:2E:82:ARG:NH1 | 2.40 | 0.54 |
| 6:2G:124:SER:O | 6:2G:124:SER:OG | 2.23 | 0.54 |
| 32:2a:1333:A:H2' | 32:2a:1334:G:O4' | 2.08 | 0.54 |
| 1:1A:674:G:H1' | 5:1F:74:ARG:HD3 | 1.90 | 0.54 |
| 6:1G:34:LEU:HD23 | 6:1G:161:THR:HG22 | 1.89 | 0.54 |
| 32:1a:957:U:H3 | 32:1a:960:U:H5'' | 1.72 | 0.54 |
| 32:1a:1027:C:N4 | 32:1a:1034:G:N1 | 2.56 | 0.54 |
| 38:1g:113:GLU:HB3 | 38:1g:118:VAL:HG13 | 1.89 | 0.54 |
| 1:2A:2206:G:H5'' | 1:2A:2207:G:C5 | 2.42 | 0.54 |
| 11:2P:95:VAL:HG13 | 11:2P:125:VAL:HG12 | 1.90 | 0.54 |
| 21:2Z:92:SER:HB2 | 21:2Z:94:GLU:OE1 | 2.08 | 0.54 |
| 32:2a:1310:G:H5' | 44:2m:77:ASN:ND2 | 2.22 | 0.54 |
| 4:1E:180:ASN:OD1 | 62:1E:402:HOH:O | 2.19 | 0.54 |
| 32:1a:1070:U:H2' | 32:1a:1071:C:C6 | 2.43 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 33:1b:16:HIS:HB2 | 33:1b:204:ASN:HB3 | 1.89 | 0.54 |
| 1:2A:1778:U:H2' | 1:2A:1784:A:N6 | 2.23 | 0.54 |
| 1:2A:1843:C:H5' | 3:2D:253:GLN:OE1 | 2.07 | 0.54 |
| 1:2A:2094:G:OP1 | 8:2I:22:LYS:HD2 | 2.08 | 0.54 |
| 1:2A:2532:G:N2 | 1:2A:2663:G:O2' | 2.41 | 0.54 |
| 7:2H:143:GLN:NE2 | 7:2H:147:ASN:OD1 | 2.40 | 0.54 |
| 11:2P:121:LYS:HB3 | 11:2P:123:LEU:HD13 | 1.89 | 0.54 |
| 32:2a:1001(A):G:C4 | 32:2a:1002:G:H1' | 2.43 | 0.54 |
| 32:2a:1155:G:H2' | 32:2a:1156:G:C8 | 2.43 | 0.54 |
| 35:2d:148:VAL:HG11 | 35:2d:158:ILE:HG21 | 1.90 | 0.54 |
| 39:2h:134:ILE:HG22 | 39:2h:135:CYS:SG | 2.47 | 0.54 |
| 1:1A:184:C:H2' | 1:1A:185:U:H6 | 1.73 | 0.53 |
| 1:1A:249:C:O2 | 30:18:12:LYS:NZ | 2.33 | 0.53 |
| 1:1A:1174:A:H4' | 1:1A:1175:U:OP1 | 2.07 | 0.53 |
| 1:1A:2790:A:H3' | 1:1A:2790:A:N3 | 2.23 | 0.53 |
| 3:1D:6:PHE:HE2 | 3:1D:18:VAL:HG13 | 1.73 | 0.53 |
| 11:1P:101:VAL:HG23 | 11:1P:106:LEU:O | 2.07 | 0.53 |
| 17:1V:76:LYS:HB2 | 17:1V:81:TYR:HB3 | 1.89 | 0.53 |
| 32:1a:343:U:O2' | 32:1a:346:G:O6 | 2.13 | 0.53 |
| 33:1b:87:ARG:NH2 | 33:1b:220:ASP:OD1 | 2.38 | 0.53 |
| 37:1f:45:LEU:HD12 | 37:1f:59:TYR:HD1 | 1.73 | 0.53 |
| 39:1h:87:SER:HA | 39:1h:93:VAL:HG23 | 1.89 | 0.53 |
| 46:1o:3:ILE:HG21 | 46:1o:34:LEU:HD21 | 1.90 | 0.53 |
| 46:1o:71:GLN:HG3 | 46:1o:78:TYR:CD2 | 2.44 | 0.53 |
| 1:2A:27:G:O2' | 1:2A:28:A:OP2 | 2.26 | 0.53 |
| 1:2A:644:A:H4' | 1:2A:645:C:N4 | 2.23 | 0.53 |
| 1:2A:1114:G:H2' | 1:2A:1115:G:H8 | 1.73 | 0.53 |
| 5:2F:109:GLY:HA2 | 5:2F:112:MET:HE3 | 1.90 | 0.53 |
| 10:2O:49:ARG:HH12 | 32:2a:1423:G:P | 2.31 | 0.53 |
| 1:1A:1429:G:H2' | 1:1A:1430:C:C6 | 2.43 | 0.53 |
| 20:1Y:6:HIS:H | 20:1Y:6:HIS:CD2 | 2.25 | 0.53 |
| 33:1b:92:TYR:HE1 | 33:1b:94:ASN:HB2 | 1.72 | 0.53 |
| 46:1o:7:GLU:O | 46:1o:11:VAL:HG23 | 2.08 | 0.53 |
| 54:1w:18:G:H4' | 54:1w:60:U:C5 | 2.43 | 0.53 |
| 1:2A:2274:A:O2' | 1:2A:2276:G:OP1 | 2.25 | 0.53 |
| 5:2F:158:THR:OG1 | 5:2F:195:ASP:OD2 | 2.23 | 0.53 |
| 25:23:6:VAL:HG22 | 25:23:56:VAL:HG12 | 1.89 | 0.53 |
| 32:2a:1159:U:O4 | 62:2a:1907:HOH:O | 2.13 | 0.53 |
| 32:2a:1327:C:H2' | 32:2a:1328:C:H6 | 1.73 | 0.53 |
| 35:2d:111:ALA:HB2 | 35:2d:120:LEU:HD12 | 1.90 | 0.53 |
| 41:2j:46:ARG:HB2 | 41:2j:46:ARG:HH11 | 1.73 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:1A:2123:G:H2' | 1:1A:2124:G:C8 | 2.43 | 0.53 |
| 4:1E:7:VAL:HG23 | 4:1E:51:PHE:CE2 | 2.41 | 0.53 |
| 26:14:61:ARG:HG3 | 26:14:62:ARG:N | 2.23 | 0.53 |
| 56:1y:40:C:H2' | 56:1y:41:C:H6 | 1.73 | 0.53 |
| 1:2A:253:C:OP2 | 30:28:5:LYS:NZ | 2.33 | 0.53 |
| 1:2A:363:G:H2' | 1:2A:363(A):A:C8 | 2.43 | 0.53 |
| 1:2A:1155:A:OP1 | 16:2U:55:ARG:HG2 | 2.09 | 0.53 |
| 1:2A:2319:G:H22 | 14:2S:3:ARG:HD2 | 1.71 | 0.53 |
| 3:2D:275:LYS:HD2 | 3:2D:276:LYS:HB2 | 1.91 | 0.53 |
| 44:2m:122:LYS:HG3 | 44:2m:123:ALA:H | 1.72 | 0.53 |
| 45:2n:23:ARG:NH1 | 45:2n:28:GLY:O | 2.40 | 0.53 |
| 56:2y:10:G:H2' | 56:2y:11:C:C6 | 2.44 | 0.53 |
| 57:2z:3:LYS:HE2 | 57:2z:17:ARG:HG3 | 1.89 | 0.53 |
| 1:1A:286:C:H2' | 1:1A:287:C:C6 | 2.44 | 0.53 |
| 1:1A:2010:G:H5'' | 18:1W:42:ARG:HB2 | 1.90 | 0.53 |
| 1:1A:2022:U:O2' | 1:1A:2617:C:H5' | 2.08 | 0.53 |
| 1:1A:2439:A:H5' | 1:1A:2439:A:C8 | 2.43 | 0.53 |
| 21:1Z:151:HIS:HA | 21:1Z:171:ILE:HG23 | 1.89 | 0.53 |
| 50:1s:48:THR:HA | 50:1s:60:VAL:O | 2.09 | 0.53 |
| 1:2A:900:A:H2' | 1:2A:901:A:H8 | 1.72 | 0.53 |
| 1:2A:1937:A:H1' | 1:2A:1939:5MU:H71 | 1.89 | 0.53 |
| 1:2A:1998:G:H4' | 1:2A:2724:C:O2' | 2.06 | 0.53 |
| 1:2A:2577:A:OP2 | 27:25:3:LYS:NZ | 2.31 | 0.53 |
| 23:21:2:SER:HB3 | 23:21:46:LEU:HD12 | 1.91 | 0.53 |
| 32:2a:187:C:H2' | 32:2a:188:C:H6 | 1.74 | 0.53 |
| 32:2a:573:A:N3 | 32:2a:883:C:O2' | 2.37 | 0.53 |
| 56:2y:14:A:N6 | 56:2y:21:A:H2 | 2.01 | 0.53 |
| 1:1A:234:C:H2' | 1:1A:235:U:H6 | 1.73 | 0.53 |
| 1:1A:1170:G:H1 | 1:1A:1179:C:H42 | 1.57 | 0.53 |
| 1:1A:2396:G:H5' | 23:11:25:LYS:HE2 | 1.91 | 0.53 |
| 17:1V:40:LEU:HB2 | 17:1V:46:VAL:HB | 1.89 | 0.53 |
| 23:11:3:LYS:HB2 | 23:11:61:ARG:HH12 | 1.72 | 0.53 |
| 31:19:25:VAL:HB | 31:19:34:GLN:HB2 | 1.91 | 0.53 |
| 35:1d:180:GLY:O | 35:1d:182:LYS:HG3 | 2.08 | 0.53 |
| 36:1e:78:HIS:HD2 | 36:1e:79:GLU:O | 1.92 | 0.53 |
| 41:1j:30:SER:HB3 | 41:1j:81:THR:OG1 | 2.08 | 0.53 |
| 32:2a:1070:U:H2' | 32:2a:1071:C:C6 | 2.44 | 0.53 |
| 32:2a:1194:U:H2' | 32:2a:1195:C:C6 | 2.43 | 0.53 |
| 5:1F:116:ASP:OD1 | 5:1F:119:ARG:NH2 | 2.39 | 0.53 |
| 8:1I:6:LEU:O | 8:1I:7:GLU:HG3 | 2.09 | 0.53 |
| 21:1Z:139:VAL:HG22 | 21:1Z:155:LEU:HD21 | 1.90 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 32:1a:1313:U:OP2 | 50:1s:5:LEU:HG | 2.09 | 0.53 |
| 43:1l:117:ARG:HG2 | 43:1l:122:THR:HB | 1.90 | 0.53 |
| 54:1w:75:C:HO3' | 54:1w:76:F3N:P | 2.30 | 0.53 |
| 55:1x:19:G:H4' | 55:1x:20:U:OP2 | 2.09 | 0.53 |
| 6:2G:15:VAL:HG13 | 6:2G:175:LEU:HD12 | 1.90 | 0.53 |
| 8:2I:38:LEU:H | 8:2I:38:LEU:HD12 | 1.74 | 0.53 |
| 14:2S:11:LYS:HG2 | 14:2S:91:PRO:HB3 | 1.91 | 0.53 |
| 22:20:32:ARG:H | 22:20:35:ASN:ND2 | 2.07 | 0.53 |
| 22:20:50:ASN:HB3 | 22:20:63:VAL:HG22 | 1.90 | 0.53 |
| 34:2c:92:ALA:HB2 | 34:2c:99:VAL:CB | 2.39 | 0.53 |
| 41:2j:50:ILE:HD11 | 41:2j:57:LYS:HD2 | 1.90 | 0.53 |
| 52:2u:9:ARG:O | 52:2u:13:ILE:HG13 | 2.09 | 0.53 |
| 1:1A:278:A:P | 1:1A:278:A:H8 | 2.31 | 0.53 |
| 1:1A:322:A:OP1 | 5:1F:168:ARG:HD2 | 2.08 | 0.53 |
| 1:1A:363(A):A:H2' | 1:1A:363(B):G:C8 | 2.44 | 0.53 |
| 1:1A:739:G:OP1 | 62:1A:4244:HOH:O | 2.19 | 0.53 |
| 1:1A:747:U:O2 | 1:1A:2014:A:H1' | 2.08 | 0.53 |
| 1:1A:1379:A:H4' | 1:1A:1380:G:OP2 | 2.09 | 0.53 |
| 1:1A:1796:U:H2' | 1:1A:1797:C:C6 | 2.44 | 0.53 |
| 32:1a:382:A:H2' | 32:1a:383:A:C8 | 2.42 | 0.53 |
| 32:1a:702:A:OP2 | 62:1a:1921:HOH:O | 2.18 | 0.53 |
| 32:1a:1348:U:H4' | 40:1i:120:ARG:HD2 | 1.89 | 0.53 |
| 36:1e:41:VAL:HG23 | 36:1e:67:VAL:HG12 | 1.90 | 0.53 |
| 48:1q:55:ASP:O | 48:1q:57:VAL:HG13 | 2.08 | 0.53 |
| 1:2A:288:C:H2' | 1:2A:289:A:C8 | 2.43 | 0.53 |
| 6:2G:126:ASP:OD2 | 6:2G:130:ASN:ND2 | 2.32 | 0.53 |
| 32:2a:45:U:H2' | 32:2a:46:G:C8 | 2.44 | 0.53 |
| 32:2a:73:G:H1 | 32:2a:96:U:H3 | 1.55 | 0.53 |
| 48:1q:56:VAL:HG12 | 48:1q:77:VAL:HB | 1.90 | 0.53 |
| 1:2A:400:G:O6 | 62:2A:3939:HOH:O | 2.16 | 0.53 |
| 3:2D:180:GLY:HA3 | 3:2D:275:LYS:HG2 | 1.91 | 0.53 |
| 23:21:64:ALA:HA | 23:21:67:ILE:HG13 | 1.90 | 0.53 |
| 33:2b:59:GLU:HG3 | 33:2b:63:MET:HE2 | 1.90 | 0.53 |
| 37:2f:9:VAL:HG23 | 37:2f:87:ARG:HB2 | 1.90 | 0.53 |
| 46:2o:25:THR:HG21 | 46:2o:70:LEU:HB2 | 1.91 | 0.53 |
| 1:1A:2376:A:H2' | 1:1A:2377:A:O4' | 2.09 | 0.53 |
| 1:1A:2523:G:C2' | 1:1A:2524:G:H5' | 2.39 | 0.53 |
| 1:1A:2693:A:H2' | 1:1A:2694:G:C8 | 2.43 | 0.53 |
| 32:1a:198:G:H2' | 32:1a:199:G:H8 | 1.73 | 0.53 |
| 32:1a:1062:U:H2' | 32:1a:1063:C:C6 | 2.44 | 0.53 |
| 1:2A:18:C:H2' | 1:2A:19:C:H6 | 1.74 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:2A:309:G:N3 | 1:2A:329:G:O2' | 2.39 | 0.53 |
| 32:2a:659:U:OP2 | 46:2o:8:LYS:NZ | 2.40 | 0.53 |
| 32:2a:939:G:H5' | 38:2g:102:ARG:CZ | 2.38 | 0.53 |
| 32:2a:1005:A:H5'' | 32:2a:1006:C:H5 | 1.74 | 0.53 |
| 32:2a:1151:A:H5'' | 41:2j:42:THR:HG23 | 1.91 | 0.53 |
| 32:2a:1327:C:H2' | 32:2a:1328:C:C6 | 2.44 | 0.53 |
| 35:2d:111:ALA:HB1 | 35:2d:116:GLN:HB3 | 1.90 | 0.53 |
| 31:19:17:ILE:HD13 | 31:19:26:ILE:HD13 | 1.91 | 0.53 |
| 1:2A:2107:C:N4 | 1:2A:2182:G:H1 | 2.06 | 0.53 |
| 4:2E:7:VAL:HG12 | 4:2E:9:VAL:HG13 | 1.90 | 0.53 |
| 6:2G:171:ALA:O | 6:2G:175:LEU:HG | 2.09 | 0.53 |
| 43:2l:38:THR:O | 43:2l:79:GLU:HG3 | 2.09 | 0.53 |
| 6:1G:165:THR:OG1 | 6:1G:168:GLU:HG3 | 2.09 | 0.52 |
| 20:1Y:20:TYR:CE2 | 20:1Y:43:ASN:HA | 2.44 | 0.52 |
| 21:1Z:80:ARG:HD3 | 21:1Z:82:ARG:NH1 | 2.25 | 0.52 |
| 33:1b:69:LEU:HB3 | 33:1b:162:ILE:HG22 | 1.90 | 0.52 |
| 1:2A:190:A:OP2 | 23:21:39:LYS:HE3 | 2.10 | 0.52 |
| 1:2A:1114:G:H2' | 1:2A:1115:G:C8 | 2.43 | 0.52 |
| 12:2Q:32:TYR:HH | 12:2Q:111:GLU:CD | 2.15 | 0.52 |
| 32:2a:1316:G:N2 | 32:2a:1318:A:H3' | 2.23 | 0.52 |
| 32:2a:1435:G:H2' | 32:2a:1436:U:C6 | 2.44 | 0.52 |
| 33:2b:63:MET:HG3 | 33:2b:225:ALA:HB1 | 1.91 | 0.52 |
| 54:2w:12:U:H2' | 54:2w:13:C:H5'' | 1.91 | 0.52 |
| 1:1A:2722:G:H2' | 1:1A:2723:C:C6 | 2.43 | 0.52 |
| 4:1E:143:ASN:HD22 | 4:1E:147:PRO:HD2 | 1.74 | 0.52 |
| 25:13:7:LYS:HE3 | 25:13:32:GLN:NE2 | 2.25 | 0.52 |
| 32:1a:60:A:H4' | 32:1a:61:G:H5' | 1.92 | 0.52 |
| 47:1p:72:ARG:O | 47:1p:75:ARG:HB3 | 2.09 | 0.52 |
| 1:2A:443:A:H1' | 1:2A:1201:C:O4' | 2.09 | 0.52 |
| 1:2A:2273:A:O2' | 1:2A:2274:A:H5' | 2.10 | 0.52 |
| 6:2G:105:LYS:NZ | 6:2G:143:GLU:OE2 | 2.39 | 0.52 |
| 8:2I:75:LEU:HD22 | 8:2I:105:HIS:CD2 | 2.43 | 0.52 |
| 8:2I:93:THR:HG22 | 8:2I:119:PRO:HB3 | 1.91 | 0.52 |
| 32:2a:189(A):C:H2' | 32:2a:189(B):C:H6 | 1.73 | 0.52 |
| 32:2a:730:G:C5 | 32:2a:731:G:H1' | 2.44 | 0.52 |
| 32:2a:1225:A:OP1 | 44:2m:103:THR:OG1 | 2.24 | 0.52 |
| 4:1E:176:ILE:HB | 4:1E:181:LEU:HB2 | 1.91 | 0.52 |
| 5:1F:53:THR:HB | 5:1F:56:GLU:OE1 | 2.09 | 0.52 |
| 16:1U:8:VAL:HG13 | 16:1U:12:ARG:HD2 | 1.92 | 0.52 |
| 36:1e:93:PRO:HG2 | 39:1h:105:ARG:NE | 2.24 | 0.52 |
| 1:2A:613:G:N2 | 1:2A:614(C):A:O2' | 2.43 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:2A:1019:U:O2' | 1:2A:1021:A:H2 | 1.92 | 0.52 |
| 1:2A:2134:A:H2' | 1:2A:2134:A:N3 | 2.23 | 0.52 |
| 1:2A:2498:C:OP1 | 62:2A:3948:HOH:O | 2.19 | 0.52 |
| 7:2H:121:ILE:HD11 | 7:2H:140:LYS:HG2 | 1.89 | 0.52 |
| 15:2T:122:ASP:HA | 15:2T:125:ARG:HG2 | 1.90 | 0.52 |
| 37:2f:99:ALA:HB1 | 49:2r:23:LYS:NZ | 2.23 | 0.52 |
| 51:2t:63:ILE:HG21 | 51:2t:81:LYS:HG3 | 1.91 | 0.52 |
| 56:2y:58:A:H1' | 56:2y:60:U:N3 | 2.24 | 0.52 |
| 1:1A:1188:U:H4' | 17:1V:79:VAL:HG22 | 1.91 | 0.52 |
| 6:1G:66:GLN:HG3 | 26:14:1:MET:HE1 | 1.91 | 0.52 |
| 33:1b:158:LEU:HD13 | 33:1b:182:ILE:HD11 | 1.90 | 0.52 |
| 38:1g:85:TYR:HB3 | 38:1g:87:VAL:HG23 | 1.92 | 0.52 |
| 41:1j:38:ILE:HD11 | 41:1j:71:LEU:HB3 | 1.91 | 0.52 |
| 1:2A:881:G:H3' | 1:2A:882:G:H8 | 1.74 | 0.52 |
| 3:2D:26:LYS:NZ | 3:2D:28:GLU:O | 2.33 | 0.52 |
| 32:2a:22:G:H4' | 32:2a:885:G:C8 | 2.45 | 0.52 |
| 32:2a:114:U:O2' | 32:2a:115:G:H5' | 2.09 | 0.52 |
| 40:2i:56:LEU:HG | 40:2i:57:GLY:H | 1.73 | 0.52 |
| 51:2t:9:ASN:O | 51:2t:10:LEU:HB2 | 2.08 | 0.52 |
| 1:1A:1173:G:OP2 | 1:1A:1173:G:H2' | 2.09 | 0.52 |
| 1:1A:1587:A:H2' | 1:1A:1588:C:H6 | 1.74 | 0.52 |
| 32:1a:437:U:H5'' | 35:1d:155:LEU:HD21 | 1.90 | 0.52 |
| 55:1x:23:C:H2' | 55:1x:24:U:C6 | 2.45 | 0.52 |
| 1:2A:957:A:H5' | 12:2Q:76:LYS:HD2 | 1.90 | 0.52 |
| 1:2A:2118:U:N3 | 1:2A:2149:G:H1' | 2.24 | 0.52 |
| 1:2A:2683:C:OP1 | 15:2T:53:ARG:NH2 | 2.37 | 0.52 |
| 6:2G:98:ARG:CZ | 26:24:1:MET:HE3 | 2.39 | 0.52 |
| 32:2a:1271:G:N1 | 32:2a:1272:G:N7 | 2.58 | 0.52 |
| 34:2c:101:LEU:HD13 | 34:2c:102:ASN:N | 2.25 | 0.52 |
| 39:2h:51:VAL:HG21 | 39:2h:60:ARG:HB2 | 1.92 | 0.52 |
| 1:1A:1165:U:H2' | 1:1A:1166:C:C6 | 2.44 | 0.52 |
| 1:1A:2328:A:H2' | 1:1A:2329:G:C8 | 2.45 | 0.52 |
| 5:1F:172:TRP:CD1 | 5:1F:172:TRP:H | 2.28 | 0.52 |
| 24:12:52:ASP:O | 24:12:56:GLN:HG3 | 2.10 | 0.52 |
| 32:1a:276:G:O3' | 48:1q:68:ARG:NH1 | 2.43 | 0.52 |
| 32:1a:1136:U:H5'' | 32:1a:1137:C:N3 | 2.24 | 0.52 |
| 32:1a:1151:A:HO2' | 32:1a:1152:A:H8 | 1.55 | 0.52 |
| 35:1d:31:CYS:HB2 | 61:1d:302:SF4:S3 | 2.49 | 0.52 |
| 40:1i:6:GLY:O | 40:1i:17:VAL:HG12 | 2.09 | 0.52 |
| 43:1l:42:THR:HA | 43:1l:53:ARG:O | 2.09 | 0.52 |
| 47:1p:19:ILE:HB | 47:1p:37:GLY:HA3 | 1.91 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:2A:1270:C:H5'' | 1:2A:1271:G:O5' | 2.10 | 0.52 |
| 1:2A:1316:U:H2' | 1:2A:1317:A:C8 | 2.44 | 0.52 |
| 2:2B:42:C:N3 | 6:2G:93:THR:OG1 | 2.35 | 0.52 |
| 32:2a:745:C:OP1 | 32:2a:851:G:O2' | 2.23 | 0.52 |
| 32:2a:1251:A:H2' | 32:2a:1252:A:C8 | 2.44 | 0.52 |
| 32:2a:1320:C:N3 | 50:2s:36:ARG:NH2 | 2.57 | 0.52 |
| 33:2b:77:ALA:HA | 33:2b:80:ILE:HG22 | 1.91 | 0.52 |
| 34:2c:71:ALA:HA | 34:2c:106:VAL:HB | 1.92 | 0.52 |
| 42:2k:98:LEU:O | 42:2k:101:SER:OG | 2.24 | 0.52 |
| 44:2m:24:GLY:HA3 | 44:2m:66:LEU:HD23 | 1.91 | 0.52 |
| 1:1A:1292:U:H2' | 1:1A:1293:C:C6 | 2.45 | 0.52 |
| 15:1T:56:GLY:O | 15:1T:59:THR:HG22 | 2.09 | 0.52 |
| 32:1a:738:C:H2' | 32:1a:739:C:H6 | 1.74 | 0.52 |
| 32:1a:1530:G:H4' | 32:1a:1530:G:OP1 | 2.10 | 0.52 |
| 1:2A:236:C:H2' | 1:2A:237:C:H6 | 1.74 | 0.52 |
| 1:2A:321:G:OP1 | 5:2F:135:LYS:NZ | 2.42 | 0.52 |
| 4:2E:38:THR:HG23 | 4:2E:41:LYS:HB3 | 1.90 | 0.52 |
| 16:2U:86:ALA:HB2 | 16:2U:116:ALA:HB2 | 1.92 | 0.52 |
| 17:2V:72:VAL:HB | 17:2V:85:LYS:HB3 | 1.90 | 0.52 |
| 35:2d:20:TYR:CD1 | 35:2d:26:CYS:HB3 | 2.40 | 0.52 |
| 1:1A:2079:U:OP1 | 23:11:21:ARG:NH2 | 2.39 | 0.52 |
| 1:1A:2428:G:OP1 | 62:1A:4203:HOH:O | 2.19 | 0.52 |
| 1:1A:2693:A:H2' | 1:1A:2694:G:H8 | 1.75 | 0.52 |
| 21:1Z:52:SER:O | 21:1Z:52:SER:OG | 2.16 | 0.52 |
| 21:1Z:105:VAL:N | 21:1Z:139:VAL:O | 2.43 | 0.52 |
| 32:1a:33:A:H2' | 32:1a:34:C:C6 | 2.45 | 0.52 |
| 33:1b:16:HIS:O | 33:1b:18:GLY:N | 2.43 | 0.52 |
| 40:1i:33:PHE:HD2 | 40:1i:34:ASN:ND2 | 2.07 | 0.52 |
| 2:2B:42:C:O2 | 6:2G:93:THR:N | 2.39 | 0.52 |
| 6:2G:97:ASP:O | 6:2G:101:ILE:HG13 | 2.09 | 0.52 |
| 30:18:4:MET:HE3 | 30:18:63:PRO:HG3 | 1.92 | 0.52 |
| 32:1a:243:A:C2 | 32:1a:246:A:C8 | 2.98 | 0.52 |
| 32:1a:625:G:H4' | 47:1p:16:HIS:CD2 | 2.44 | 0.52 |
| 32:1a:1101:A:H4' | 32:1a:1102:A:O5' | 2.10 | 0.52 |
| 43:1l:117:ARG:HB3 | 43:1l:122:THR:O | 2.09 | 0.52 |
| 51:1t:90:GLN:O | 51:1t:93:GLU:HB2 | 2.09 | 0.52 |
| 1:2A:572:A:OP2 | 17:2V:78:LYS:NZ | 2.42 | 0.52 |
| 1:2A:856:C:O4' | 22:20:27:GLU:HB3 | 2.10 | 0.52 |
| 2:2B:14:U:H1' | 2:2B:108:U:O2' | 2.09 | 0.52 |
| 9:2N:1:MET:HE1 | 16:2U:94:ASN:ND2 | 2.25 | 0.52 |
| 32:2a:176:C:H2' | 32:2a:177:C:H6 | 1.75 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 32:2a:967:5MC:H2' | 32:2a:968:A:N7 | 2.25 | 0.52 |
| 32:2a:1027:C:C4 | 32:2a:1034:G:O6 | 2.63 | 0.52 |
| 34:2c:113:ALA:N | 34:2c:114:PRO:HD2 | 2.25 | 0.52 |
| 1:1A:1007:C:OP1 | 9:1N:37:LYS:HE2 | 2.10 | 0.52 |
| 1:1A:1266:G:O5' | 18:1W:15:ARG:NH2 | 2.43 | 0.52 |
| 1:1A:2127:G:H2' | 1:1A:2128:C:C6 | 2.45 | 0.52 |
| 1:1A:2298:A:H2' | 1:1A:2299:G:O4' | 2.10 | 0.52 |
| 3:1D:4:LYS:HB3 | 3:1D:18:VAL:HG22 | 1.91 | 0.52 |
| 3:1D:92:ILE:HD12 | 3:1D:104:TYR:CD1 | 2.44 | 0.52 |
| 7:1H:6:ARG:HH22 | 7:1H:54:ARG:NH2 | 2.08 | 0.52 |
| 9:1N:67:LEU:O | 9:1N:88:GLU:HG3 | 2.10 | 0.52 |
| 32:1a:942:G:H21 | 40:1i:124:GLN:NE2 | 2.07 | 0.52 |
| 32:1a:1429:C:H2' | 32:1a:1430:C:C6 | 2.45 | 0.52 |
| 33:1b:16:HIS:HB3 | 33:1b:210:SER:OG | 2.10 | 0.52 |
| 1:2A:631:A:OP1 | 11:2P:65:ARG:NH1 | 2.43 | 0.52 |
| 1:2A:2162:G:H4' | 1:2A:2172:U:H2' | 1.92 | 0.52 |
| 1:2A:2238:G:H5'' | 62:2A:3976:HOH:O | 2.09 | 0.52 |
| 2:2B:103:G:N2 | 21:2Z:73:GLN:HE22 | 1.99 | 0.52 |
| 8:2I:40:THR:O | 8:2I:44:LEU:HB2 | 2.10 | 0.52 |
| 10:2O:26:LYS:O | 10:2O:30:ALA:HB2 | 2.10 | 0.52 |
| 15:2T:117:ASP:OD2 | 15:2T:120:ARG:NE | 2.40 | 0.52 |
| 32:2a:1118:C:H1' | 32:2a:1179:A:C5 | 2.44 | 0.52 |
| 33:2b:71:VAL:HB | 33:2b:164:VAL:HG22 | 1.91 | 0.52 |
| 33:2b:80:ILE:O | 33:2b:80:ILE:HG12 | 2.09 | 0.52 |
| 34:2c:121:ALA:O | 34:2c:125:GLU:HG2 | 2.09 | 0.52 |
| 44:2m:20:THR:C | 44:2m:22:ILE:H | 2.18 | 0.52 |
| 47:2p:18:ARG:HD3 | 47:2p:35:LYS:HD2 | 1.91 | 0.52 |
| 52:2u:6:ARG:HG2 | 52:2u:15:ARG:HD2 | 1.92 | 0.52 |
| 1:1A:1301:A:O2' | 1:1A:1302:A:H3' | 2.09 | 0.51 |
| 1:1A:1779:U:H2' | 62:1A:4279:HOH:O | 2.10 | 0.51 |
| 1:1A:2319:G:H22 | 14:1S:3:ARG:CD | 2.24 | 0.51 |
| 6:1G:126:ASP:HB2 | 6:1G:130:ASN:O | 2.09 | 0.51 |
| 8:1I:4:ILE:HD13 | 8:1I:47:LEU:HG | 1.92 | 0.51 |
| 32:1a:334:C:H2' | 32:1a:335:C:C6 | 2.45 | 0.51 |
| 1:2A:1430:C:H2' | 1:2A:1431:U:H6 | 1.75 | 0.51 |
| 7:2H:3:ARG:NH1 | 7:2H:5:GLY:H | 2.08 | 0.51 |
| 8:2I:130:TYR:CE2 | 8:2I:132:PRO:HB3 | 2.43 | 0.51 |
| 12:2Q:43:THR:HA | 12:2Q:94:VAL:HG12 | 1.92 | 0.51 |
| 18:2W:12:ILE:HD13 | 18:2W:17:VAL:HG13 | 1.91 | 0.51 |
| 28:26:32:ASN:OD1 | 28:26:32:ASN:N | 2.38 | 0.51 |
| 32:2a:1077:G:H5' | 32:2a:1078:U:OP2 | 2.11 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 35:2d:86:LYS:H | 35:2d:86:LYS:HD2 | 1.74 | 0.51 |
| 41:2j:33:GLN:HG2 | 41:2j:34:VAL:H | 1.74 | 0.51 |
| 42:2k:19:ALA:HA | 42:2k:32:ILE:HD13 | 1.92 | 0.51 |
| 1:1A:286:C:H2' | 1:1A:287:C:H6 | 1.75 | 0.51 |
| 1:1A:573:G:O2' | 1:1A:574:C:H3' | 2.09 | 0.51 |
| 1:1A:1028:A:N6 | 1:1A:1125:G:H2' | 2.24 | 0.51 |
| 10:1O:26:LYS:O | 10:1O:30:ALA:HB2 | 2.09 | 0.51 |
| 32:1a:841:U:OP2 | 32:1a:841:U:H6 | 1.92 | 0.51 |
| 37:1f:100:ASN:HB2 | 49:1r:28:GLU:HA | 1.92 | 0.51 |
| 1:2A:176:G:O2' | 1:2A:177:G:H5' | 2.10 | 0.51 |
| 1:2A:1506:C:H2' | 1:2A:1507:A:H5' | 1.92 | 0.51 |
| 1:2A:2495:G:OP1 | 12:2Q:82:ARG:NE | 2.37 | 0.51 |
| 6:2G:101:ILE:HG22 | 6:2G:105:LYS:HE2 | 1.92 | 0.51 |
| 15:2T:74:ARG:HH11 | 15:2T:74:ARG:HG3 | 1.75 | 0.51 |
| 32:2a:148:G:H2' | 32:2a:149:A:C8 | 2.45 | 0.51 |
| 36:2e:103:GLY:O | 36:2e:106:PRO:HD2 | 2.09 | 0.51 |
| 1:1A:284:U:H2' | 1:1A:285:C:H6 | 1.75 | 0.51 |
| 5:1F:32:LEU:HB3 | 5:1F:112:MET:HE1 | 1.92 | 0.51 |
| 32:1a:1216:G:H5'' | 45:1n:5:ALA:HB2 | 1.92 | 0.51 |
| 35:1d:178:VAL:C | 35:1d:180:GLY:H | 2.18 | 0.51 |
| 39:1h:41:ARG:NH2 | 39:1h:123:GLU:OE2 | 2.43 | 0.51 |
| 48:1q:43:LEU:HD12 | 48:1q:68:ARG:HB3 | 1.90 | 0.51 |
| 54:1w:47:U:H5'' | 54:1w:48:C:H5' | 1.93 | 0.51 |
| 56:1y:19:G:C2 | 56:1y:56:C:N3 | 2.78 | 0.51 |
| 56:1y:47:U:H2' | 56:1y:50:U:OP1 | 2.11 | 0.51 |
| 56:1y:56:C:H2' | 56:1y:57:G:H8 | 1.75 | 0.51 |
| 1:2A:1493:C:N4 | 1:2A:2206:G:O2' | 2.37 | 0.51 |
| 1:2A:2135:A:C8 | 1:2A:2136:C:H5 | 2.28 | 0.51 |
| 6:2G:44:GLY:C | 6:2G:46:ALA:H | 2.16 | 0.51 |
| 8:2I:129:THR:HA | 8:2I:138:ILE:O | 2.10 | 0.51 |
| 20:2Y:2:ARG:NH2 | 20:2Y:4:LYS:HD3 | 2.25 | 0.51 |
| 20:2Y:6:HIS:H | 20:2Y:6:HIS:CD2 | 2.28 | 0.51 |
| 26:24:45:GLY:C | 26:24:47:GLN:N | 2.69 | 0.51 |
| 26:24:57:GLU:HA | 26:24:60:GLN:HB2 | 1.93 | 0.51 |
| 32:2a:624:C:H2' | 32:2a:625:G:C8 | 2.44 | 0.51 |
| 32:2a:1152:A:H5' | 41:2j:70:ARG:HH22 | 1.75 | 0.51 |
| 32:2a:1446:U:O4 | 62:2a:1913:HOH:O | 2.19 | 0.51 |
| 36:2e:18:ARG:NH2 | 36:2e:25:ARG:HG2 | 2.25 | 0.51 |
| 1:1A:292:C:H2' | 1:1A:293:U:H6 | 1.76 | 0.51 |
| 7:1H:101:ARG:NH2 | 7:1H:121:ILE:O | 2.44 | 0.51 |
| 32:1a:990:C:O2' | 32:1a:991:U:H5' | 2.11 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 51:1t:40:ALA:HB2 | 51:1t:55:ILE:HG22 | 1.92 | 0.51 |
| 8:2I:75:LEU:HD13 | 8:2I:105:HIS:NE2 | 2.26 | 0.51 |
| 20:2Y:19:LYS:HD3 | 20:2Y:20:TYR:CE2 | 2.45 | 0.51 |
| 32:2a:1070:U:H2' | 32:2a:1071:C:H6 | 1.75 | 0.51 |
| 33:2b:48:MET:HG3 | 33:2b:49:GLU:N | 2.26 | 0.51 |
| 35:2d:180:GLY:HA3 | 35:2d:182:LYS:HD2 | 1.92 | 0.51 |
| 44:2m:13:LYS:HA | 44:2m:44:ARG:NH1 | 2.11 | 0.51 |
| 1:1A:2319:G:H22 | 14:1S:3:ARG:HD3 | 1.74 | 0.51 |
| 4:1E:116:VAL:HG13 | 4:1E:122:PHE:HB2 | 1.92 | 0.51 |
| 21:1Z:92:SER:O | 21:1Z:130:PRO:HG2 | 2.11 | 0.51 |
| 32:1a:560:U:O2' | 32:1a:561:U:OP2 | 2.24 | 0.51 |
| 32:1a:1179:A:O3' | 40:1i:103:THR:HB | 2.11 | 0.51 |
| 32:1a:1302:U:C5 | 44:1m:17:VAL:HG21 | 2.45 | 0.51 |
| 35:1d:108:LEU:HD21 | 35:1d:174:LEU:HD22 | 1.92 | 0.51 |
| 1:2A:350:U:H2' | 1:2A:351:G:O4' | 2.10 | 0.51 |
| 1:2A:2134:A:N6 | 1:2A:2157:G:H4' | 2.18 | 0.51 |
| 1:2A:2748:A:H5' | 7:2H:4:ILE:HD12 | 1.92 | 0.51 |
| 2:2B:3:C:H2' | 2:2B:4:C:C6 | 2.45 | 0.51 |
| 14:2S:87:PHE:CE1 | 14:2S:102:ALA:HB2 | 2.45 | 0.51 |
| 32:2a:112:G:O2' | 32:2a:354:G:O2' | 2.21 | 0.51 |
| 32:2a:1004:A:H61 | 32:2a:1037:C:H1' | 1.75 | 0.51 |
| 32:2a:1118:C:H1' | 32:2a:1179:A:C4 | 2.44 | 0.51 |
| 41:2j:49:VAL:CG2 | 45:2n:41:ARG:HB2 | 2.38 | 0.51 |
| 1:1A:192:C:OP1 | 62:1A:4237:HOH:O | 2.18 | 0.51 |
| 1:1A:1075:C:C2 | 1:1A:1076:C:H2' | 2.45 | 0.51 |
| 1:1A:2136:C:N3 | 1:1A:2155:G:C2 | 2.79 | 0.51 |
| 11:1P:82:GLY:HA2 | 11:1P:113:LYS:O | 2.11 | 0.51 |
| 36:1e:144:THR:H | 36:1e:147:ASP:HB2 | 1.74 | 0.51 |
| 43:1l:42:THR:HG22 | 43:1l:54:LYS:HD2 | 1.93 | 0.51 |
| 1:2A:748:G:C8 | 18:2W:89:ALA:HB1 | 2.46 | 0.51 |
| 2:2B:94:C:H2' | 2:2B:95:C:H6 | 1.74 | 0.51 |
| 14:2S:7:TYR:O | 14:2S:11:LYS:HG3 | 2.10 | 0.51 |
| 32:2a:165:C:H2' | 32:2a:166:G:C8 | 2.43 | 0.51 |
| 32:2a:299:G:H2' | 32:2a:300:A:C8 | 2.46 | 0.51 |
| 32:2a:921:U:O2 | 36:2e:19:MET:HB2 | 2.10 | 0.51 |
| 32:2a:977:A:O2' | 32:2a:981:U:N3 | 2.35 | 0.51 |
| 38:2g:137:LYS:O | 38:2g:141:VAL:HG23 | 2.11 | 0.51 |
| 1:1A:2474:C:H5'' | 1:1A:2475:C:OP2 | 2.10 | 0.51 |
| 32:1a:486:U:H2' | 32:1a:487:A:H8 | 1.76 | 0.51 |
| 32:1a:1027:C:N3 | 32:1a:1034:G:C2 | 2.79 | 0.51 |
| 32:1a:1391:U:H2' | 32:1a:1392:G:C8 | 2.46 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 37:1f:4:TYR:CD1 | 37:1f:92:LYS:HA | 2.46 | 0.51 |
| 42:1k:59:TYR:CZ | 42:1k:63:LEU:HD11 | 2.46 | 0.51 |
| 1:2A:301:G:N7 | 62:2A:4005:HOH:O | 2.34 | 0.51 |
| 1:2A:1469:A:H2' | 1:2A:1470:G:O4' | 2.11 | 0.51 |
| 1:2A:1740:G:H2' | 1:2A:1741:A:C8 | 2.46 | 0.51 |
| 1:2A:1794:U:H2' | 1:2A:1795:C:C6 | 2.46 | 0.51 |
| 32:2a:403:C:O2' | 35:2d:122:ARG:NH2 | 2.44 | 0.51 |
| 32:2a:976:G:H5' | 32:2a:1358:U:O2' | 2.11 | 0.51 |
| 32:2a:1060:C:H5 | 34:2c:2:GLY:HA3 | 1.76 | 0.51 |
| 33:2b:162:ILE:HD11 | 33:2b:177:ALA:CB | 2.40 | 0.51 |
| 42:2k:67:ASP:O | 42:2k:71:LYS:HG3 | 2.10 | 0.51 |
| 1:1A:887:A:C2 | 1:1A:890:A:C8 | 2.99 | 0.51 |
| 1:1A:1038:C:H42 | 1:1A:1117:G:H1 | 1.58 | 0.51 |
| 1:1A:2135:A:H2' | 1:1A:2135:A:N3 | 2.26 | 0.51 |
| 4:1E:56:PRO:HG3 | 4:1E:74:PRO:HG2 | 1.92 | 0.51 |
| 32:1a:179:A:H2' | 32:1a:180:U:C6 | 2.45 | 0.51 |
| 32:1a:198:G:H2' | 32:1a:199:G:C8 | 2.46 | 0.51 |
| 32:1a:738:C:H2' | 32:1a:739:C:C6 | 2.45 | 0.51 |
| 32:1a:760:G:O2' | 48:1q:98:LEU:HD23 | 2.11 | 0.51 |
| 32:1a:1038:C:H2' | 32:1a:1039:C:H6 | 1.75 | 0.51 |
| 42:1k:99:GLN:HG3 | 42:1k:105:VAL:HG21 | 1.93 | 0.51 |
| 52:1u:9:ARG:HG3 | 52:1u:21:TYR:O | 2.11 | 0.51 |
| 1:2A:686:G:C2 | 29:27:11:LYS:HE3 | 2.45 | 0.51 |
| 6:2G:149:VAL:HG22 | 6:2G:150:ASP:H | 1.76 | 0.51 |
| 9:2N:96:GLU:CD | 9:2N:96:GLU:H | 2.19 | 0.51 |
| 32:2a:155:C:H2' | 32:2a:156:G:O4' | 2.11 | 0.51 |
| 32:2a:554:C:H2' | 32:2a:555:C:H6 | 1.75 | 0.51 |
| 32:2a:979:C:OP1 | 32:2a:1223:C:N4 | 2.43 | 0.51 |
| 32:2a:1368:G:OP1 | 40:2i:111:ARG:NH2 | 2.43 | 0.51 |
| 34:2c:70:VAL:HG12 | 34:2c:72:LYS:H | 1.74 | 0.51 |
| 46:2o:3:ILE:HG21 | 46:2o:34:LEU:HD21 | 1.92 | 0.51 |
| 1:1A:1651:G:N2 | 1:1A:2007:C:C2 | 2.79 | 0.51 |
| 32:1a:820:U:H4' | 32:1a:821:G:OP2 | 2.10 | 0.51 |
| 34:1c:177:THR:HG22 | 34:1c:180:ALA:H | 1.76 | 0.51 |
| 42:1k:24:SER:O | 42:1k:88:GLY:HA3 | 2.11 | 0.51 |
| 1:2A:1641:A:H2' | 1:2A:1642:G:O4' | 2.10 | 0.51 |
| 1:2A:2276:G:C2' | 1:2A:2277:G:H5' | 2.41 | 0.51 |
| 1:2A:2886:G:H2' | 1:2A:2887:U:H6 | 1.76 | 0.51 |
| 1:2A:2888:C:H2' | 1:2A:2889:C:C6 | 2.46 | 0.51 |
| 18:2W:88:ARG:NH1 | 18:2W:94:ASP:OD2 | 2.44 | 0.51 |
| 32:2a:586:C:H42 | 32:2a:755:G:H1 | 1.59 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 36:2e:71:LEU:C | 36:2e:72:GLN:HE21 | 2.18 | 0.51 |
| 1:1A:2101:G:H2' | 1:1A:2102:U:C6 | 2.46 | 0.51 |
| 1:1A:2557:G:H2' | 1:1A:2558:C:C6 | 2.46 | 0.51 |
| 6:1G:114:ILE:HG13 | 6:1G:140:ILE:HG12 | 1.92 | 0.51 |
| 7:1H:56:SER:OG | 7:1H:57:ASP:N | 2.42 | 0.51 |
| 17:1V:1:MET:HE2 | 17:1V:43:GLU:H | 1.75 | 0.51 |
| 32:1a:232:G:H1' | 32:1a:262:A:N1 | 2.26 | 0.51 |
| 33:1b:223:ILE:HA | 33:1b:226:ARG:HG2 | 1.93 | 0.51 |
| 38:1g:12:LEU:HD22 | 38:1g:24:THR:HG22 | 1.93 | 0.51 |
| 50:1s:24:ALA:O | 50:1s:26:GLY:N | 2.37 | 0.51 |
| 1:2A:467:G:OP1 | 29:27:33:ARG:HD2 | 2.11 | 0.51 |
| 1:2A:1239:G:H2' | 1:2A:1240:U:O4' | 2.11 | 0.51 |
| 1:2A:1885:A:H2' | 1:2A:1886:C:O4' | 2.11 | 0.51 |
| 1:2A:2572:A:C8 | 4:2E:144:ARG:HD3 | 2.46 | 0.51 |
| 11:2P:38:GLN:O | 11:2P:39:LYS:CB | 2.58 | 0.51 |
| 25:23:23:LEU:HD12 | 25:23:50:VAL:HG21 | 1.93 | 0.51 |
| 28:26:25:LYS:HE2 | 28:26:51:GLU:OE1 | 2.11 | 0.51 |
| 32:2a:973:G:H3' | 32:2a:974:A:H5'' | 1.91 | 0.51 |
| 32:2a:976:G:OP2 | 32:2a:1358:U:O2' | 2.24 | 0.51 |
| 37:2f:19:LEU:HD23 | 37:2f:19:LEU:O | 2.11 | 0.51 |
| 1:1A:579:G:H2' | 1:1A:580:C:C6 | 2.46 | 0.50 |
| 1:1A:1688:U:O2 | 1:1A:1700:A:H5' | 2.11 | 0.50 |
| 5:1F:152:GLU:OE1 | 5:1F:191:ARG:HD2 | 2.11 | 0.50 |
| 21:1Z:158:PRO:HB2 | 21:1Z:159:PRO:CD | 2.40 | 0.50 |
| 32:1a:489:C:H2' | 32:1a:490:G:H8 | 1.75 | 0.50 |
| 34:1c:6:HIS:HD2 | 34:1c:8:ILE:N | 2.01 | 0.50 |
| 51:1t:64:ASP:OD2 | 51:1t:81:LYS:NZ | 2.39 | 0.50 |
| 1:2A:271(H):G:H5' | 23:21:81:LYS:HD3 | 1.93 | 0.50 |
| 1:2A:272(G):C:H42 | 1:2A:363(C):G:H1 | 1.57 | 0.50 |
| 1:2A:784:A:C6 | 3:2D:229:VAL:HG11 | 2.46 | 0.50 |
| 1:2A:2131:G:N2 | 1:2A:2131:G:OP2 | 2.41 | 0.50 |
| 3:2D:148:GLU:HB2 | 3:2D:151:LYS:HD2 | 1.93 | 0.50 |
| 5:2F:133:ASN:N | 5:2F:138:GLU:OE1 | 2.44 | 0.50 |
| 7:2H:9:ILE:N | 7:2H:50:VAL:O | 2.36 | 0.50 |
| 10:2O:16:ALA:HB2 | 10:2O:52:VAL:HG21 | 1.92 | 0.50 |
| 13:2R:28:LEU:HD23 | 13:2R:48:VAL:HG21 | 1.93 | 0.50 |
| 19:2X:1:MET:N | 24:22:29:LYS:HE3 | 2.26 | 0.50 |
| 21:2Z:99:TYR:CE1 | 21:2Z:125:LEU:HB2 | 2.46 | 0.50 |
| 32:2a:461:A:O2' | 32:2a:470:C:H5' | 2.10 | 0.50 |
| 32:2a:944:G:OP1 | 62:2a:1914:HOH:O | 2.19 | 0.50 |
| 32:2a:955:U:O2' | 50:2s:83:HIS:HD2 | 1.94 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 32:2a:967:5MC:H2' | 32:2a:968:A:C8 | 2.46 | 0.50 |
| 32:2a:1239:A:H62 | 32:2a:1299:A:H62 | 1.59 | 0.50 |
| 33:2b:78:GLN:HE22 | 33:2b:95:GLN:HE22 | 1.57 | 0.50 |
| 38:2g:108:ALA:HA | 38:2g:111:ARG:HD2 | 1.92 | 0.50 |
| 1:1A:784:A:C6 | 3:1D:229:VAL:HG11 | 2.47 | 0.50 |
| 1:1A:1041:C:N4 | 1:1A:1114:G:H1 | 2.07 | 0.50 |
| 1:1A:2751:G:H4' | 7:1H:4:ILE:HD11 | 1.93 | 0.50 |
| 16:1U:76:TYR:CE2 | 16:1U:80:ILE:HG13 | 2.46 | 0.50 |
| 24:12:22:GLU:OE2 | 24:12:68:ARG:NH2 | 2.43 | 0.50 |
| 32:1a:977:A:C8 | 32:1a:1223:C:N3 | 2.79 | 0.50 |
| 33:1b:174:VAL:O | 33:1b:178:ARG:HG2 | 2.11 | 0.50 |
| 1:2A:298:G:H5'' | 1:2A:299:A:OP1 | 2.11 | 0.50 |
| 1:2A:307:G:N2 | 1:2A:310:A:O5' | 2.42 | 0.50 |
| 1:2A:1495:A:H2' | 1:2A:1496:A:H8 | 1.76 | 0.50 |
| 1:2A:2330:G:O2' | 22:20:41:ARG:O | 2.26 | 0.50 |
| 1:2A:2432:A:C6 | 1:2A:2433:A:C6 | 3.00 | 0.50 |
| 23:21:19:GLN:O | 23:21:35:THR:HG22 | 2.11 | 0.50 |
| 35:2d:176:LEU:HD12 | 35:2d:182:LYS:O | 2.11 | 0.50 |
| 53:2v:16:A:H2' | 53:2v:17:U:O4' | 2.11 | 0.50 |
| 54:2w:63:G:H2' | 54:2w:64:A:H8 | 1.76 | 0.50 |
| 1:1A:305:U:H2' | 1:1A:306:U:C6 | 2.46 | 0.50 |
| 1:1A:800:A:N7 | 62:1A:4326:HOH:O | 2.35 | 0.50 |
| 32:1a:690:G:C6 | 32:1a:691:G:C6 | 3.00 | 0.50 |
| 32:1a:1291:G:O2' | 40:1i:38:GLN:OE1 | 2.23 | 0.50 |
| 33:1b:16:HIS:C | 33:1b:18:GLY:H | 2.20 | 0.50 |
| 35:1d:149:ALA:HB3 | 35:1d:152:SER:HB2 | 1.92 | 0.50 |
| 1:2A:1477:A:H2' | 1:2A:1478:G:O4' | 2.12 | 0.50 |
| 1:2A:1996:C:H4' | 1:2A:1997:G:OP1 | 2.10 | 0.50 |
| 1:2A:2473:U:H2' | 1:2A:2474:C:H6 | 1.74 | 0.50 |
| 26:24:62:ARG:HB2 | 26:24:63:TYR:CE2 | 2.45 | 0.50 |
| 32:2a:1299:A:H2' | 32:2a:1299:A:N3 | 2.26 | 0.50 |
| 33:2b:13:ALA:C | 33:2b:15:VAL:H | 2.19 | 0.50 |
| 1:1A:864:G:O2' | 1:1A:865:C:H5' | 2.11 | 0.50 |
| 1:1A:1021:A:OP2 | 9:1N:65:LYS:NZ | 2.45 | 0.50 |
| 1:1A:1062:G:C5' | 1:1A:1070:A:HO2' | 2.25 | 0.50 |
| 3:1D:275:LYS:HG3 | 3:1D:276:LYS:H | 1.76 | 0.50 |
| 21:1Z:4:ARG:NH2 | 21:1Z:60:GLU:OE2 | 2.43 | 0.50 |
| 42:1k:66:LEU:HG | 42:1k:97:ALA:HB1 | 1.92 | 0.50 |
| 1:2A:236:C:H2' | 1:2A:237:C:C6 | 2.46 | 0.50 |
| 1:2A:304:G:H1 | 1:2A:313:C:H42 | 1.60 | 0.50 |
| 1:2A:1777:U:O2' | 1:2A:1778:U:H5' | 2.11 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:2A:1796:U:H2' | 1:2A:1797:C:C6 | 2.46 | 0.50 |
| 1:2A:2880:C:O3' | 13:2R:90:ARG:NH1 | 2.45 | 0.50 |
| 6:2G:142:PRO:O | 26:24:31:ILE:HD12 | 2.10 | 0.50 |
| 9:2N:67:LEU:C | 9:2N:88:GLU:HG3 | 2.36 | 0.50 |
| 10:2O:15:GLY:O | 10:2O:47:ILE:HG12 | 2.10 | 0.50 |
| 32:2a:109:A:H2' | 32:2a:326:G:N2 | 2.26 | 0.50 |
| 32:2a:300:A:H1' | 32:2a:565:U:O2 | 2.12 | 0.50 |
| 40:2i:26:VAL:HG22 | 40:2i:61:ALA:HB3 | 1.92 | 0.50 |
| 55:2x:53:G:C8 | 55:2x:54:5MU:H72 | 2.47 | 0.50 |
| 1:1A:848:G:O6 | 1:1A:928:G:H2' | 2.12 | 0.50 |
| 1:1A:2139:C:H2' | 1:1A:2140:C:O4' | 2.11 | 0.50 |
| 6:1G:47:LYS:HG3 | 6:1G:48:GLU:H | 1.75 | 0.50 |
| 7:1H:6:ARG:HH22 | 7:1H:54:ARG:HH22 | 1.58 | 0.50 |
| 15:1T:105:LEU:HD22 | 15:1T:109:GLU:HB3 | 1.94 | 0.50 |
| 26:14:61:ARG:HD3 | 50:1s:42:PRO:HG3 | 1.92 | 0.50 |
| 32:1a:4:U:C4 | 39:1h:105:ARG:HD3 | 2.47 | 0.50 |
| 34:1c:36:ASP:O | 34:1c:40:ARG:HG3 | 2.11 | 0.50 |
| 36:1e:75:THR:HG23 | 36:1e:76:ILE:O | 2.12 | 0.50 |
| 41:1j:81:THR:C | 41:1j:83:GLU:N | 2.69 | 0.50 |
| 1:2A:1410:G:H2' | 1:2A:1411:C:C6 | 2.46 | 0.50 |
| 1:2A:2022:U:O2' | 1:2A:2617:C:H5' | 2.12 | 0.50 |
| 1:2A:2655:G:O2' | 1:2A:2664:G:O6 | 2.28 | 0.50 |
| 12:2Q:57:HIS:CD2 | 12:2Q:117:ALA:HB2 | 2.46 | 0.50 |
| 25:23:44:ARG:O | 25:23:48:GLU:HG3 | 2.10 | 0.50 |
| 32:2a:242:C:H2' | 32:2a:243:A:H5' | 1.94 | 0.50 |
| 43:2l:34:ARG:HG3 | 43:2l:105:TYR:CE2 | 2.46 | 0.50 |
| 49:2r:58:LEU:HB3 | 49:2r:62:GLU:HB2 | 1.93 | 0.50 |
| 50:2s:80:TYR:O | 50:2s:82:GLY:N | 2.38 | 0.50 |
| 1:1A:467:G:OP1 | 29:17:33:ARG:NH1 | 2.44 | 0.50 |
| 1:1A:1815:A:P | 3:1D:54:ARG:HH22 | 2.34 | 0.50 |
| 32:1a:1118:C:H1' | 32:1a:1179:A:C4 | 2.46 | 0.50 |
| 32:1a:1457:G:OP1 | 51:1t:39:LYS:NZ | 2.38 | 0.50 |
| 43:1l:39:VAL:HG11 | 43:1l:41:ARG:HH11 | 1.76 | 0.50 |
| 44:1m:2:ALA:N | 44:1m:8:GLU:OE1 | 2.45 | 0.50 |
| 1:2A:375:C:H2' | 1:2A:376:C:H6 | 1.75 | 0.50 |
| 1:2A:731:C:OP1 | 62:2A:3952:HOH:O | 2.20 | 0.50 |
| 1:2A:854:G:O6 | 62:2A:3951:HOH:O | 2.19 | 0.50 |
| 1:2A:879:G:C6 | 1:2A:880:G:C2 | 2.99 | 0.50 |
| 1:2A:1359:A:H2 | 1:2A:1372:U:O4 | 1.94 | 0.50 |
| 1:2A:2564:A:C2 | 1:2A:2647:U:H4' | 2.47 | 0.50 |
| 32:2a:1298:C:C4 | 38:2g:114:ARG:HD3 | 2.47 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|----------------------|--------------------------|-------------------|
| 33:2b:16:HIS:CG | 33:2b:17:PHE:N | 2.79 | 0.50 |
| 1:1A:570:G:H2' | 1:1A:2030:A:N7 | 2.27 | 0.50 |
| 8:1I:31:LEU:HD21 | 8:1I:38:LEU:HD22 | 1.94 | 0.50 |
| 17:1V:98:GLU:OE2 | 17:1V:100:ARG:NH1 | 2.45 | 0.50 |
| 32:1a:1004:A:N6 | 32:1a:1036:G:N2 | 2.59 | 0.50 |
| 35:1d:173:TRP:CZ3 | 35:1d:174:LEU:HG | 2.47 | 0.50 |
| 50:1s:11:VAL:HG11 | 50:1s:16:LEU:HB2 | 1.92 | 0.50 |
| 50:1s:69:HIS:HB3 | 50:1s:73:GLU:CD | 2.37 | 0.50 |
| 51:1t:56:MET:HE3 | 51:1t:85:MET:HE2 | 1.93 | 0.50 |
| 1:2A:2727:G:O2' | 10:2O:70:LYS:NZ | 2.44 | 0.50 |
| 4:2E:8:LYS:HD2 | 4:2E:188:VAL:HG12 | 1.93 | 0.50 |
| 32:2a:176:C:H2' | 32:2a:177:C:C6 | 2.47 | 0.50 |
| 32:2a:1206:G:O2' | 34:2c:193:TYR:HA | 2.11 | 0.50 |
| 40:2i:4:TYR:CE1 | 40:2i:88:TYR:HA | 2.46 | 0.50 |
| 1:1A:673:C:OP1 | 5:1F:54:ARG:NH1 | 2.43 | 0.50 |
| 1:1A:1272:A:OP2 | 62:1A:4208:HOH:O | 2.20 | 0.50 |
| 1:1A:1420:U:HO2' | 1:1A:1421:G:P | 2.35 | 0.50 |
| 1:1A:2262:U:OP1 | 1:1A:2387:U:O2' | 2.20 | 0.50 |
| 2:1B:29:A:H2' | 2:1B:30:C:O4' | 2.12 | 0.50 |
| 5:1F:33:LEU:HB3 | 11:1P:6:LEU:HD21 | 1.94 | 0.50 |
| 32:1a:92:C:H2' | 32:1a:93:G:C8 | 2.47 | 0.50 |
| 32:1a:1095:U:P | 32:1a:1108:G:H1 | 2.35 | 0.50 |
| 50:1s:52:TYR:HA | 50:1s:56:GLN:O | 2.11 | 0.50 |
| 1:2A:910:A:N1 | 1:2A:2277:G:H1' | 2.27 | 0.50 |
| 1:2A:2839:G:H5' | 13:2R:46:GLY:CA | 2.38 | 0.50 |
| 7:2H:59:ARG:O | 7:2H:63:SER:OG | 2.30 | 0.50 |
| 26:24:46:GLN:C | 26:24:48:ARG:N | 2.66 | 0.50 |
| 32:2a:1145:C:H4' | 32:2a:1146:A:H8 | 1.77 | 0.50 |
| 32:2a:1256:A:OP1 | 34:2c:26:LYS:NZ | 2.32 | 0.50 |
| 32:2a:1509:C:H2' | 32:2a:1510:U:O4' | 2.12 | 0.50 |
| 33:2b:96:ARG:HG2 | 33:2b:98:LEU:HD23 | 1.94 | 0.50 |
| 41:2j:62:HIS:HB3 | 45:2n:59:ALA:HB3 | 1.93 | 0.50 |
| 48:2q:67:LYS:O | 48:2q:68:ARG:HB2 | 2.11 | 0.50 |
| 1:1A:2100:G:O2' | 1:1A:2101:G:H5' | 2.12 | 0.50 |
| 32:1a:13:U:O2' | 62:1a:1909:HOH:O | 2.05 | 0.50 |
| 32:1a:527:G7M:HN71 | 43:1l:92:0TD:H3 | 1.94 | 0.50 |
| 32:1a:535:A:H5'' | 62:1a:1930:HOH:O | 2.11 | 0.50 |
| 32:1a:1030:C:H3' | 32:1a:1030(A):G:H5'' | 1.94 | 0.50 |
| 32:1a:1126:U:O2 | 32:1a:1280:A:H2' | 2.12 | 0.50 |
| 33:1b:105:PHE:O | 33:1b:107:THR:N | 2.44 | 0.50 |
| 41:1j:81:THR:HG22 | 41:1j:85:LEU:HG | 1.94 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:2A:284:U:H2' | 1:2A:285:C:C6 | 2.47 | 0.50 |
| 1:2A:811:U:H2' | 11:2P:21:ARG:HA | 1.94 | 0.50 |
| 1:2A:893:C:H2' | 1:2A:894:C:C4 | 2.47 | 0.50 |
| 1:2A:956:G:N2 | 1:2A:959:A:H3' | 2.27 | 0.50 |
| 1:2A:1204:A:N6 | 1:2A:1240:U:H2' | 2.27 | 0.50 |
| 5:2F:135:LYS:HB2 | 5:2F:138:GLU:HG3 | 1.94 | 0.50 |
| 11:2P:63:PRO:HG2 | 30:28:25:MET:HB2 | 1.94 | 0.50 |
| 23:21:50:ARG:HG2 | 23:21:59:THR:CG2 | 2.39 | 0.50 |
| 32:2a:1027:C:C2 | 32:2a:1034:G:N1 | 2.79 | 0.50 |
| 37:2f:96:PRO:HB3 | 49:2r:30:ASP:OD2 | 2.11 | 0.50 |
| 56:2y:18:G:H4' | 56:2y:60:U:H5 | 1.77 | 0.50 |
| 1:1A:1607:C:H4' | 1:1A:1608:A:O5' | 2.11 | 0.49 |
| 1:1A:2406:U:H2' | 1:1A:2406:U:OP2 | 2.12 | 0.49 |
| 1:1A:2492:U:H2' | 1:1A:2493:U:C6 | 2.47 | 0.49 |
| 2:1B:88:C:H2' | 2:1B:89:G:O4' | 2.12 | 0.49 |
| 6:1G:179:PRO:HG3 | 26:14:43:TYR:CZ | 2.47 | 0.49 |
| 7:1H:73:ALA:HA | 7:1H:76:VAL:HG22 | 1.94 | 0.49 |
| 32:1a:78:G:HO2' | 32:1a:79:G:H8 | 1.58 | 0.49 |
| 33:1b:54:THR:HG21 | 33:1b:201:ILE:HD11 | 1.93 | 0.49 |
| 48:1q:67:LYS:O | 48:1q:68:ARG:HB2 | 2.12 | 0.49 |
| 1:2A:11:G:C2' | 1:2A:12:U:H5' | 2.42 | 0.49 |
| 1:2A:307:G:H22 | 1:2A:310:A:P | 2.34 | 0.49 |
| 1:2A:361:G:O2' | 1:2A:362:U:H5' | 2.11 | 0.49 |
| 1:2A:2322:A:H2' | 1:2A:2323:G:O4' | 2.12 | 0.49 |
| 1:2A:2461:C:H2' | 1:2A:2462:U:C6 | 2.47 | 0.49 |
| 2:2B:8:U:H3 | 2:2B:113:G:H1 | 1.59 | 0.49 |
| 8:2I:76:THR:HG22 | 8:2I:141:LYS:CB | 2.42 | 0.49 |
| 26:24:58:ARG:HD2 | 50:2s:68:GLY:N | 2.27 | 0.49 |
| 26:24:60:GLN:O | 26:24:62:ARG:HG2 | 2.12 | 0.49 |
| 1:1A:1798:U:H5' | 3:1D:259:THR:CG2 | 2.26 | 0.49 |
| 1:1A:2314:C:H2' | 1:1A:2315:G:H8 | 1.77 | 0.49 |
| 1:1A:2464:C:H1' | 62:1A:5616:HOH:O | 2.11 | 0.49 |
| 6:1G:16:ARG:O | 6:1G:20:ILE:HG13 | 2.12 | 0.49 |
| 32:1a:342:C:H2' | 32:1a:343:U:C6 | 2.47 | 0.49 |
| 32:1a:342:C:H2' | 32:1a:343:U:O4' | 2.12 | 0.49 |
| 33:1b:44:LEU:H | 33:1b:44:LEU:HD12 | 1.78 | 0.49 |
| 46:1o:54:ARG:HG2 | 46:1o:58:MET:HE2 | 1.94 | 0.49 |
| 56:1y:19:G:C6 | 56:1y:56:C:N4 | 2.80 | 0.49 |
| 1:2A:1027:A:C2 | 1:2A:2488:A:H5' | 2.47 | 0.49 |
| 1:2A:2557:G:H2' | 1:2A:2558:C:H6 | 1.75 | 0.49 |
| 1:2A:2818:G:OP2 | 13:2R:42:LYS:NZ | 2.45 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:2F:192:LEU:HD13 | 5:2F:194:MET:HE2 | 1.94 | 0.49 |
| 32:2a:1004:A:N3 | 32:2a:1038:C:C2 | 2.80 | 0.49 |
| 32:2a:1263:C:H2' | 32:2a:1264:C:C6 | 2.46 | 0.49 |
| 32:2a:1296:C:H4' | 32:2a:1302:U:C5 | 2.47 | 0.49 |
| 32:2a:1456:G:O2' | 51:2t:39:LYS:HE3 | 2.12 | 0.49 |
| 42:2k:18:ARG:NH2 | 42:2k:35:PRO:O | 2.38 | 0.49 |
| 1:1A:483:A:O2' | 20:1Y:49:VAL:O | 2.24 | 0.49 |
| 1:1A:1062:G:H22 | 1:1A:1077:A:N6 | 2.09 | 0.49 |
| 19:1X:54:VAL:HG22 | 19:1X:81:VAL:HG12 | 1.94 | 0.49 |
| 32:1a:922:G:H4' | 36:1e:20:GLN:HA | 1.94 | 0.49 |
| 47:1p:49:LEU:HD12 | 47:1p:50:LYS:H | 1.77 | 0.49 |
| 1:2A:100:G:O2' | 24:22:7:ARG:NH2 | 2.44 | 0.49 |
| 1:2A:994:C:O2' | 1:2A:996:A:OP1 | 2.26 | 0.49 |
| 1:2A:1539:G:H2' | 1:2A:1540:U:O4' | 2.11 | 0.49 |
| 2:2B:7:G:H21 | 14:2S:38:GLN:NE2 | 1.93 | 0.49 |
| 19:2X:31:HIS:HD2 | 19:2X:33:LYS:H | 1.59 | 0.49 |
| 32:2a:273:A:N7 | 62:2a:1929:HOH:O | 2.35 | 0.49 |
| 32:2a:1153:C:C4 | 32:2a:1154:G:N7 | 2.80 | 0.49 |
| 51:2t:10:LEU:HG | 51:2t:12:ALA:H | 1.78 | 0.49 |
| 1:1A:1588:C:H2' | 1:1A:1589:C:C6 | 2.48 | 0.49 |
| 8:1I:69:LYS:HA | 8:1I:138:ILE:HG12 | 1.94 | 0.49 |
| 9:1N:13:TRP:CE2 | 9:1N:133:GLN:HG2 | 2.47 | 0.49 |
| 23:11:19:GLN:O | 23:11:35:THR:HG22 | 2.12 | 0.49 |
| 32:1a:149:A:H2' | 32:1a:150:C:H6 | 1.77 | 0.49 |
| 32:1a:189:G:C4 | 32:1a:189(L):G:N2 | 2.81 | 0.49 |
| 32:1a:636:U:H2' | 32:1a:637:G:H8 | 1.77 | 0.49 |
| 32:1a:1016:A:H2' | 32:1a:1017:G:O4' | 2.12 | 0.49 |
| 44:1m:87:TYR:O | 44:1m:91:ARG:HG2 | 2.13 | 0.49 |
| 54:1w:75:C:O3' | 54:1w:76:F3N:O5' | 2.30 | 0.49 |
| 1:2A:869:G:C4 | 1:2A:870:A:C8 | 3.01 | 0.49 |
| 1:2A:1489:U:O2' | 1:2A:1490:A:H8 | 1.95 | 0.49 |
| 1:2A:1889:A:H2' | 1:2A:1890:A:C8 | 2.47 | 0.49 |
| 21:2Z:145:GLU:N | 21:2Z:148:ASP:HB2 | 2.27 | 0.49 |
| 32:2a:1236:A:O2' | 32:2a:1304:G:H4' | 2.13 | 0.49 |
| 33:2b:212:GLN:NE2 | 33:2b:235:SER:HA | 2.27 | 0.49 |
| 38:2g:78:ARG:HG3 | 38:2g:156:TRP:HZ3 | 1.78 | 0.49 |
| 1:1A:284:U:H2' | 1:1A:285:C:C6 | 2.48 | 0.49 |
| 1:1A:996:A:OP2 | 16:1U:93:LYS:NZ | 2.39 | 0.49 |
| 32:1a:1239:A:H4' | 32:1a:1240:U:H5'' | 1.95 | 0.49 |
| 36:1e:95:ALA:HB1 | 36:1e:96:PRO:HD2 | 1.93 | 0.49 |
| 44:1m:126:LYS:HB2 | 44:1m:126:LYS:NZ | 2.26 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 1:2A:2118:U:OP2 | 1:2A:2147:G:O2' | 2.31 | 0.49 |
| 1:2A:2169:A:H2' | 1:2A:2170:A:C8 | 2.48 | 0.49 |
| 1:2A:2711:A:OP2 | 62:2A:3944:HOH:O | 2.20 | 0.49 |
| 7:2H:154:PRO:HB3 | 7:2H:163:TYR:CE1 | 2.48 | 0.49 |
| 15:2T:16:ARG:NH2 | 15:2T:18:ASP:OD2 | 2.46 | 0.49 |
| 32:2a:116:A:H8 | 32:2a:116:A:O5' | 1.96 | 0.49 |
| 32:2a:392:G:H2' | 32:2a:393:A:H8 | 1.76 | 0.49 |
| 32:2a:410:G:OP1 | 35:2d:30:LYS:NZ | 2.42 | 0.49 |
| 32:2a:975:A:H4' | 32:2a:976:G:H5'' | 1.94 | 0.49 |
| 32:2a:1367:C:O2' | 41:2j:62:HIS:HE1 | 1.94 | 0.49 |
| 35:2d:25:ARG:O | 35:2d:28:SER:HB3 | 2.12 | 0.49 |
| 36:2e:87:SER:HB3 | 36:2e:131:ILE:HD13 | 1.94 | 0.49 |
| 1:1A:292:C:H2' | 1:1A:293:U:C6 | 2.48 | 0.49 |
| 1:1A:652(T):C:H2' | 1:1A:652(U):G:O4' | 2.13 | 0.49 |
| 1:1A:890:A:C5 | 1:1A:892:G:H1' | 2.48 | 0.49 |
| 1:1A:1843:C:H5' | 3:1D:253:GLN:OE1 | 2.12 | 0.49 |
| 23:11:23:LYS:HB3 | 23:11:29:GLY:HA3 | 1.93 | 0.49 |
| 35:1d:70:ILE:HD11 | 35:1d:74:GLN:HB3 | 1.94 | 0.49 |
| 40:1i:17:VAL:HG11 | 40:1i:80:GLY:C | 2.37 | 0.49 |
| 42:1k:34:ASP:HB2 | 42:1k:35:PRO:HD2 | 1.94 | 0.49 |
| 42:1k:48:ILE:HD12 | 42:1k:63:LEU:CB | 2.42 | 0.49 |
| 1:2A:579:G:H2' | 1:2A:580:C:C6 | 2.48 | 0.49 |
| 1:2A:1889:A:N1 | 1:2A:2234:G:H1' | 2.28 | 0.49 |
| 4:2E:143:ASN:HB2 | 4:2E:147:PRO:HD2 | 1.93 | 0.49 |
| 5:2F:10:PRO:HB3 | 5:2F:17:ARG:NH1 | 2.26 | 0.49 |
| 8:2I:81:VAL:HG21 | 8:2I:88:ILE:HD13 | 1.95 | 0.49 |
| 8:2I:92:VAL:CG1 | 8:2I:120:ILE:HB | 2.41 | 0.49 |
| 32:2a:792:A:H4' | 32:2a:793:U:H5'' | 1.93 | 0.49 |
| 32:2a:1004:A:N1 | 32:2a:1037:C:H1' | 2.28 | 0.49 |
| 32:2a:1111:A:N1 | 34:2c:177:THR:OG1 | 2.30 | 0.49 |
| 32:2a:1265:G:C4 | 32:2a:1271:G:N2 | 2.81 | 0.49 |
| 32:2a:1517:G:N7 | 32:2a:1518:MA6:H103 | 2.27 | 0.49 |
| 41:2j:81:THR:C | 41:2j:83:GLU:H | 2.18 | 0.49 |
| 56:2y:68:C:C4 | 56:2y:69:G:C8 | 3.01 | 0.49 |
| 1:1A:583:G:OP2 | 16:1U:10:ARG:HD2 | 2.12 | 0.49 |
| 1:1A:1057:A:N6 | 1:1A:1087:G:OP1 | 2.46 | 0.49 |
| 1:1A:2104:G:H2' | 1:1A:2105:C:C6 | 2.48 | 0.49 |
| 1:1A:2107:C:H42 | 1:1A:2182:G:H1 | 1.61 | 0.49 |
| 1:1A:2153:G:H2' | 1:1A:2154:G:C8 | 2.48 | 0.49 |
| 1:1A:2615:U:H2' | 1:1A:2616:C:H6 | 1.78 | 0.49 |
| 35:1d:157:LEU:HD22 | 35:1d:161:ASN:HD21 | 1.77 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 39:1h:51:VAL:HG21 | 39:1h:60:ARG:HB2 | 1.95 | 0.49 |
| 42:1k:62:GLN:HB2 | 42:1k:93:GLN:HG3 | 1.95 | 0.49 |
| 42:1k:85:ARG:NH2 | 42:1k:111:ASP:OD2 | 2.31 | 0.49 |
| 56:1y:37:MIA:H2' | 56:1y:38:A:C8 | 2.48 | 0.49 |
| 1:2A:370:G:OP2 | 62:2A:3953:HOH:O | 2.20 | 0.49 |
| 1:2A:1149:G:H2' | 1:2A:1150:C:C6 | 2.48 | 0.49 |
| 1:2A:2064:C:H2' | 1:2A:2065:C:C6 | 2.48 | 0.49 |
| 1:2A:2886:G:H2' | 1:2A:2887:U:C6 | 2.48 | 0.49 |
| 9:2N:110:GLY:O | 9:2N:114:ARG:HG3 | 2.12 | 0.49 |
| 11:2P:8:PRO:HB2 | 11:2P:12:ALA:HB3 | 1.94 | 0.49 |
| 12:2Q:29:PHE:O | 21:2Z:122:ARG:NH2 | 2.46 | 0.49 |
| 15:2T:67:SER:O | 15:2T:67:SER:OG | 2.30 | 0.49 |
| 26:24:44:THR:O | 26:24:46:GLN:N | 2.44 | 0.49 |
| 26:24:58:ARG:HD2 | 50:2s:68:GLY:H | 1.77 | 0.49 |
| 32:2a:757:U:H2' | 32:2a:758:G:O4' | 2.13 | 0.49 |
| 32:2a:1092:A:N3 | 32:2a:1183:A:N6 | 2.60 | 0.49 |
| 32:2a:1179:A:H2' | 32:2a:1180:A:O4' | 2.13 | 0.49 |
| 44:2m:19:LEU:HB3 | 44:2m:25:ILE:HG21 | 1.93 | 0.49 |
| 32:1a:1014:A:H4' | 50:1s:14:HIS:CE1 | 2.48 | 0.49 |
| 32:1a:1370:G:C2 | 32:1a:1371:G:C8 | 3.00 | 0.49 |
| 34:1c:134:ILE:HG22 | 34:1c:168:ALA:HB3 | 1.94 | 0.49 |
| 35:1d:112:VAL:HG23 | 35:1d:116:GLN:NE2 | 2.24 | 0.49 |
| 1:2A:413:C:H42 | 1:2A:2410:G:H1 | 1.61 | 0.49 |
| 4:2E:45:THR:O | 4:2E:82:ARG:HD2 | 2.13 | 0.49 |
| 6:2G:15:VAL:HG13 | 6:2G:175:LEU:HB2 | 1.95 | 0.49 |
| 6:2G:70:VAL:HA | 6:2G:90:LEU:HD23 | 1.94 | 0.49 |
| 7:2H:20:ALA:HB1 | 7:2H:21:PRO:HD2 | 1.95 | 0.49 |
| 20:2Y:5:MET:HE2 | 20:2Y:32:PRO:HA | 1.94 | 0.49 |
| 33:2b:16:HIS:HB2 | 33:2b:204:ASN:HD22 | 1.78 | 0.49 |
| 35:2d:47:ARG:HB2 | 35:2d:47:ARG:NH1 | 2.27 | 0.49 |
| 39:2h:51:VAL:HG21 | 39:2h:60:ARG:NH1 | 2.28 | 0.49 |
| 1:1A:11:G:C2' | 1:1A:12:U:H5' | 2.41 | 0.49 |
| 1:1A:1817:G:OP1 | 3:1D:88:ARG:NH2 | 2.45 | 0.49 |
| 1:1A:2086:U:H2' | 1:1A:2087:G:C8 | 2.48 | 0.49 |
| 5:1F:31:HIS:NE2 | 5:1F:35:GLU:OE2 | 2.45 | 0.49 |
| 8:1I:33:ARG:O | 8:1I:35:LEU:N | 2.46 | 0.49 |
| 10:1O:35:VAL:HG21 | 10:1O:69:ILE:HD13 | 1.95 | 0.49 |
| 25:13:35:ARG:HE | 25:13:37:LEU:HD21 | 1.78 | 0.49 |
| 32:1a:664:G:N2 | 32:1a:741:G:H1 | 2.07 | 0.49 |
| 32:1a:769:G:H4' | 32:1a:1513:A:H4' | 1.93 | 0.49 |
| 32:1a:1272:G:H2' | 32:1a:1273:G:O4' | 2.12 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 32:1a:1292:U:H5' | 40:1i:38:GLN:OE1 | 2.13 | 0.49 |
| 32:1a:1298:C:H4' | 32:1a:1299:A:C4 | 2.48 | 0.49 |
| 32:1a:1441:G:H5'' | 32:1a:1442:G:H5' | 1.94 | 0.49 |
| 1:2A:1745(A):C:H5' | 1:2A:1746:G:OP2 | 2.12 | 0.49 |
| 1:2A:2137:C:N4 | 1:2A:2155:G:O6 | 2.45 | 0.49 |
| 1:2A:2704:C:H2' | 1:2A:2705:A:O4' | 2.13 | 0.49 |
| 10:2O:87:ILE:HD12 | 10:2O:91:LEU:HA | 1.94 | 0.49 |
| 36:2e:36:ASP:C | 36:2e:38:GLN:H | 2.19 | 0.49 |
| 39:2h:12:ARG:NH1 | 39:2h:27:PRO:HD3 | 2.28 | 0.49 |
| 47:2p:72:ARG:HG3 | 47:2p:73:LEU:N | 2.27 | 0.49 |
| 2:1B:96:U:H2' | 2:1B:97:G:C8 | 2.48 | 0.49 |
| 26:14:63:TYR:N | 26:14:64:GLY:HA2 | 2.28 | 0.49 |
| 32:1a:17:U:H2' | 32:1a:18:C:C6 | 2.48 | 0.49 |
| 36:1e:34:VAL:HG12 | 36:1e:62:ALA:HB1 | 1.95 | 0.49 |
| 51:1t:13:LEU:O | 51:1t:17:ARG:HG3 | 2.13 | 0.49 |
| 54:1w:2:C:H2' | 54:1w:3:C:H6 | 1.77 | 0.49 |
| 55:1x:64:G:H2' | 55:1x:65:C:H6 | 1.77 | 0.49 |
| 1:2A:1357:U:H2' | 1:2A:1358:G:O4' | 2.13 | 0.49 |
| 1:2A:1721:G:H8 | 1:2A:1741:A:H62 | 1.59 | 0.49 |
| 6:2G:179:PRO:HG3 | 26:24:43:TYR:CZ | 2.48 | 0.49 |
| 7:2H:11:VAL:HG21 | 7:2H:50:VAL:HG23 | 1.94 | 0.49 |
| 7:2H:88:LEU:HD11 | 7:2H:165:ALA:HA | 1.95 | 0.49 |
| 21:2Z:22:GLY:O | 21:2Z:23:LYS:HD3 | 2.12 | 0.49 |
| 1:1A:71:A:N7 | 19:1X:31:HIS:HE1 | 2.11 | 0.48 |
| 1:1A:1300:U:H4' | 1:1A:1301:A:H5'' | 1.94 | 0.48 |
| 1:1A:1495:A:H2' | 1:1A:1496:A:C8 | 2.47 | 0.48 |
| 1:1A:1786:A:H1' | 1:1A:1938:A:N6 | 2.27 | 0.48 |
| 1:1A:1876:A:H2' | 1:1A:1877:A:C8 | 2.48 | 0.48 |
| 1:1A:2123:G:H2' | 1:1A:2124:G:O4' | 2.12 | 0.48 |
| 28:16:26:ASN:HD21 | 28:16:28:ARG:NH2 | 2.10 | 0.48 |
| 36:1e:31:LEU:HD22 | 36:1e:43:LEU:HD11 | 1.95 | 0.48 |
| 41:1j:55:LYS:O | 41:1j:55:LYS:HG2 | 2.12 | 0.48 |
| 42:1k:48:ILE:HD12 | 42:1k:63:LEU:HB2 | 1.95 | 0.48 |
| 1:2A:81:G:H21 | 20:2Y:1:MET:HE1 | 1.78 | 0.48 |
| 1:2A:774:A:H2' | 1:2A:774:A:N3 | 2.28 | 0.48 |
| 1:2A:2786:U:OP1 | 4:2E:69:LYS:HD2 | 2.13 | 0.48 |
| 4:2E:92:THR:O | 4:2E:95:ILE:HG23 | 2.13 | 0.48 |
| 32:2a:391:G:C6 | 32:2a:392:G:C5 | 3.01 | 0.48 |
| 32:2a:1252:A:H2' | 32:2a:1253:G:O4' | 2.13 | 0.48 |
| 33:2b:54:THR:O | 33:2b:57:PHE:N | 2.45 | 0.48 |
| 36:2e:60:TYR:OH | 36:2e:64:ARG:NH1 | 2.46 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 40:2i:8:GLY:HA2 | 40:2i:79:LEU:HD23 | 1.95 | 0.48 |
| 1:1A:717:G:H2' | 1:1A:718:A:O4' | 2.12 | 0.48 |
| 1:1A:1030:G:OP2 | 12:1Q:128:LYS:NZ | 2.44 | 0.48 |
| 1:1A:1826:G:H2' | 1:1A:1827:C:O4' | 2.14 | 0.48 |
| 1:1A:2537:U:H2' | 1:1A:2538:C:C6 | 2.48 | 0.48 |
| 2:1B:31:C:N4 | 14:1S:32:LEU:HD13 | 2.28 | 0.48 |
| 8:1I:103:ARG:HG2 | 8:1I:104:GLN:N | 2.28 | 0.48 |
| 15:1T:65:LYS:HE2 | 15:1T:67:SER:HB2 | 1.95 | 0.48 |
| 32:1a:420:U:H2' | 32:1a:422:C:C5 | 2.49 | 0.48 |
| 33:1b:62:ALA:C | 33:1b:64:ARG:H | 2.21 | 0.48 |
| 52:1u:3:LYS:HB3 | 52:1u:14:TRP:CD1 | 2.48 | 0.48 |
| 1:2A:1899:G:H2' | 1:2A:1899:G:N3 | 2.27 | 0.48 |
| 12:2Q:138:ASP:OD1 | 21:2Z:81:ARG:NH1 | 2.46 | 0.48 |
| 20:2Y:13:VAL:HG12 | 20:2Y:74:PRO:HA | 1.95 | 0.48 |
| 32:2a:689:C:H2' | 32:2a:690:G:O4' | 2.13 | 0.48 |
| 33:2b:175:ARG:HH12 | 33:2b:179:LYS:NZ | 2.11 | 0.48 |
| 1:1A:1062:G:H22 | 1:1A:1077:A:H61 | 1.61 | 0.48 |
| 1:1A:2228:G:OP1 | 3:1D:261:LYS:NZ | 2.35 | 0.48 |
| 1:1A:2295:C:OP1 | 14:1S:10:ARG:NH1 | 2.46 | 0.48 |
| 3:1D:183:ARG:HG2 | 3:1D:184:LYS:N | 2.28 | 0.48 |
| 10:1O:49:ARG:NH2 | 32:1a:1423:G:OP1 | 2.34 | 0.48 |
| 27:15:40:LYS:HE3 | 27:15:44:THR:O | 2.13 | 0.48 |
| 35:1d:162:LEU:HD13 | 35:1d:181:MET:HG2 | 1.95 | 0.48 |
| 56:1y:42:C:H2' | 56:1y:43:C:C6 | 2.49 | 0.48 |
| 1:2A:18:C:O2' | 1:2A:554:U:OP1 | 2.30 | 0.48 |
| 1:2A:1022:G:H22 | 1:2A:1142(A):A:H2 | 1.59 | 0.48 |
| 1:2A:1773:A:H5'' | 62:2A:4445:HOH:O | 2.13 | 0.48 |
| 1:2A:2723:C:OP2 | 4:2E:109:LYS:NZ | 2.45 | 0.48 |
| 1:2A:2862:G:C6 | 1:2A:2863:C:C4 | 3.02 | 0.48 |
| 7:2H:3:ARG:HH11 | 7:2H:4:ILE:H | 1.61 | 0.48 |
| 11:2P:39:LYS:HB2 | 11:2P:45:LEU:CG | 2.44 | 0.48 |
| 32:2a:983:A:H5' | 32:2a:984:C:OP2 | 2.13 | 0.48 |
| 38:2g:78:ARG:HD2 | 38:2g:154:TYR:O | 2.13 | 0.48 |
| 55:2x:8:4SU:O2 | 55:2x:21:A:H2 | 1.97 | 0.48 |
| 1:1A:1270:C:H5'' | 1:1A:1271:G:O5' | 2.14 | 0.48 |
| 3:1D:177:LEU:HD12 | 3:1D:181:GLU:HB3 | 1.96 | 0.48 |
| 15:1T:41:ARG:NH2 | 15:1T:43:GLN:HE21 | 2.11 | 0.48 |
| 32:1a:1239:A:H62 | 32:1a:1299:A:N6 | 2.11 | 0.48 |
| 32:1a:1296:C:H5'' | 44:1m:44:ARG:HH22 | 1.77 | 0.48 |
| 1:2A:430:G:H5'' | 1:2A:431:U:OP2 | 2.14 | 0.48 |
| 1:2A:2888:C:H2' | 1:2A:2889:C:H6 | 1.78 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:2B:73:A:C4 | 2:2B:105:A:C2 | 3.01 | 0.48 |
| 3:2D:218:ARG:HB3 | 3:2D:219:PRO:HD2 | 1.95 | 0.48 |
| 6:2G:47:LYS:HB2 | 6:2G:86:MET:HE2 | 1.95 | 0.48 |
| 32:2a:202:U:H5' | 32:2a:203:U:H5 | 1.78 | 0.48 |
| 32:2a:1225:A:H2' | 32:2a:1226:C:C5 | 2.48 | 0.48 |
| 38:2g:16:LEU:HD11 | 40:2i:45:ALA:HB2 | 1.96 | 0.48 |
| 41:2j:78:ASN:C | 41:2j:80:LYS:H | 2.20 | 0.48 |
| 43:2l:32:PHE:HB3 | 43:2l:84:LEU:HD11 | 1.96 | 0.48 |
| 1:1A:2146:C:O2 | 1:1A:2147:G:N1 | 2.46 | 0.48 |
| 1:1A:2811:G:N2 | 1:1A:2891:G:H1' | 2.28 | 0.48 |
| 7:1H:7:LEU:HD12 | 7:1H:8:PRO:HD2 | 1.95 | 0.48 |
| 13:1R:38:VAL:O | 13:1R:42:LYS:HG3 | 2.12 | 0.48 |
| 32:1a:258:G:H2' | 32:1a:259:G:C8 | 2.48 | 0.48 |
| 32:1a:1131:G:OP1 | 40:1i:20:ARG:NH2 | 2.41 | 0.48 |
| 44:1m:49:THR:HG23 | 44:1m:52:GLU:OE1 | 2.12 | 0.48 |
| 50:1s:42:PRO:O | 50:1s:45:VAL:HG23 | 2.13 | 0.48 |
| 1:2A:307:G:N1 | 1:2A:310:A:OP2 | 2.41 | 0.48 |
| 1:2A:2516:G:C6 | 1:2A:2517:C:C4 | 3.01 | 0.48 |
| 6:2G:131:TYR:HE2 | 6:2G:133:LEU:HD22 | 1.79 | 0.48 |
| 12:2Q:2:LEU:HD13 | 12:2Q:69:PHE:CD1 | 2.48 | 0.48 |
| 18:2W:14:PRO:O | 18:2W:18:ARG:HG3 | 2.13 | 0.48 |
| 32:2a:427:U:C4 | 32:2a:428:G:C6 | 3.01 | 0.48 |
| 32:2a:1047:G:H5'' | 45:2n:4:LYS:HD3 | 1.96 | 0.48 |
| 38:2g:97:GLN:O | 38:2g:101:LEU:HG | 2.12 | 0.48 |
| 46:2o:53:HIS:CE1 | 46:2o:57:LEU:HD11 | 2.48 | 0.48 |
| 4:1E:1:MET:HE2 | 4:1E:202:LYS:HE3 | 1.95 | 0.48 |
| 6:1G:47:LYS:HG3 | 6:1G:48:GLU:N | 2.29 | 0.48 |
| 20:1Y:6:HIS:HE1 | 20:1Y:72:VAL:O | 1.97 | 0.48 |
| 21:1Z:76:LEU:HD23 | 21:1Z:83:PRO:HA | 1.95 | 0.48 |
| 26:14:61:ARG:HG3 | 26:14:62:ARG:H | 1.79 | 0.48 |
| 32:1a:939:G:H5' | 38:1g:102:ARG:NH1 | 2.29 | 0.48 |
| 48:1q:45:HIS:CD2 | 48:1q:47:PRO:HG3 | 2.48 | 0.48 |
| 51:1t:87:LYS:O | 51:1t:91:LEU:HG | 2.14 | 0.48 |
| 1:2A:886:C:O2' | 1:2A:889:C:N4 | 2.46 | 0.48 |
| 1:2A:2751:G:C8 | 7:2H:2:SER:HA | 2.45 | 0.48 |
| 1:2A:2892:A:H2' | 1:2A:2893:G:H5' | 1.94 | 0.48 |
| 3:2D:206:LEU:HD22 | 3:2D:211:ARG:HG2 | 1.96 | 0.48 |
| 6:2G:117:PHE:HZ | 6:2G:179:PRO:HG2 | 1.78 | 0.48 |
| 9:2N:4:TYR:CD2 | 16:2U:100:VAL:HG11 | 2.48 | 0.48 |
| 12:2Q:17:LEU:HD22 | 12:2Q:96:VAL:HG13 | 1.95 | 0.48 |
| 32:2a:1060:C:C5 | 34:2c:2:GLY:HA3 | 2.48 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 32:2a:1347:G:H5'' | 40:2i:107:ARG:HB3 | 1.95 | 0.48 |
| 35:2d:8:VAL:HA | 35:2d:11:LEU:HD13 | 1.96 | 0.48 |
| 42:2k:85:ARG:HG2 | 42:2k:111:ASP:O | 2.13 | 0.48 |
| 1:1A:244:A:H2' | 1:1A:245:G:O4' | 2.13 | 0.48 |
| 1:1A:340:A:H2' | 1:1A:341:G:O4' | 2.14 | 0.48 |
| 12:1Q:21:THR:HG22 | 12:1Q:99:PRO:O | 2.13 | 0.48 |
| 14:1S:83:LYS:HB3 | 14:1S:111:GLU:OE1 | 2.12 | 0.48 |
| 32:1a:963:G:H5' | 62:1a:2019:HOH:O | 2.13 | 0.48 |
| 33:1b:101:MET:HG2 | 33:1b:152:PHE:CE1 | 2.48 | 0.48 |
| 33:1b:163:PHE:HD1 | 33:1b:185:ILE:HG13 | 1.78 | 0.48 |
| 37:1f:19:LEU:HD21 | 37:1f:59:TYR:CZ | 2.48 | 0.48 |
| 1:2A:1557:C:OP2 | 1:2A:1558:A:O2' | 2.28 | 0.48 |
| 1:2A:2105:C:H2' | 1:2A:2106:G:C8 | 2.49 | 0.48 |
| 1:2A:2516:G:C6 | 1:2A:2517:C:N4 | 2.82 | 0.48 |
| 21:2Z:77:ASP:CG | 21:2Z:80:ARG:HH11 | 2.21 | 0.48 |
| 32:2a:451:A:N6 | 32:2a:480:U:H2' | 2.28 | 0.48 |
| 32:2a:952:U:H2' | 32:2a:953:G:C8 | 2.47 | 0.48 |
| 32:2a:1101:A:H4' | 32:2a:1102:A:O5' | 2.14 | 0.48 |
| 33:2b:118:LEU:HD21 | 33:2b:141:GLU:HB3 | 1.95 | 0.48 |
| 41:2j:91:PRO:HB2 | 41:2j:94:VAL:HG23 | 1.95 | 0.48 |
| 1:1A:1588:C:H2' | 1:1A:1589:C:H6 | 1.78 | 0.48 |
| 1:1A:2162:G:H1' | 1:1A:2173:A:H1' | 1.96 | 0.48 |
| 1:1A:2530:A:N7 | 7:1H:172:LYS:NZ | 2.61 | 0.48 |
| 6:1G:27:ASN:HB3 | 6:1G:30:GLU:HG3 | 1.94 | 0.48 |
| 15:1T:113:LYS:O | 15:1T:114:LEU:HD23 | 2.14 | 0.48 |
| 19:1X:39:ILE:O | 19:1X:43:VAL:HG23 | 2.14 | 0.48 |
| 32:1a:922:G:C6 | 32:1a:923:A:C6 | 3.02 | 0.48 |
| 1:2A:674:G:O2' | 5:2F:74:ARG:HD3 | 2.13 | 0.48 |
| 1:2A:1183:G:H5'' | 25:23:30:ARG:NH2 | 2.29 | 0.48 |
| 1:2A:1266:G:O5' | 18:2W:15:ARG:NH2 | 2.46 | 0.48 |
| 1:2A:2418:A:H2' | 1:2A:2419:U:C6 | 2.48 | 0.48 |
| 6:2G:58:GLN:O | 6:2G:62:LEU:HG | 2.13 | 0.48 |
| 20:2Y:28:LYS:HG3 | 20:2Y:40:GLU:HB2 | 1.95 | 0.48 |
| 23:21:52:ARG:NH2 | 23:21:57:GLU:HB2 | 2.29 | 0.48 |
| 26:24:50:VAL:HG21 | 44:2m:64:TRP:C | 2.38 | 0.48 |
| 32:2a:1058:G:H2' | 32:2a:1059:C:C6 | 2.49 | 0.48 |
| 32:2a:1271:G:C2 | 32:2a:1272:G:C8 | 3.02 | 0.48 |
| 33:2b:178:ARG:HH12 | 39:2h:68:ARG:HH22 | 1.61 | 0.48 |
| 35:2d:78:LEU:HD23 | 35:2d:96:LEU:HB3 | 1.95 | 0.48 |
| 42:2k:41:THR:HG21 | 42:2k:71:LYS:HB2 | 1.94 | 0.48 |
| 42:2k:45:GLY:O | 42:2k:50:TYR:HB2 | 2.14 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 45:2n:60:SER:O | 45:2n:60:SER:OG | 2.32 | 0.48 |
| 1:1A:118:A:C8 | 1:1A:119:A:C8 | 3.02 | 0.48 |
| 1:1A:247:G:H4' | 1:1A:386:G:C6 | 2.49 | 0.48 |
| 1:1A:312:G:H5' | 1:1A:331:A:O2' | 2.14 | 0.48 |
| 1:1A:1548:C:H2' | 1:1A:1549:C:H6 | 1.78 | 0.48 |
| 6:1G:116:ASP:OD2 | 44:1m:68:GLY:HA3 | 2.14 | 0.48 |
| 10:1O:13:ASN:HD21 | 10:1O:96:THR:H | 1.62 | 0.48 |
| 11:1P:38:GLN:O | 11:1P:39:LYS:CB | 2.62 | 0.48 |
| 12:1Q:135:ASP:N | 12:1Q:138:ASP:OD2 | 2.45 | 0.48 |
| 32:1a:56:U:H2' | 32:1a:57:G:C8 | 2.48 | 0.48 |
| 36:1e:110:LEU:HD13 | 36:1e:118:ILE:HG21 | 1.94 | 0.48 |
| 37:1f:16:GLN:H | 37:1f:16:GLN:CD | 2.21 | 0.48 |
| 40:1i:46:ALA:HB2 | 40:1i:74:ILE:HG23 | 1.94 | 0.48 |
| 41:1j:81:THR:C | 41:1j:83:GLU:H | 2.21 | 0.48 |
| 1:2A:588:U:H2' | 1:2A:589:C:C6 | 2.49 | 0.48 |
| 1:2A:1211:U:H4' | 1:2A:1212:G:OP2 | 2.14 | 0.48 |
| 1:2A:2699:C:H2' | 1:2A:2700:C:O4' | 2.13 | 0.48 |
| 16:2U:106:PHE:O | 16:2U:110:VAL:HG23 | 2.14 | 0.48 |
| 32:2a:189(A):C:H2' | 32:2a:189(B):C:C6 | 2.48 | 0.48 |
| 32:2a:1066:C:O2' | 32:2a:1067:A:H5' | 2.13 | 0.48 |
| 33:2b:200:ILE:H | 33:2b:200:ILE:HD12 | 1.78 | 0.48 |
| 34:2c:6:HIS:HD2 | 34:2c:8:ILE:H | 1.61 | 0.48 |
| 34:2c:41:GLY:O | 34:2c:43:LEU:N | 2.47 | 0.48 |
| 34:2c:155:GLY:HA3 | 34:2c:196:LEU:HD22 | 1.95 | 0.48 |
| 47:2p:1:MET:H3 | 47:2p:24:ALA:HB2 | 1.78 | 0.48 |
| 54:2w:18:G:O2' | 54:2w:57:G:N2 | 2.31 | 0.48 |
| 1:1A:740:U:OP2 | 62:1A:4245:HOH:O | 2.20 | 0.48 |
| 1:1A:883:G:O2' | 1:1A:884:C:H5 | 1.97 | 0.48 |
| 1:1A:1076:C:H4' | 1:1A:1077:A:OP1 | 2.14 | 0.48 |
| 1:1A:2364:C:H2' | 1:1A:2365:G:O4' | 2.14 | 0.48 |
| 32:1a:532:A:N6 | 32:1a:1206:G:O2' | 2.47 | 0.48 |
| 32:1a:1029:C:H41 | 32:1a:1030(A):G:N2 | 2.12 | 0.48 |
| 33:1b:134:GLU:O | 33:1b:138:LEU:HG | 2.14 | 0.48 |
| 33:1b:207:ALA:O | 33:1b:211:ILE:HG13 | 2.14 | 0.48 |
| 54:1w:18:G:H4' | 54:1w:60:U:C6 | 2.49 | 0.48 |
| 1:2A:247:G:H4' | 1:2A:386:G:C5 | 2.49 | 0.48 |
| 1:2A:286:C:H2' | 1:2A:287:C:H6 | 1.79 | 0.48 |
| 1:2A:1886:C:H2' | 1:2A:1887:C:H6 | 1.78 | 0.48 |
| 1:2A:2080:G:H5' | 23:21:35:THR:HG23 | 1.95 | 0.48 |
| 1:2A:2250:G:OP1 | 12:2Q:85:LYS:NZ | 2.47 | 0.48 |
| 4:2E:50:GLY:HA3 | 4:2E:75:VAL:HG21 | 1.96 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 9:2N:69:GLN:O | 9:2N:71:ILE:HG13 | 2.14 | 0.48 |
| 14:2S:19:LYS:C | 14:2S:21:THR:H | 2.22 | 0.48 |
| 15:2T:7:ILE:O | 15:2T:11:GLU:HG3 | 2.13 | 0.48 |
| 16:2U:50:ARG:HH22 | 17:2V:72:VAL:HG13 | 1.79 | 0.48 |
| 32:2a:922:G:N3 | 32:2a:1398:A:H2 | 2.12 | 0.48 |
| 32:2a:954:G:H2' | 32:2a:955:U:O4' | 2.14 | 0.48 |
| 33:2b:231:GLU:H | 33:2b:232:PRO:HD3 | 1.79 | 0.48 |
| 36:2e:41:VAL:O | 36:2e:66:MET:HA | 2.14 | 0.48 |
| 40:2i:17:VAL:HG11 | 40:2i:81:ILE:HA | 1.95 | 0.48 |
| 56:2y:9:A:O5' | 56:2y:46:G7M:N2 | 2.45 | 0.48 |
| 56:2y:9:A:H4' | 56:2y:46:G7M:H5' | 1.96 | 0.48 |
| 1:1A:1071:G:H4' | 1:1A:1089:G:OP2 | 2.14 | 0.47 |
| 1:1A:1593:G:H2' | 1:1A:1594:G:C8 | 2.49 | 0.47 |
| 4:1E:101:ARG:HB2 | 4:1E:201:THR:HG21 | 1.96 | 0.47 |
| 11:1P:135:LEU:HD23 | 11:1P:135:LEU:HA | 1.66 | 0.47 |
| 23:11:8:SER:HB3 | 23:11:66:HIS:CD2 | 2.48 | 0.47 |
| 33:1b:80:ILE:O | 33:1b:84:GLU:HG2 | 2.13 | 0.47 |
| 34:1c:162:GLN:NE2 | 53:1v:24:A:O2' | 2.47 | 0.47 |
| 40:1i:11:LYS:C | 40:1i:13:ALA:H | 2.22 | 0.47 |
| 1:2A:222:A:H5'' | 1:2A:421:U:OP1 | 2.14 | 0.47 |
| 1:2A:2162:G:H2' | 1:2A:2163:C:H6 | 1.78 | 0.47 |
| 1:2A:2238:G:H2' | 1:2A:2238:G:N3 | 2.29 | 0.47 |
| 2:2B:103:G:H21 | 21:2Z:73:GLN:NE2 | 1.98 | 0.47 |
| 12:2Q:99:PRO:HG2 | 21:2Z:79:ARG:HH22 | 1.79 | 0.47 |
| 15:2T:6:LEU:HD23 | 15:2T:6:LEU:HA | 1.67 | 0.47 |
| 20:2Y:5:MET:HE1 | 20:2Y:35:TYR:HA | 1.95 | 0.47 |
| 32:2a:972:C:O2' | 41:2j:55:LYS:O | 2.31 | 0.47 |
| 32:2a:1166:G:N2 | 32:2a:1170:A:OP2 | 2.47 | 0.47 |
| 32:2a:1258:G:H8 | 32:2a:1258:G:OP2 | 1.97 | 0.47 |
| 38:2g:53:LYS:HB3 | 38:2g:53:LYS:HE2 | 1.69 | 0.47 |
| 41:2j:49:VAL:O | 41:2j:61:GLU:N | 2.45 | 0.47 |
| 42:2k:73:MET:SD | 42:2k:103:LEU:HD11 | 2.53 | 0.47 |
| 1:1A:536:A:H2' | 1:1A:537:C:C6 | 2.49 | 0.47 |
| 1:1A:993:G:OP1 | 16:1U:50:ARG:NH2 | 2.46 | 0.47 |
| 1:1A:1054:A:N1 | 1:1A:1105:U:O2 | 2.48 | 0.47 |
| 1:1A:2291:U:OP1 | 1:1A:2380:C:O2' | 2.25 | 0.47 |
| 1:1A:2576:G:H1' | 62:1A:4813:HOH:O | 2.12 | 0.47 |
| 7:1H:12:PRO:HD2 | 7:1H:15:VAL:HG22 | 1.96 | 0.47 |
| 32:1a:1510:U:H2' | 32:1a:1511:G:C8 | 2.50 | 0.47 |
| 41:1j:13:HIS:HD2 | 41:1j:14:LYS:H | 1.62 | 0.47 |
| 1:2A:1204:A:H61 | 1:2A:1240:U:H2' | 1.80 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:2A:2086:U:H2' | 1:2A:2087:G:C8 | 2.49 | 0.47 |
| 1:2A:2097:C:H2' | 1:2A:2098:U:O4' | 2.13 | 0.47 |
| 1:2A:2493:U:H2' | 1:2A:2494:G:O4' | 2.14 | 0.47 |
| 10:2O:115:VAL:HG13 | 10:2O:121:VAL:HG21 | 1.95 | 0.47 |
| 25:23:5:LYS:HE2 | 25:23:34:GLU:OE2 | 2.14 | 0.47 |
| 32:2a:554:C:H2' | 32:2a:555:C:C6 | 2.48 | 0.47 |
| 32:2a:1054:C:C4 | 54:2w:34:G:H1' | 2.49 | 0.47 |
| 32:2a:1206:G:C6 | 32:2a:1207:2MG:C5 | 3.02 | 0.47 |
| 32:2a:1226:C:H4' | 32:2a:1227:A:OP1 | 2.15 | 0.47 |
| 35:2d:59:ARG:NH1 | 35:2d:59:ARG:HA | 2.29 | 0.47 |
| 40:2i:18:PHE:O | 40:2i:61:ALA:HA | 2.14 | 0.47 |
| 42:2k:102:GLY:C | 42:2k:103:LEU:HD12 | 2.40 | 0.47 |
| 44:2m:4:ILE:HG23 | 44:2m:5:ALA:H | 1.79 | 0.47 |
| 55:2x:50:U:H3 | 55:2x:64:G:H1 | 1.60 | 0.47 |
| 1:1A:897:C:C2 | 1:1A:898:C:C5 | 3.02 | 0.47 |
| 1:1A:1113:U:H2' | 1:1A:1114:G:C8 | 2.50 | 0.47 |
| 1:1A:1899:G:O2' | 1:1A:1900:A:OP2 | 2.30 | 0.47 |
| 22:10:11:ARG:HG2 | 62:10:207:HOH:O | 2.13 | 0.47 |
| 32:1a:673:G:H2' | 32:1a:674:G:C8 | 2.49 | 0.47 |
| 32:1a:1098:C:C2 | 32:1a:1099:G:C8 | 3.02 | 0.47 |
| 32:1a:1269:A:H2 | 32:1a:1312:G:N3 | 2.12 | 0.47 |
| 56:1y:13:C:H2' | 56:1y:14:A:H5'' | 1.96 | 0.47 |
| 1:2A:10:G:H8 | 1:2A:10:G:OP2 | 1.97 | 0.47 |
| 1:2A:1448:G:H2' | 1:2A:1449:A:C8 | 2.49 | 0.47 |
| 1:2A:1834:U:H4' | 1:2A:1969:A:C6 | 2.50 | 0.47 |
| 1:2A:2666:C:H5'' | 1:2A:2667:C:OP2 | 2.15 | 0.47 |
| 21:2Z:31:ARG:HD3 | 21:2Z:94:GLU:CD | 2.39 | 0.47 |
| 32:2a:7:G:H5' | 32:2a:298:A:O4' | 2.14 | 0.47 |
| 32:2a:160:A:H1' | 32:2a:344:A:C5 | 2.49 | 0.47 |
| 32:2a:545:C:OP1 | 35:2d:61:LYS:NZ | 2.44 | 0.47 |
| 35:2d:3:ARG:NH1 | 35:2d:115:ARG:HE | 2.12 | 0.47 |
| 47:2p:22:THR:HA | 47:2p:33:ILE:HG13 | 1.97 | 0.47 |
| 1:1A:196:A:O2' | 1:1A:805:G:O6 | 2.28 | 0.47 |
| 1:1A:1175:U:H4' | 1:1A:1176:G:OP1 | 2.14 | 0.47 |
| 1:1A:2056:G:O2' | 27:15:8:LYS:HD3 | 2.15 | 0.47 |
| 6:1G:41:GLN:HG2 | 6:1G:154:GLY:O | 2.14 | 0.47 |
| 6:1G:179:PRO:HG3 | 26:14:43:TYR:OH | 2.14 | 0.47 |
| 32:1a:195:A:H1' | 32:1a:222:U:O2' | 2.14 | 0.47 |
| 32:1a:1149:C:OP1 | 40:1i:9:ARG:NH2 | 2.38 | 0.47 |
| 32:1a:1239:A:H62 | 32:1a:1299:A:H62 | 1.61 | 0.47 |
| 33:1b:15:VAL:HG13 | 33:1b:209:ARG:HG3 | 1.96 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 34:1c:52:LEU:HD12 | 34:1c:53:ALA:N | 2.26 | 0.47 |
| 34:1c:175:LEU:H | 34:1c:175:LEU:HD12 | 1.80 | 0.47 |
| 55:1x:23:C:H2' | 55:1x:24:U:H6 | 1.78 | 0.47 |
| 1:2A:730:C:H5' | 62:2A:4067:HOH:O | 2.13 | 0.47 |
| 1:2A:1594:G:H2' | 1:2A:1595:G:O4' | 2.14 | 0.47 |
| 1:2A:2360:A:H2' | 1:2A:2361:A:O4' | 2.13 | 0.47 |
| 5:2F:172:TRP:H | 5:2F:172:TRP:CD1 | 2.30 | 0.47 |
| 6:2G:120:LEU:HB3 | 6:2G:131:TYR:OH | 2.15 | 0.47 |
| 7:2H:13:LYS:HA | 7:2H:14:GLY:HA2 | 1.52 | 0.47 |
| 17:2V:76:LYS:HB2 | 17:2V:81:TYR:HB3 | 1.95 | 0.47 |
| 22:20:23:VAL:HG22 | 22:20:38:VAL:HG22 | 1.97 | 0.47 |
| 32:2a:340:U:H2' | 32:2a:341:C:C6 | 2.49 | 0.47 |
| 32:2a:564:C:H5' | 48:2q:32:TYR:CE1 | 2.48 | 0.47 |
| 32:2a:1291:G:C6 | 32:2a:1292:U:C4 | 3.02 | 0.47 |
| 34:2c:47:LEU:HD12 | 34:2c:68:VAL:HG11 | 1.95 | 0.47 |
| 37:2f:100:ASN:HB2 | 49:2r:28:GLU:HA | 1.97 | 0.47 |
| 38:2g:26:PHE:O | 38:2g:30:ILE:HD12 | 2.15 | 0.47 |
| 47:2p:58:TYR:O | 47:2p:61:SER:OG | 2.26 | 0.47 |
| 54:2w:39:PSU:H2' | 54:2w:40:C:C6 | 2.50 | 0.47 |
| 1:1A:2123:G:H2' | 1:1A:2124:G:H8 | 1.78 | 0.47 |
| 1:1A:2176:A:H2' | 1:1A:2177:C:C6 | 2.49 | 0.47 |
| 16:1U:105:VAL:HG22 | 17:1V:45:THR:CG2 | 2.44 | 0.47 |
| 19:1X:31:HIS:CD2 | 19:1X:32:PRO:HD2 | 2.50 | 0.47 |
| 32:1a:1302:U:H5 | 44:1m:17:VAL:HG21 | 1.79 | 0.47 |
| 33:1b:82:ARG:HD2 | 33:1b:92:TYR:OH | 2.15 | 0.47 |
| 33:1b:134:GLU:HA | 33:1b:137:ARG:HE | 1.79 | 0.47 |
| 39:1h:97:VAL:O | 39:1h:100:ILE:HG13 | 2.14 | 0.47 |
| 39:1h:116:LYS:HD3 | 39:1h:127:LEU:HD23 | 1.96 | 0.47 |
| 43:1l:53:ARG:HG3 | 43:1l:93:LEU:HD21 | 1.96 | 0.47 |
| 46:1o:37:ASN:O | 46:1o:41:GLU:HG2 | 2.14 | 0.47 |
| 49:1r:66:LEU:O | 49:1r:69:THR:OG1 | 2.28 | 0.47 |
| 55:1x:17:C:OP2 | 55:1x:17(A):U:O2' | 2.29 | 0.47 |
| 1:2A:1379:A:H4' | 1:2A:1380:G:OP2 | 2.13 | 0.47 |
| 1:2A:1589:C:H2' | 1:2A:1590:U:H6 | 1.79 | 0.47 |
| 12:2Q:57:HIS:CE1 | 12:2Q:116:GLU:HG2 | 2.49 | 0.47 |
| 32:2a:438:G:H4' | 35:2d:123:HIS:ND1 | 2.29 | 0.47 |
| 32:2a:509:A:H5'' | 35:2d:55:ALA:HB2 | 1.96 | 0.47 |
| 32:2a:1026:G:N3 | 32:2a:1026:G:H2' | 2.30 | 0.47 |
| 32:2a:1315:U:O2' | 32:2a:1360:A:N3 | 2.42 | 0.47 |
| 32:2a:1381:U:H1' | 38:2g:79:ARG:HD2 | 1.97 | 0.47 |
| 33:2b:32:ILE:HD13 | 33:2b:40:HIS:HB3 | 1.97 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 46:2o:7:GLU:O | 46:2o:11:VAL:HG23 | 2.15 | 0.47 |
| 1:1A:1579:A:H2' | 1:1A:1580:A:C8 | 2.49 | 0.47 |
| 7:1H:12:PRO:HD2 | 7:1H:15:VAL:CG2 | 2.45 | 0.47 |
| 23:11:23:LYS:HB2 | 56:1y:74:C:H4' | 1.95 | 0.47 |
| 32:1a:975:A:H5' | 32:1a:975:A:C8 | 2.45 | 0.47 |
| 32:1a:976:G:OP2 | 32:1a:1358:U:O2' | 2.25 | 0.47 |
| 33:1b:185:ILE:HG23 | 33:1b:199:TYR:HD2 | 1.79 | 0.47 |
| 38:1g:12:LEU:HD12 | 38:1g:12:LEU:H | 1.78 | 0.47 |
| 44:1m:126:LYS:HB3 | 53:1v:19:U:O4' | 2.14 | 0.47 |
| 54:1w:72:C:O5' | 54:1w:72:C:H6 | 1.97 | 0.47 |
| 1:2A:324:A:N6 | 1:2A:338:G:O2' | 2.47 | 0.47 |
| 1:2A:880:G:H2' | 1:2A:881:G:H8 | 1.79 | 0.47 |
| 1:2A:2801(A):A:N3 | 1:2A:2895:U:O2' | 2.46 | 0.47 |
| 4:2E:48:GLN:HA | 4:2E:80:GLU:HA | 1.95 | 0.47 |
| 8:2I:2:LYS:HA | 8:2I:19:VAL:O | 2.15 | 0.47 |
| 12:2Q:34:LEU:HB2 | 12:2Q:118:LEU:HD22 | 1.96 | 0.47 |
| 12:2Q:63:LYS:HG2 | 12:2Q:65:PHE:CE2 | 2.49 | 0.47 |
| 21:2Z:72:ARG:HH11 | 21:2Z:89:PHE:HD2 | 1.62 | 0.47 |
| 32:2a:1125:U:H6 | 32:2a:1126:U:HO2' | 1.62 | 0.47 |
| 32:2a:1142:G:C8 | 32:2a:1143:G:C8 | 3.02 | 0.47 |
| 32:2a:1264:C:C4 | 32:2a:1272:G:O6 | 2.68 | 0.47 |
| 32:2a:1469:G:H2' | 32:2a:1470:G:H8 | 1.78 | 0.47 |
| 36:2e:9:LYS:HB2 | 36:2e:112:LEU:HD11 | 1.95 | 0.47 |
| 47:2p:6:LEU:HD23 | 47:2p:17:TYR:CG | 2.49 | 0.47 |
| 47:2p:15:PRO:HD2 | 47:2p:42:ARG:HD2 | 1.95 | 0.47 |
| 1:1A:548:A:H61 | 17:1V:18:LEU:HA | 1.79 | 0.47 |
| 1:1A:1315:C:OP2 | 62:1A:4221:HOH:O | 2.20 | 0.47 |
| 1:1A:1406:U:H2' | 1:1A:1407:C:C6 | 2.50 | 0.47 |
| 1:1A:2022:U:OP1 | 62:1A:4247:HOH:O | 2.20 | 0.47 |
| 1:1A:2157:G:H4' | 1:1A:2158:A:OP1 | 2.15 | 0.47 |
| 1:1A:2649:U:H2' | 1:1A:2650:U:C6 | 2.49 | 0.47 |
| 6:1G:3:LEU:HD12 | 6:1G:5:VAL:HG12 | 1.95 | 0.47 |
| 6:1G:132:ASN:HA | 6:1G:157:ILE:O | 2.15 | 0.47 |
| 8:1I:4:ILE:HG12 | 8:1I:18:VAL:HG22 | 1.96 | 0.47 |
| 15:1T:127:ALA:C | 15:1T:129:ARG:H | 2.21 | 0.47 |
| 32:1a:78:G:C6 | 32:1a:91:C:N4 | 2.82 | 0.47 |
| 32:1a:100:C:H2' | 32:1a:101:A:C8 | 2.50 | 0.47 |
| 32:1a:519:C:OP2 | 43:1l:50:SER:OG | 2.33 | 0.47 |
| 32:1a:713:G:H2' | 32:1a:714:G:C8 | 2.50 | 0.47 |
| 32:1a:872:A:C5 | 32:1a:874:G:C8 | 3.03 | 0.47 |
| 32:1a:974:A:H8 | 32:1a:974:A:OP1 | 1.97 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 32:1a:1486:G:H2' | 32:1a:1487:G:O4' | 2.15 | 0.47 |
| 44:1m:108:ARG:HA | 44:1m:108:ARG:HD3 | 1.49 | 0.47 |
| 49:1r:53:ARG:C | 49:1r:55:ARG:H | 2.23 | 0.47 |
| 1:2A:528:A:N1 | 1:2A:2042:A:H2' | 2.30 | 0.47 |
| 1:2A:864:G:C6 | 1:2A:865:C:N4 | 2.83 | 0.47 |
| 1:2A:888:C:OP1 | 44:2m:93:ARG:HD2 | 2.14 | 0.47 |
| 1:2A:1951:U:O4 | 62:2A:3946:HOH:O | 2.19 | 0.47 |
| 1:2A:2113:U:H2' | 1:2A:2114:A:H8 | 1.79 | 0.47 |
| 1:2A:2114:A:H62 | 1:2A:2115:G:H21 | 1.61 | 0.47 |
| 1:2A:2807:G:C2 | 1:2A:2893:G:O6 | 2.67 | 0.47 |
| 2:2B:105:A:H5' | 2:2B:106:G:OP2 | 2.14 | 0.47 |
| 6:2G:146:TYR:O | 6:2G:149:VAL:HG12 | 2.15 | 0.47 |
| 18:2W:12:ILE:HG13 | 18:2W:42:ARG:NH1 | 2.28 | 0.47 |
| 21:2Z:70:LEU:HD12 | 21:2Z:71:VAL:H | 1.79 | 0.47 |
| 28:26:12:GLU:OE1 | 28:26:52:VAL:HG11 | 2.15 | 0.47 |
| 32:2a:151:A:H2' | 32:2a:152:A:O4' | 2.15 | 0.47 |
| 32:2a:441:A:H3' | 32:2a:442:C:C6 | 2.48 | 0.47 |
| 32:2a:618:C:C2 | 32:2a:622:A:N6 | 2.83 | 0.47 |
| 32:2a:1346:A:N1 | 32:2a:1374:A:H5'' | 2.30 | 0.47 |
| 35:2d:61:LYS:HD2 | 35:2d:207:TYR:OH | 2.15 | 0.47 |
| 35:2d:163:GLU:C | 35:2d:165:MET:H | 2.22 | 0.47 |
| 36:2e:105:VAL:HB | 36:2e:106:PRO:HD3 | 1.97 | 0.47 |
| 39:2h:14:ARG:O | 39:2h:18:ARG:HD2 | 2.15 | 0.47 |
| 40:2i:4:TYR:HA | 40:2i:87:GLN:HE22 | 1.80 | 0.47 |
| 46:2o:87:ILE:HG22 | 46:2o:88:ARG:H | 1.80 | 0.47 |
| 47:2p:3:LYS:O | 47:2p:21:VAL:HA | 2.14 | 0.47 |
| 50:2s:80:TYR:C | 50:2s:82:GLY:H | 2.21 | 0.47 |
| 51:2t:98:PRO:O | 51:2t:99:LEU:HB2 | 2.14 | 0.47 |
| 1:1A:1812:A:O2' | 3:1D:45:ASN:N | 2.44 | 0.47 |
| 1:1A:2348:U:O4 | 1:1A:2382:G:N1 | 2.48 | 0.47 |
| 8:1I:88:ILE:HD12 | 8:1I:121:LYS:C | 2.40 | 0.47 |
| 9:1N:91:LEU:HG | 9:1N:98:VAL:HG21 | 1.97 | 0.47 |
| 14:1S:48:LEU:HD23 | 14:1S:82:ILE:HD11 | 1.96 | 0.47 |
| 14:1S:71:ARG:NH1 | 14:1S:107:GLU:OE1 | 2.48 | 0.47 |
| 32:1a:350:G:H2' | 32:1a:351:G:C8 | 2.50 | 0.47 |
| 32:1a:436:C:H2' | 32:1a:437:U:C6 | 2.48 | 0.47 |
| 32:1a:545:C:H5' | 35:1d:72:GLU:HG2 | 1.96 | 0.47 |
| 32:1a:848:C:H2' | 32:1a:849:C:H6 | 1.80 | 0.47 |
| 32:1a:1320:C:O2 | 50:1s:36:ARG:NH2 | 2.46 | 0.47 |
| 36:1e:148:VAL:HG21 | 39:1h:107:LEU:HD23 | 1.96 | 0.47 |
| 38:1g:77:SER:HA | 38:1g:85:TYR:O | 2.14 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 44:1m:49:THR:OG1 | 44:1m:52:GLU:HG3 | 2.14 | 0.47 |
| 1:2A:136:G:O2' | 1:2A:137:C:H5' | 2.13 | 0.47 |
| 1:2A:1668:A:O2' | 1:2A:1674:G:N7 | 2.47 | 0.47 |
| 1:2A:2139:C:C2 | 1:2A:2153:G:N2 | 2.82 | 0.47 |
| 4:2E:1:MET:O | 4:2E:84:PHE:HB2 | 2.15 | 0.47 |
| 32:2a:123:C:OP1 | 32:2a:312:C:H5' | 2.15 | 0.47 |
| 32:2a:1238:A:N7 | 32:2a:1303:C:H1' | 2.30 | 0.47 |
| 32:2a:1279:A:OP2 | 41:2j:9:ARG:NH2 | 2.48 | 0.47 |
| 32:2a:1323:G:H2' | 32:2a:1324:A:C8 | 2.50 | 0.47 |
| 1:1A:1797:C:H4' | 3:1D:257:LEU:O | 2.14 | 0.47 |
| 9:1N:96:GLU:CD | 9:1N:96:GLU:H | 2.23 | 0.47 |
| 12:1Q:63:LYS:HG2 | 12:1Q:65:PHE:CZ | 2.50 | 0.47 |
| 14:1S:78:LEU:HD11 | 14:1S:109:GLY:O | 2.15 | 0.47 |
| 32:1a:130:A:O2' | 32:1a:131:C:O5' | 2.31 | 0.47 |
| 33:1b:44:LEU:HA | 33:1b:47:THR:OG1 | 2.15 | 0.47 |
| 34:1c:113:ALA:HB3 | 34:1c:114:PRO:HD3 | 1.97 | 0.47 |
| 34:1c:150:LYS:HG3 | 34:1c:169:ALA:HB2 | 1.96 | 0.47 |
| 42:1k:20:TYR:CE1 | 42:1k:83:ILE:HD12 | 2.50 | 0.47 |
| 50:1s:15:LEU:O | 50:1s:19:VAL:HG23 | 2.15 | 0.47 |
| 1:2A:288:C:H2' | 1:2A:289:A:H8 | 1.80 | 0.47 |
| 1:2A:489:G:N7 | 18:2W:49:LYS:NZ | 2.63 | 0.47 |
| 1:2A:2102:U:H2' | 1:2A:2103:C:C6 | 2.50 | 0.47 |
| 32:2a:841:U:H6 | 32:2a:841:U:P | 2.38 | 0.47 |
| 32:2a:901:A:H5'' | 32:2a:902:G:OP2 | 2.15 | 0.47 |
| 32:2a:1010:G:N2 | 32:2a:1020:U:H1' | 2.30 | 0.47 |
| 32:2a:1287:A:H2' | 32:2a:1288:A:C8 | 2.50 | 0.47 |
| 32:2a:1345:U:H2' | 62:2a:1991:HOH:O | 2.15 | 0.47 |
| 32:2a:1469:G:H2' | 32:2a:1470:G:C8 | 2.50 | 0.47 |
| 35:2d:119:GLN:HG3 | 35:2d:123:HIS:CD2 | 2.46 | 0.47 |
| 45:2n:27:CYS:SG | 45:2n:28:GLY:N | 2.87 | 0.47 |
| 46:2o:54:ARG:O | 46:2o:58:MET:HG3 | 2.15 | 0.47 |
| 56:2y:9:A:C2' | 56:2y:11:C:H41 | 2.25 | 0.47 |
| 1:1A:775:G:C4 | 1:1A:794:G:C8 | 3.03 | 0.47 |
| 1:1A:1062:G:P | 1:1A:1070:A:H1' | 2.55 | 0.47 |
| 1:1A:1636:C:H2' | 1:1A:1637:A:C8 | 2.50 | 0.47 |
| 1:1A:2165:G:H1 | 1:1A:2171:A:H2' | 1.79 | 0.47 |
| 1:1A:2171:A:O2' | 1:1A:2172:U:H5'' | 2.15 | 0.47 |
| 1:1A:2312:U:OP1 | 6:1G:73:ALA:HA | 2.15 | 0.47 |
| 5:1F:184:TYR:CD2 | 5:1F:188:ARG:HD2 | 2.50 | 0.47 |
| 15:1T:26:ASP:OD1 | 15:1T:120:ARG:NH2 | 2.44 | 0.47 |
| 21:1Z:125:LEU:HG | 21:1Z:164:ALA:HB3 | 1.96 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 32:1a:96:U:H2' | 32:1a:97:G:H8 | 1.79 | 0.47 |
| 32:1a:688:G:H2' | 32:1a:689:C:H6 | 1.79 | 0.47 |
| 32:1a:748:C:O5' | 32:1a:748:C:H6 | 1.98 | 0.47 |
| 32:1a:1278:U:H5' | 32:1a:1279:A:O4' | 2.15 | 0.47 |
| 32:1a:1347:G:O2' | 32:1a:1373:G:O6 | 2.28 | 0.47 |
| 34:1c:54:ARG:HG2 | 34:1c:56:ASP:OD1 | 2.15 | 0.47 |
| 1:2A:946:G:OP1 | 62:2A:3954:HOH:O | 2.20 | 0.47 |
| 1:2A:2495:G:H5'' | 12:2Q:82:ARG:HG2 | 1.96 | 0.47 |
| 6:2G:45:GLU:H | 6:2G:45:GLU:HG2 | 1.37 | 0.47 |
| 21:2Z:155:LEU:HB2 | 21:2Z:157:LEU:HD12 | 1.96 | 0.47 |
| 25:23:26:LEU:O | 25:23:35:ARG:HD3 | 2.15 | 0.47 |
| 26:24:67:TYR:OH | 50:2s:43:GLU:OE2 | 2.23 | 0.47 |
| 32:2a:202:U:H3' | 32:2a:203:U:C6 | 2.50 | 0.47 |
| 32:2a:706:A:H5'' | 42:2k:22:HIS:CE1 | 2.50 | 0.47 |
| 32:2a:1380:U:C4 | 38:2g:3:ARG:HG2 | 2.50 | 0.47 |
| 36:2e:41:VAL:O | 36:2e:67:VAL:HG12 | 2.14 | 0.47 |
| 56:2y:15:G:N2 | 56:2y:48:C:H42 | 2.13 | 0.47 |
| 1:1A:1064:C:N3 | 1:1A:1074:G:O6 | 2.47 | 0.46 |
| 1:1A:2099:U:O2 | 1:1A:2190:G:N2 | 2.35 | 0.46 |
| 1:1A:2785:C:OP1 | 4:1E:41:LYS:HE3 | 2.15 | 0.46 |
| 4:1E:175:VAL:O | 4:1E:177:PRO:HD3 | 2.15 | 0.46 |
| 14:1S:3:ARG:HD2 | 14:1S:4:LEU:O | 2.14 | 0.46 |
| 15:1T:96:ARG:CZ | 15:1T:96:ARG:HB3 | 2.43 | 0.46 |
| 32:1a:353:A:H5' | 32:1a:353:A:H8 | 1.80 | 0.46 |
| 32:1a:507:C:OP2 | 32:1a:508:C:O2' | 2.27 | 0.46 |
| 35:1d:13:ARG:HB3 | 35:1d:38:TYR:O | 2.15 | 0.46 |
| 40:1i:73:GLN:O | 40:1i:77:ILE:HD12 | 2.15 | 0.46 |
| 44:1m:15:VAL:HB | 44:1m:34:LEU:HD11 | 1.98 | 0.46 |
| 45:1n:26:ARG:NE | 45:1n:47:LEU:HD21 | 2.30 | 0.46 |
| 1:2A:1268:A:C2 | 1:2A:2013:A:C4 | 3.03 | 0.46 |
| 1:2A:1813:G:O6 | 62:2A:3950:HOH:O | 2.19 | 0.46 |
| 5:2F:51:THR:HG21 | 5:2F:92:PRO:HD2 | 1.97 | 0.46 |
| 7:2H:85:LYS:HE2 | 7:2H:164:TYR:CE1 | 2.50 | 0.46 |
| 32:2a:189(C):C:H2' | 32:2a:189(D):C:O4' | 2.14 | 0.46 |
| 32:2a:1095:U:H2' | 32:2a:1096:C:H6 | 1.79 | 0.46 |
| 32:2a:1168:A:H2' | 32:2a:1169:A:C8 | 2.50 | 0.46 |
| 32:2a:1256:A:H61 | 32:2a:1278:U:C1' | 2.26 | 0.46 |
| 32:2a:1417:G:O6 | 62:2a:1912:HOH:O | 2.18 | 0.46 |
| 33:2b:16:HIS:HB2 | 33:2b:204:ASN:CB | 2.44 | 0.46 |
| 33:2b:51:LEU:HD23 | 33:2b:51:LEU:HA | 1.68 | 0.46 |
| 33:2b:198:ASP:N | 33:2b:198:ASP:OD1 | 2.47 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 37:2f:35:ALA:HA | 37:2f:67:MET:HB3 | 1.97 | 0.46 |
| 1:1A:306:U:H2' | 1:1A:307:G:O4' | 2.16 | 0.46 |
| 1:1A:876:C:H42 | 1:1A:901:A:N6 | 2.13 | 0.46 |
| 1:1A:1550:C:OP1 | 1:1A:1720:U:O2' | 2.30 | 0.46 |
| 1:1A:1920:OMC:HM22 | 1:1A:1921:G:O4' | 2.15 | 0.46 |
| 1:1A:2115:G:C2 | 1:1A:2117:A:N7 | 2.83 | 0.46 |
| 1:1A:2662:A:H2' | 1:1A:2663:G:O4' | 2.14 | 0.46 |
| 1:1A:2892:A:N6 | 1:1A:2893:G:C6 | 2.83 | 0.46 |
| 6:1G:83:ARG:O | 6:1G:86:MET:HG3 | 2.15 | 0.46 |
| 8:1I:8:PRO:O | 8:1I:9:LEU:HD23 | 2.15 | 0.46 |
| 18:1W:68:ARG:HG2 | 18:1W:110:LYS:O | 2.15 | 0.46 |
| 23:11:18:ILE:HG12 | 23:11:37:ILE:HD13 | 1.98 | 0.46 |
| 32:1a:262:A:C6 | 32:1a:263:A:C6 | 3.02 | 0.46 |
| 32:1a:1057:G:H2' | 32:1a:1058:G:O4' | 2.14 | 0.46 |
| 55:1x:8:4SU:O2 | 55:1x:21:A:H2 | 1.98 | 0.46 |
| 1:2A:92:A:H2' | 1:2A:93:G:H8 | 1.80 | 0.46 |
| 1:2A:171:G:H2' | 1:2A:172:C:H6 | 1.80 | 0.46 |
| 1:2A:300:A:P | 20:2Y:86:ARG:HH12 | 2.39 | 0.46 |
| 1:2A:1803:A:H4' | 3:2D:259:THR:HG23 | 1.98 | 0.46 |
| 1:2A:2532:G:H2' | 1:2A:2533:A:C8 | 2.51 | 0.46 |
| 3:2D:146:GLU:HA | 3:2D:153:ALA:HA | 1.97 | 0.46 |
| 12:2Q:19:GLY:O | 12:2Q:98:LYS:HD3 | 2.16 | 0.46 |
| 32:2a:996:A:C6 | 32:2a:997:U:C4 | 3.04 | 0.46 |
| 32:2a:1036:G:H5'' | 32:2a:1037:C:OP2 | 2.15 | 0.46 |
| 32:2a:1064:G:OP1 | 32:2a:1386:G:H4' | 2.15 | 0.46 |
| 32:2a:1269:A:C2 | 32:2a:1313:U:O4' | 2.67 | 0.46 |
| 51:2t:36:LEU:CD1 | 51:2t:58:LYS:HG3 | 2.45 | 0.46 |
| 1:1A:415:A:H2' | 1:1A:416:C:C6 | 2.50 | 0.46 |
| 1:1A:783:A:N3 | 1:1A:783:A:H2' | 2.31 | 0.46 |
| 1:1A:2110:G:OP1 | 1:1A:2111:C:H5 | 1.98 | 0.46 |
| 1:1A:2810:A:N6 | 1:1A:2891:G:O2' | 2.39 | 0.46 |
| 2:1B:24:G:N7 | 2:1B:56:G:H2' | 2.30 | 0.46 |
| 5:1F:126:VAL:HG21 | 5:1F:129:PHE:CZ | 2.50 | 0.46 |
| 32:1a:994:A:N1 | 32:1a:1047:G:H4' | 2.30 | 0.46 |
| 32:1a:1264:C:H42 | 32:1a:1271:G:H1 | 1.62 | 0.46 |
| 32:1a:1402:4OC:O5' | 32:1a:1402:4OC:H6 | 2.16 | 0.46 |
| 54:1w:43:C:H2' | 54:1w:44:G:C8 | 2.51 | 0.46 |
| 1:2A:668:G:H5' | 1:2A:669:G:OP2 | 2.16 | 0.46 |
| 1:2A:850:C:H6 | 1:2A:850:C:O5' | 1.98 | 0.46 |
| 4:2E:163:GLU:HG2 | 4:2E:164:ARG:N | 2.30 | 0.46 |
| 7:2H:10:PRO:O | 7:2H:12:PRO:HD3 | 2.14 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 11:2P:97:PRO:HD3 | 11:2P:126:VAL:O | 2.16 | 0.46 |
| 32:2a:1187:G:H2' | 32:2a:1188:A:C8 | 2.50 | 0.46 |
| 33:2b:58:ILE:O | 33:2b:62:ALA:N | 2.45 | 0.46 |
| 36:2e:99:GLY:O | 36:2e:117:ASP:HA | 2.15 | 0.46 |
| 36:2e:100:VAL:O | 36:2e:107:ARG:NH2 | 2.41 | 0.46 |
| 36:2e:139:LEU:O | 36:2e:142:LEU:HB2 | 2.15 | 0.46 |
| 36:2e:144:THR:OG1 | 36:2e:146:ALA:HB3 | 2.16 | 0.46 |
| 37:2f:100:ASN:HD21 | 49:2r:23:LYS:HE3 | 1.80 | 0.46 |
| 47:2p:43:LYS:HG2 | 47:2p:48:TRP:CE2 | 2.49 | 0.46 |
| 48:2q:82:MET:O | 48:2q:86:GLU:HG2 | 2.15 | 0.46 |
| 51:2t:14:LYS:HA | 51:2t:17:ARG:CZ | 2.45 | 0.46 |
| 1:1A:414:C:H2' | 1:1A:415:A:C8 | 2.49 | 0.46 |
| 1:1A:1805:U:O2 | 3:1D:50:THR:HB | 2.16 | 0.46 |
| 1:1A:2001:A:OP1 | 13:1R:9:LYS:NZ | 2.47 | 0.46 |
| 4:1E:47:VAL:HG11 | 4:1E:86:PRO:HD2 | 1.97 | 0.46 |
| 8:1I:114:LEU:HD11 | 8:1I:128:LEU:HB3 | 1.96 | 0.46 |
| 10:1O:49:ARG:HH12 | 32:1a:1423:G:P | 2.38 | 0.46 |
| 11:1P:50:ARG:HD3 | 30:18:7:HIS:CD2 | 2.51 | 0.46 |
| 21:1Z:152:ALA:O | 21:1Z:155:LEU:HB2 | 2.14 | 0.46 |
| 32:1a:452:A:OP1 | 47:1p:43:LYS:NZ | 2.43 | 0.46 |
| 32:1a:1053:G:N7 | 32:1a:1200:C:H5'' | 2.31 | 0.46 |
| 39:1h:51:VAL:HG12 | 39:1h:52:ASP:H | 1.80 | 0.46 |
| 44:1m:15:VAL:HG22 | 44:1m:43:THR:O | 2.15 | 0.46 |
| 1:2A:2320:A:N3 | 1:2A:2320:A:H2' | 2.30 | 0.46 |
| 3:2D:38:LYS:HA | 3:2D:38:LYS:HD2 | 1.57 | 0.46 |
| 16:2U:89:GLU:O | 17:2V:11:GLN:NE2 | 2.42 | 0.46 |
| 16:2U:91:ASP:O | 16:2U:95:LEU:HB2 | 2.15 | 0.46 |
| 21:2Z:159:PRO:HA | 21:2Z:160:GLY:HA2 | 1.59 | 0.46 |
| 24:22:35:LEU:HD23 | 24:22:35:LEU:HA | 1.72 | 0.46 |
| 32:2a:152:A:OP2 | 32:2a:153:C:N4 | 2.36 | 0.46 |
| 32:2a:434:U:H2' | 32:2a:435:C:C6 | 2.50 | 0.46 |
| 32:2a:441:A:H3' | 32:2a:442:C:H6 | 1.79 | 0.46 |
| 32:2a:533:A:O2' | 32:2a:534:U:H5'' | 2.16 | 0.46 |
| 38:2g:38:LEU:O | 38:2g:42:ILE:HG13 | 2.16 | 0.46 |
| 44:2m:80:ARG:O | 44:2m:84:ILE:HG12 | 2.15 | 0.46 |
| 54:2w:76:F3N:N | 55:2x:76:31H:O2' | 2.48 | 0.46 |
| 3:1D:206:LEU:HA | 3:1D:211:ARG:NH1 | 2.31 | 0.46 |
| 7:1H:3:ARG:CZ | 7:1H:5:GLY:H | 2.29 | 0.46 |
| 7:1H:90:LYS:HE3 | 7:1H:163:TYR:CD2 | 2.51 | 0.46 |
| 13:1R:20:LEU:O | 13:1R:24:GLN:HG3 | 2.16 | 0.46 |
| 32:1a:1149:C:H2' | 32:1a:1150:U:C6 | 2.51 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 44:1m:79:LYS:HA | 44:1m:82:MET:HE2 | 1.98 | 0.46 |
| 46:1o:39:LEU:HD23 | 46:1o:56:LEU:HB2 | 1.97 | 0.46 |
| 56:1y:6:G:C6 | 56:1y:7:A:C6 | 3.03 | 0.46 |
| 2:2B:1:U:H2' | 2:2B:2:C:C6 | 2.50 | 0.46 |
| 2:2B:8:U:O3' | 14:2S:25:ARG:NH2 | 2.47 | 0.46 |
| 5:2F:89:VAL:HG12 | 5:2F:90:PHE:CD2 | 2.51 | 0.46 |
| 5:2F:178:PRO:HG2 | 5:2F:179:GLU:OE2 | 2.15 | 0.46 |
| 18:2W:12:ILE:HG13 | 18:2W:42:ARG:HH11 | 1.81 | 0.46 |
| 21:2Z:69:THR:HG22 | 21:2Z:90:VAL:HA | 1.98 | 0.46 |
| 26:24:68:ARG:NH1 | 26:24:69:LYS:H | 2.13 | 0.46 |
| 32:2a:137:C:H2' | 32:2a:138:G:C8 | 2.51 | 0.46 |
| 32:2a:415:A:H2' | 32:2a:416:G:O4' | 2.15 | 0.46 |
| 32:2a:1226:C:P | 44:2m:91:ARG:HH12 | 2.39 | 0.46 |
| 44:2m:38:GLY:O | 44:2m:39:ILE:HG13 | 2.15 | 0.46 |
| 1:1A:2094:G:O2' | 1:1A:2095:C:H5' | 2.15 | 0.46 |
| 1:1A:2207:G:H2' | 1:1A:2208:A:H2 | 1.81 | 0.46 |
| 1:1A:2235:G:N7 | 62:1A:4335:HOH:O | 2.35 | 0.46 |
| 8:1I:95:LYS:NZ | 8:1I:99:GLU:OE2 | 2.49 | 0.46 |
| 19:1X:57:LEU:N | 19:1X:57:LEU:HD23 | 2.31 | 0.46 |
| 32:1a:377:G:OP1 | 47:1p:3:LYS:HD3 | 2.15 | 0.46 |
| 34:1c:30:ARG:HB3 | 45:1n:36:PHE:O | 2.14 | 0.46 |
| 35:1d:63:LYS:HD3 | 35:1d:197:PRO:O | 2.15 | 0.46 |
| 35:1d:194:LEU:HD12 | 35:1d:195:ALA:N | 2.31 | 0.46 |
| 37:1f:37:VAL:HA | 37:1f:65:VAL:HG12 | 1.98 | 0.46 |
| 47:1p:60:LEU:HD12 | 47:1p:60:LEU:HA | 1.84 | 0.46 |
| 1:2A:974:G:OP1 | 1:2A:1187:G:O2' | 2.27 | 0.46 |
| 1:2A:2298:A:N6 | 1:2A:2318:G:H8 | 2.14 | 0.46 |
| 5:2F:53:THR:HG23 | 5:2F:55:GLY:N | 2.27 | 0.46 |
| 6:2G:109:VAL:HG21 | 6:2G:142:PRO:HG3 | 1.96 | 0.46 |
| 10:2O:2:ILE:HG23 | 10:2O:6:THR:HG21 | 1.96 | 0.46 |
| 11:2P:98:GLU:O | 11:2P:102:ARG:HG3 | 2.15 | 0.46 |
| 24:22:63:VAL:O | 24:22:67:LYS:HG2 | 2.15 | 0.46 |
| 32:2a:624:C:H4' | 47:2p:11:SER:HB3 | 1.97 | 0.46 |
| 32:2a:818:G:O2' | 32:2a:819:A:H5' | 2.16 | 0.46 |
| 32:2a:1183:A:O2' | 32:2a:1184:G:OP1 | 2.32 | 0.46 |
| 32:2a:1387:G:H2' | 32:2a:1388:C:C6 | 2.51 | 0.46 |
| 33:2b:79:ASP:C | 33:2b:81:VAL:H | 2.23 | 0.46 |
| 34:2c:178:LEU:C | 34:2c:180:ALA:H | 2.23 | 0.46 |
| 37:2f:63:TYR:N | 37:2f:63:TYR:CD2 | 2.84 | 0.46 |
| 38:2g:23:VAL:O | 38:2g:27:ILE:HG13 | 2.16 | 0.46 |
| 42:2k:22:HIS:HB3 | 42:2k:29:ILE:HB | 1.98 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 56:2y:26:A:N1 | 56:2y:44:G:C6 | 2.83 | 0.46 |
| 56:2y:68:C:N4 | 56:2y:69:G:N7 | 2.63 | 0.46 |
| 1:1A:531:C:OP1 | 1:1A:561:G:N1 | 2.47 | 0.46 |
| 6:1G:110:ALA:O | 6:1G:113:ARG:N | 2.30 | 0.46 |
| 14:1S:39:ILE:HB | 14:1S:49:VAL:HG13 | 1.98 | 0.46 |
| 14:1S:93:LYS:HG2 | 14:1S:95:HIS:HB2 | 1.97 | 0.46 |
| 21:1Z:52:SER:C | 21:1Z:54:HIS:H | 2.24 | 0.46 |
| 32:1a:21:G:H2' | 32:1a:22:G:C8 | 2.50 | 0.46 |
| 32:1a:413:G:N2 | 32:1a:428:G:H1' | 2.31 | 0.46 |
| 32:1a:438:G:H4' | 35:1d:123:HIS:ND1 | 2.30 | 0.46 |
| 32:1a:509:A:H5'' | 35:1d:55:ALA:HB2 | 1.97 | 0.46 |
| 32:1a:1277:C:O2' | 32:1a:1279:A:H1' | 2.16 | 0.46 |
| 55:1x:64:G:H2' | 55:1x:65:C:C6 | 2.51 | 0.46 |
| 56:1y:44:G:H8 | 56:1y:44:G:OP2 | 1.98 | 0.46 |
| 1:2A:93:G:H2' | 1:2A:94:C:H6 | 1.79 | 0.46 |
| 1:2A:244:A:H2' | 1:2A:245:G:O4' | 2.16 | 0.46 |
| 1:2A:921:G:H2' | 1:2A:922:U:C6 | 2.50 | 0.46 |
| 1:2A:1839:G:C8 | 1:2A:1927:A:H1' | 2.50 | 0.46 |
| 2:2B:77:U:OP1 | 21:2Z:19:ARG:NH2 | 2.49 | 0.46 |
| 2:2B:78:A:C2 | 2:2B:100:A:C4 | 3.04 | 0.46 |
| 7:2H:107:VAL:HG23 | 7:2H:109:PHE:CD2 | 2.51 | 0.46 |
| 18:2W:29:LEU:HD22 | 18:2W:69:LEU:HD12 | 1.97 | 0.46 |
| 24:22:32:LEU:HD13 | 24:22:53:LEU:HB3 | 1.97 | 0.46 |
| 32:2a:325:A:H2' | 32:2a:326:G:O4' | 2.16 | 0.46 |
| 32:2a:922:G:C6 | 32:2a:923:A:C6 | 3.03 | 0.46 |
| 32:2a:1012:U:H2' | 32:2a:1013:G:C8 | 2.50 | 0.46 |
| 32:2a:1352:C:H2' | 32:2a:1353:G:C8 | 2.50 | 0.46 |
| 38:2g:79:ARG:NH1 | 38:2g:80:VAL:HG22 | 2.31 | 0.46 |
| 44:2m:50:GLU:O | 44:2m:54:VAL:HG23 | 2.15 | 0.46 |
| 50:2s:61:TYR:HE2 | 50:2s:63:THR:HG22 | 1.80 | 0.46 |
| 1:1A:389:G:O6 | 11:1P:70:GLN:HB2 | 2.16 | 0.46 |
| 1:1A:1924:C:H4' | 55:1x:13:C:O2' | 2.15 | 0.46 |
| 1:1A:2695:C:H2' | 1:1A:2696:U:C6 | 2.51 | 0.46 |
| 21:1Z:137:ILE:HA | 21:1Z:156:LYS:HZ1 | 1.80 | 0.46 |
| 23:11:50:ARG:HG2 | 23:11:59:THR:HG22 | 1.98 | 0.46 |
| 32:1a:341:C:H2' | 32:1a:342:C:H6 | 1.81 | 0.46 |
| 32:1a:1037:C:H2' | 32:1a:1038:C:C6 | 2.50 | 0.46 |
| 32:1a:1513:A:H2' | 32:1a:1514:C:C6 | 2.51 | 0.46 |
| 33:1b:73:THR:OG1 | 33:1b:170:GLU:OE1 | 2.33 | 0.46 |
| 33:1b:97:TRP:CZ2 | 33:1b:102:LEU:HD13 | 2.51 | 0.46 |
| 33:1b:102:LEU:HD23 | 33:1b:182:ILE:HD12 | 1.96 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:1d:158:ILE:H | 35:1d:158:ILE:HG13 | 1.52 | 0.46 |
| 37:1f:1:MET:HA | 37:1f:68:PRO:HA | 1.98 | 0.46 |
| 46:1o:56:LEU:O | 46:1o:60:VAL:HG23 | 2.15 | 0.46 |
| 50:1s:43:GLU:OE1 | 50:1s:43:GLU:N | 2.49 | 0.46 |
| 1:2A:212:G:H2' | 1:2A:213:A:O4' | 2.16 | 0.46 |
| 1:2A:884:C:H3' | 1:2A:885:C:C6 | 2.51 | 0.46 |
| 1:2A:908:C:O2' | 1:2A:909:A:H5' | 2.16 | 0.46 |
| 1:2A:1591:G:H2' | 1:2A:1592:C:H6 | 1.79 | 0.46 |
| 26:24:57:GLU:CB | 26:24:58:ARG:HA | 2.46 | 0.46 |
| 32:2a:611:A:H61 | 32:2a:629:G:H1 | 1.63 | 0.46 |
| 32:2a:646:U:H2' | 32:2a:647:C:C6 | 2.51 | 0.46 |
| 33:2b:142:LEU:HD21 | 33:2b:146:GLN:NE2 | 2.31 | 0.46 |
| 37:2f:97:PHE:CD2 | 49:2r:65:ILE:HD12 | 2.51 | 0.46 |
| 47:2p:69:THR:O | 47:2p:69:THR:OG1 | 2.33 | 0.46 |
| 48:2q:29:HIS:HB3 | 48:2q:33:GLY:N | 2.31 | 0.46 |
| 55:2x:19:G:H4' | 55:2x:20:U:OP2 | 2.15 | 0.46 |
| 56:2y:12:U:C2 | 56:2y:24:G:N2 | 2.84 | 0.46 |
| 1:1A:207:A:H2' | 1:1A:208:C:O4' | 2.15 | 0.46 |
| 1:1A:1085:A:H2' | 1:1A:1086:A:N3 | 2.30 | 0.46 |
| 1:1A:2051:A:H8 | 1:1A:2051:A:OP2 | 1.99 | 0.46 |
| 1:1A:2128:C:N4 | 1:1A:2160:G:H1 | 2.11 | 0.46 |
| 1:1A:2422:A:O4' | 56:1y:76:A:N6 | 2.49 | 0.46 |
| 17:1V:14:VAL:HG12 | 17:1V:18:LEU:HD23 | 1.98 | 0.46 |
| 30:18:29:LYS:HG2 | 30:18:44:LYS:HB3 | 1.98 | 0.46 |
| 32:1a:159:G:H21 | 32:1a:161:A:H3' | 1.80 | 0.46 |
| 32:1a:221:C:H2' | 32:1a:222:U:H6 | 1.80 | 0.46 |
| 35:1d:129:ASN:OD1 | 35:1d:145:GLU:N | 2.42 | 0.46 |
| 46:1o:55:GLY:O | 46:1o:59:MET:HG3 | 2.16 | 0.46 |
| 47:1p:50:LYS:HD2 | 47:1p:50:LYS:HA | 1.81 | 0.46 |
| 52:1u:3:LYS:HD3 | 52:1u:14:TRP:HD1 | 1.81 | 0.46 |
| 57:1z:8:ASP:C | 57:1z:8:ASP:OD1 | 2.59 | 0.46 |
| 2:2B:61:G:C6 | 2:2B:62:C:C4 | 3.03 | 0.46 |
| 5:2F:32:LEU:HD13 | 5:2F:112:MET:HE1 | 1.97 | 0.46 |
| 21:2Z:98:MET:O | 21:2Z:125:LEU:HD12 | 2.16 | 0.46 |
| 32:2a:67:C:H2' | 32:2a:68:G:H8 | 1.80 | 0.46 |
| 32:2a:540:G:C6 | 32:2a:541:G:C5 | 3.04 | 0.46 |
| 32:2a:973:G:OP1 | 41:2j:57:LYS:NZ | 2.41 | 0.46 |
| 32:2a:1239:A:O2' | 38:2g:114:ARG:O | 2.31 | 0.46 |
| 33:2b:98:LEU:HB2 | 33:2b:101:MET:HG3 | 1.98 | 0.46 |
| 34:2c:17:ASP:O | 34:2c:54:ARG:NH2 | 2.48 | 0.46 |
| 39:2h:21:LYS:N | 39:2h:65:TYR:OH | 2.49 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 47:2p:43:LYS:HG2 | 47:2p:48:TRP:CD2 | 2.50 | 0.46 |
| 48:2q:45:HIS:HB3 | 48:2q:72:ARG:HG2 | 1.98 | 0.46 |
| 53:2v:12:A:N3 | 53:2v:12:A:H2' | 2.30 | 0.46 |
| 1:1A:568:U:H5' | 1:1A:945:A:H62 | 1.81 | 0.46 |
| 1:1A:839:U:H2' | 1:1A:840:C:C6 | 2.51 | 0.46 |
| 1:1A:1021:A:H3' | 1:1A:1021:A:N3 | 2.31 | 0.46 |
| 1:1A:1153:C:H2' | 1:1A:1154:G:O4' | 2.16 | 0.46 |
| 1:1A:2683:C:O2 | 10:1O:70:LYS:NZ | 2.39 | 0.46 |
| 2:1B:42:C:O2' | 6:1G:66:GLN:HG2 | 2.16 | 0.46 |
| 5:1F:178:PRO:HB2 | 5:1F:201:VAL:HG21 | 1.97 | 0.46 |
| 6:1G:140:ILE:HG22 | 6:1G:141:PHE:CD2 | 2.50 | 0.46 |
| 8:1I:127:VAL:O | 8:1I:128:LEU:HD23 | 2.16 | 0.46 |
| 10:1O:16:ALA:HB2 | 10:1O:52:VAL:HG21 | 1.97 | 0.46 |
| 24:12:10:LEU:HD21 | 24:12:59:ARG:HD3 | 1.98 | 0.46 |
| 30:18:26:LYS:HG2 | 30:18:46:ARG:O | 2.15 | 0.46 |
| 32:1a:392:G:H2' | 32:1a:393:A:H8 | 1.81 | 0.46 |
| 32:1a:1279:A:OP2 | 41:1j:9:ARG:NH1 | 2.49 | 0.46 |
| 33:1b:27:LYS:HB2 | 33:1b:194:PRO:HD2 | 1.97 | 0.46 |
| 37:1f:10:LEU:HD21 | 37:1f:61:LEU:HD22 | 1.98 | 0.46 |
| 1:2A:38:A:H2' | 1:2A:39:C:C6 | 2.51 | 0.46 |
| 1:2A:635:C:O2' | 1:2A:639:U:OP1 | 2.28 | 0.46 |
| 1:2A:2177:C:H2' | 1:2A:2178:C:O4' | 2.15 | 0.46 |
| 1:2A:2431:U:OP1 | 62:2A:3956:HOH:O | 2.21 | 0.46 |
| 7:2H:68:THR:O | 7:2H:72:ILE:HG12 | 2.15 | 0.46 |
| 7:2H:70:THR:HG22 | 7:2H:74:ASN:ND2 | 2.27 | 0.46 |
| 12:2Q:85:LYS:HE2 | 22:20:7:LEU:HD12 | 1.98 | 0.46 |
| 32:2a:114:U:H1' | 32:2a:353:A:H1' | 1.98 | 0.46 |
| 32:2a:1305:G:H5' | 52:2u:4:GLY:HA3 | 1.96 | 0.46 |
| 33:2b:16:HIS:C | 33:2b:18:GLY:H | 2.24 | 0.46 |
| 33:2b:77:ALA:HA | 33:2b:80:ILE:CG2 | 2.46 | 0.46 |
| 46:2o:16:ALA:CB | 46:2o:21:ASP:HB3 | 2.38 | 0.46 |
| 1:1A:55:G:O2' | 1:1A:127:A:N1 | 2.44 | 0.45 |
| 1:1A:919:G:N2 | 1:1A:2269:A:OP2 | 2.47 | 0.45 |
| 1:1A:1698:A:C8 | 1:1A:1700:A:O4' | 2.69 | 0.45 |
| 1:1A:2100:G:H2' | 1:1A:2101:G:C8 | 2.51 | 0.45 |
| 1:1A:2324:C:H5'' | 1:1A:2325:G:H5' | 1.98 | 0.45 |
| 4:1E:40:GLU:CD | 4:1E:40:GLU:H | 2.23 | 0.45 |
| 4:1E:143:ASN:HD22 | 4:1E:147:PRO:CD | 2.28 | 0.45 |
| 13:1R:16:HIS:HD2 | 13:1R:16:HIS:O | 1.99 | 0.45 |
| 19:1X:34:ALA:HA | 19:1X:38:GLU:OE1 | 2.16 | 0.45 |
| 32:1a:165:C:O2' | 32:1a:166:G:H5' | 2.14 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 32:1a:946:A:H2' | 32:1a:947:G:C8 | 2.51 | 0.45 |
| 34:1c:181:ASN:HD22 | 34:1c:204:LEU:HB2 | 1.79 | 0.45 |
| 36:1e:137:GLU:O | 36:1e:141:GLN:HG3 | 2.16 | 0.45 |
| 40:1i:78:LYS:HG2 | 40:1i:78:LYS:O | 2.15 | 0.45 |
| 1:2A:630:G:N2 | 1:2A:633:A:OP2 | 2.46 | 0.45 |
| 1:2A:2497:A:H5'' | 62:2A:4064:HOH:O | 2.16 | 0.45 |
| 5:2F:117:ARG:HH12 | 11:2P:1:MET:N | 2.14 | 0.45 |
| 5:2F:165:ARG:HG2 | 5:2F:168:ARG:NH2 | 2.31 | 0.45 |
| 8:2I:31:LEU:HD21 | 8:2I:38:LEU:HG | 1.97 | 0.45 |
| 8:2I:50:ARG:HA | 8:2I:53:ALA:HB3 | 1.97 | 0.45 |
| 8:2I:120:ILE:HG21 | 8:2I:126:TYR:CE2 | 2.51 | 0.45 |
| 12:2Q:57:HIS:HD2 | 12:2Q:117:ALA:HB2 | 1.82 | 0.45 |
| 16:2U:28:ARG:NH1 | 16:2U:38:THR:OG1 | 2.46 | 0.45 |
| 32:2a:1272:G:N2 | 32:2a:1273:G:C6 | 2.83 | 0.45 |
| 35:2d:22:LYS:HB2 | 35:2d:26:CYS:SG | 2.56 | 0.45 |
| 36:2e:72:GLN:O | 36:2e:75:THR:HG22 | 2.16 | 0.45 |
| 52:2u:5:ASP:O | 52:2u:11:GLY:HA3 | 2.16 | 0.45 |
| 1:1A:271(H):G:H1 | 1:1A:271(P):C:H42 | 1.63 | 0.45 |
| 1:1A:590:A:H2' | 1:1A:591:C:O4' | 2.16 | 0.45 |
| 1:1A:1670:C:O2 | 4:1E:129:HIS:NE2 | 2.46 | 0.45 |
| 1:1A:2386:C:H2' | 1:1A:2387:U:C6 | 2.52 | 0.45 |
| 1:1A:2808:U:H5'' | 1:1A:2891:G:O6 | 2.16 | 0.45 |
| 5:1F:28:ILE:O | 5:1F:30:PRO:HD3 | 2.17 | 0.45 |
| 5:1F:53:THR:HG22 | 5:1F:55:GLY:H | 1.80 | 0.45 |
| 21:1Z:10:ARG:HG3 | 21:1Z:36:LYS:HB3 | 1.98 | 0.45 |
| 32:1a:280:C:N3 | 48:1q:39:SER:N | 2.64 | 0.45 |
| 32:1a:376:G:P | 47:1p:67:THR:HG21 | 2.57 | 0.45 |
| 32:1a:841:U:C4 | 32:1a:848:C:H1' | 2.52 | 0.45 |
| 32:1a:966:M2G:HM13 | 32:1a:967:5MC:H1' | 1.98 | 0.45 |
| 32:1a:1136:U:O5' | 32:1a:1136:U:H6 | 2.00 | 0.45 |
| 33:1b:165:VAL:HG13 | 33:1b:166:ASP:N | 2.28 | 0.45 |
| 1:2A:184:C:H2' | 1:2A:185:U:H6 | 1.82 | 0.45 |
| 1:2A:218:A:C2 | 1:2A:235:U:H4' | 2.51 | 0.45 |
| 1:2A:747:U:O2 | 1:2A:2014:A:H1' | 2.15 | 0.45 |
| 1:2A:1327:C:O2' | 1:2A:1328:G:H5' | 2.16 | 0.45 |
| 1:2A:2376:A:H2' | 1:2A:2377:A:O4' | 2.15 | 0.45 |
| 2:2B:66:A:N6 | 2:2B:108:U:H3' | 2.31 | 0.45 |
| 6:2G:11:TYR:HB2 | 6:2G:176:LEU:HD21 | 1.97 | 0.45 |
| 6:2G:117:PHE:CZ | 6:2G:179:PRO:HG2 | 2.51 | 0.45 |
| 15:2T:42:ILE:N | 15:2T:42:ILE:HD12 | 2.31 | 0.45 |
| 32:2a:21:G:H2' | 32:2a:22:G:C8 | 2.50 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 32:2a:651:C:N4 | 32:2a:753:A:OP2 | 2.48 | 0.45 |
| 35:2d:76:ARG:O | 35:2d:80:GLU:HG2 | 2.16 | 0.45 |
| 39:2h:138:TRP:C | 39:2h:138:TRP:CD1 | 2.93 | 0.45 |
| 41:2j:23:ILE:HD13 | 41:2j:23:ILE:HA | 1.81 | 0.45 |
| 45:2n:57:ARG:HG2 | 45:2n:58:LYS:N | 2.31 | 0.45 |
| 46:2o:81:LEU:HG | 46:2o:85:LEU:HD12 | 1.98 | 0.45 |
| 48:2q:45:HIS:NE2 | 48:2q:47:PRO:HB3 | 2.32 | 0.45 |
| 51:2t:43:LEU:O | 51:2t:47:GLY:HA2 | 2.16 | 0.45 |
| 54:2w:18:G:H4' | 54:2w:60:U:C5 | 2.51 | 0.45 |
| 1:1A:479:A:N3 | 1:1A:481:G:H5'' | 2.31 | 0.45 |
| 1:1A:657:U:H2' | 1:1A:658:C:C6 | 2.51 | 0.45 |
| 1:1A:2861:G:H8 | 1:1A:2861:G:H5'' | 1.80 | 0.45 |
| 8:1I:33:ARG:C | 8:1I:35:LEU:H | 2.25 | 0.45 |
| 19:1X:92:LEU:O | 19:1X:94:GLY:N | 2.49 | 0.45 |
| 32:1a:658:G:C2 | 32:1a:749:C:N3 | 2.85 | 0.45 |
| 33:1b:15:VAL:HG21 | 33:1b:213:LEU:HD22 | 1.98 | 0.45 |
| 33:1b:92:TYR:CE1 | 33:1b:94:ASN:HB2 | 2.51 | 0.45 |
| 33:1b:112:VAL:O | 33:1b:115:LEU:HB3 | 2.16 | 0.45 |
| 35:1d:22:LYS:HB2 | 35:1d:26:CYS:SG | 2.56 | 0.45 |
| 36:1e:135:THR:O | 36:1e:139:LEU:HG | 2.16 | 0.45 |
| 44:1m:4:ILE:HD11 | 44:1m:60:VAL:HG11 | 1.98 | 0.45 |
| 51:1t:26:ASN:OD1 | 51:1t:71:THR:OG1 | 2.34 | 0.45 |
| 1:2A:253:C:H2' | 1:2A:254:G:O4' | 2.17 | 0.45 |
| 1:2A:1637:A:H4' | 1:2A:2711:A:O2' | 2.16 | 0.45 |
| 1:2A:2748:A:C2 | 7:2H:63:SER:HB3 | 2.51 | 0.45 |
| 3:2D:182:LEU:HD23 | 3:2D:182:LEU:HA | 1.80 | 0.45 |
| 14:2S:3:ARG:NH1 | 14:2S:3:ARG:HA | 2.31 | 0.45 |
| 30:28:63:PRO:HG2 | 30:28:64:TYR:CD2 | 2.51 | 0.45 |
| 32:2a:1056:U:H5' | 34:2c:163:ALA:HB2 | 1.98 | 0.45 |
| 32:2a:1192:C:N4 | 32:2a:1193:G:C4 | 2.85 | 0.45 |
| 32:2a:1357:A:H8 | 32:2a:1357:A:O5' | 1.99 | 0.45 |
| 34:2c:35:GLU:HG2 | 34:2c:59:ARG:NH2 | 2.31 | 0.45 |
| 35:2d:98:GLU:OE1 | 35:2d:103:ASN:ND2 | 2.43 | 0.45 |
| 35:2d:108:LEU:HD13 | 35:2d:183:GLY:HA3 | 1.97 | 0.45 |
| 37:2f:25:ILE:HD13 | 37:2f:82:ARG:HD3 | 1.97 | 0.45 |
| 39:2h:83:ILE:HG13 | 39:2h:137:VAL:HG22 | 1.99 | 0.45 |
| 1:1A:278:A:H8 | 1:1A:278:A:OP2 | 1.99 | 0.45 |
| 1:1A:671:C:N4 | 62:1A:4439:HOH:O | 2.48 | 0.45 |
| 1:1A:1405:U:H2' | 1:1A:1406:U:C6 | 2.51 | 0.45 |
| 1:1A:2379:G:O2' | 14:1S:17:ARG:NH2 | 2.47 | 0.45 |
| 5:1F:53:THR:CG2 | 5:1F:55:GLY:H | 2.28 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 21:1Z:4:ARG:NE | 21:1Z:60:GLU:OE2 | 2.47 | 0.45 |
| 32:1a:111:G:H5'' | 47:1p:27:LYS:HB3 | 1.98 | 0.45 |
| 32:1a:163:C:H2' | 32:1a:164:U:C6 | 2.52 | 0.45 |
| 32:1a:1180:A:OP1 | 40:1i:103:THR:HB | 2.17 | 0.45 |
| 33:1b:185:ILE:CG2 | 33:1b:199:TYR:HB2 | 2.44 | 0.45 |
| 39:1h:87:SER:HB2 | 39:1h:93:VAL:H | 1.82 | 0.45 |
| 51:1t:92:LEU:O | 51:1t:96:GLY:HA2 | 2.17 | 0.45 |
| 55:1x:17:C:H3' | 55:1x:17(A):U:H2' | 1.99 | 0.45 |
| 1:2A:322:A:C5 | 1:2A:340:A:C2 | 3.04 | 0.45 |
| 1:2A:657:U:H2' | 1:2A:658:C:C6 | 2.51 | 0.45 |
| 1:2A:910:A:C5 | 12:2Q:13:GLN:HG3 | 2.52 | 0.45 |
| 1:2A:1946:U:H2' | 1:2A:1947:C:C6 | 2.51 | 0.45 |
| 1:2A:2365:G:N7 | 30:28:39:LYS:NZ | 2.57 | 0.45 |
| 1:2A:2523:G:O2' | 1:2A:2764:A:O2' | 2.27 | 0.45 |
| 5:2F:20:LEU:HD12 | 5:2F:20:LEU:HA | 1.76 | 0.45 |
| 9:2N:35:ARG:O | 9:2N:42:TRP:NE1 | 2.47 | 0.45 |
| 32:2a:173:U:H5'' | 32:2a:197:A:O4' | 2.16 | 0.45 |
| 32:2a:1121:U:C4 | 32:2a:1122:U:C4 | 3.04 | 0.45 |
| 43:2l:117:ARG:HB3 | 43:2l:122:THR:O | 2.17 | 0.45 |
| 44:2m:16:ASP:OD1 | 44:2m:16:ASP:N | 2.49 | 0.45 |
| 46:2o:64:ARG:HH11 | 46:2o:68:ARG:NH2 | 2.13 | 0.45 |
| 47:2p:28:ARG:HG2 | 47:2p:28:ARG:HH11 | 1.81 | 0.45 |
| 1:1A:41:C:H2' | 1:1A:42:G:O4' | 2.16 | 0.45 |
| 1:1A:271(D):G:O2' | 1:1A:271(E):U:H5' | 2.16 | 0.45 |
| 1:1A:1174:A:HI' | 1:1A:1175:U:H5'' | 1.98 | 0.45 |
| 1:1A:2080:G:OP1 | 23:11:35:THR:HG21 | 2.16 | 0.45 |
| 1:1A:2149:G:C6 | 1:1A:2150:U:C2 | 3.05 | 0.45 |
| 1:1A:2709:G:H2' | 1:1A:2710:C:C6 | 2.52 | 0.45 |
| 3:1D:237:GLU:OE2 | 62:1D:402:HOH:O | 2.21 | 0.45 |
| 7:1H:20:ALA:HB1 | 7:1H:21:PRO:HD2 | 1.98 | 0.45 |
| 32:1a:1330:U:H2' | 32:1a:1331:G:H5' | 1.97 | 0.45 |
| 32:1a:1330:U:C2' | 32:1a:1331:G:H5' | 2.47 | 0.45 |
| 35:1d:154:ASN:HA | 35:1d:159:ARG:HH21 | 1.81 | 0.45 |
| 49:1r:47:THR:O | 49:1r:83:GLU:N | 2.37 | 0.45 |
| 1:2A:2438:U:O2' | 1:2A:2440:C:OP1 | 2.26 | 0.45 |
| 5:2F:176:LEU:HD23 | 5:2F:176:LEU:HA | 1.82 | 0.45 |
| 12:2Q:38:GLU:HB2 | 12:2Q:127:ILE:HB | 1.99 | 0.45 |
| 21:2Z:128:VAL:HG23 | 21:2Z:161:VAL:HB | 1.99 | 0.45 |
| 32:2a:900:A:H2' | 32:2a:901:A:C8 | 2.52 | 0.45 |
| 32:2a:1289:A:OP1 | 52:2u:10:ARG:NH2 | 2.49 | 0.45 |
| 34:2c:23:TYR:CG | 34:2c:24:ALA:N | 2.84 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 36:2e:62:ALA:C | 36:2e:64:ARG:H | 2.24 | 0.45 |
| 38:2g:58:PRO:O | 38:2g:61:VAL:N | 2.49 | 0.45 |
| 43:2l:75:HIS:ND1 | 43:2l:77:LEU:HB2 | 2.32 | 0.45 |
| 51:2t:22:ARG:O | 51:2t:26:ASN:HB2 | 2.17 | 0.45 |
| 57:2z:2:LYS:HB3 | 57:2z:3:LYS:H | 1.54 | 0.45 |
| 1:1A:577:G:O2' | 1:1A:1254:A:OP1 | 2.34 | 0.45 |
| 1:1A:910:A:N1 | 1:1A:2277:G:H1' | 2.31 | 0.45 |
| 1:1A:1419:A:O2' | 1:1A:1421:G:N7 | 2.28 | 0.45 |
| 5:1F:182:ASN:HD21 | 5:1F:185:ASP:CG | 2.24 | 0.45 |
| 18:1W:5:ALA:C | 18:1W:6:ILE:HG13 | 2.41 | 0.45 |
| 26:14:53:GLU:HB2 | 26:14:55:ARG:O | 2.17 | 0.45 |
| 26:14:57:GLU:HA | 26:14:58:ARG:HA | 1.80 | 0.45 |
| 32:1a:660:G:OP1 | 46:1o:5:LYS:HD3 | 2.17 | 0.45 |
| 36:1e:86:ALA:O | 36:1e:125:SER:N | 2.38 | 0.45 |
| 40:1i:3:GLN:HG2 | 40:1i:20:ARG:NE | 2.31 | 0.45 |
| 50:1s:24:ALA:C | 50:1s:26:GLY:H | 2.24 | 0.45 |
| 56:1y:39:PSU:H2' | 56:1y:40:C:C6 | 2.51 | 0.45 |
| 57:1z:2:LYS:HB2 | 57:1z:2:LYS:HE3 | 1.77 | 0.45 |
| 1:2A:1116:C:H2' | 1:2A:1117:G:C8 | 2.52 | 0.45 |
| 1:2A:1364:G:P | 23:21:3:LYS:HG3 | 2.57 | 0.45 |
| 6:2G:41:GLN:HB3 | 6:2G:43:LEU:HD22 | 1.98 | 0.45 |
| 8:2I:48:GLU:HA | 8:2I:51:ILE:HG22 | 1.98 | 0.45 |
| 21:2Z:6:LYS:HD3 | 21:2Z:8:TYR:HE2 | 1.81 | 0.45 |
| 28:26:12:GLU:OE1 | 28:26:19:ARG:NH1 | 2.49 | 0.45 |
| 32:2a:938:A:N7 | 62:2a:1932:HOH:O | 2.36 | 0.45 |
| 32:2a:1244:C:C2 | 32:2a:1294:G:N2 | 2.85 | 0.45 |
| 33:2b:17:PHE:HA | 33:2b:44:LEU:HD21 | 1.98 | 0.45 |
| 43:2l:24:VAL:HB | 43:2l:27:LEU:HD12 | 1.97 | 0.45 |
| 56:2y:7:A:OP2 | 56:2y:7:A:H2' | 2.16 | 0.45 |
| 1:1A:548:A:H3' | 1:1A:548:A:OP2 | 2.16 | 0.45 |
| 1:1A:1814:G:H4' | 3:1D:51:VAL:HG21 | 1.99 | 0.45 |
| 1:1A:1891:G:O6 | 62:1A:4238:HOH:O | 2.17 | 0.45 |
| 1:1A:2591:C:H2' | 1:1A:2592:G:C8 | 2.52 | 0.45 |
| 23:11:50:ARG:HD2 | 23:11:57:GLU:OE1 | 2.16 | 0.45 |
| 27:15:52:TYR:HB3 | 27:15:57:VAL:HG21 | 1.98 | 0.45 |
| 32:1a:278:G:OP2 | 48:1q:92:ARG:NH2 | 2.50 | 0.45 |
| 32:1a:309:G:O2' | 32:1a:607:A:N1 | 2.50 | 0.45 |
| 32:1a:382:A:H2' | 32:1a:383:A:H8 | 1.82 | 0.45 |
| 32:1a:1025:U:O2 | 32:1a:1036:G:C6 | 2.69 | 0.45 |
| 33:1b:187:LEU:HD12 | 33:1b:201:ILE:O | 2.17 | 0.45 |
| 36:1e:62:ALA:C | 36:1e:64:ARG:H | 2.25 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 39:1h:121:ASP:OD2 | 39:1h:125:ARG:NH2 | 2.50 | 0.45 |
| 42:1k:48:ILE:O | 42:1k:50:TYR:N | 2.50 | 0.45 |
| 44:1m:121:LYS:HE2 | 44:1m:121:LYS:HB2 | 1.62 | 0.45 |
| 50:1s:3:ARG:NE | 50:1s:8:GLY:O | 2.50 | 0.45 |
| 54:1w:76:F3N:OP1 | 62:1w:201:HOH:O | 2.21 | 0.45 |
| 56:1y:7:A:HO2' | 56:1y:49:C:H5' | 1.82 | 0.45 |
| 1:2A:764:A:H5'' | 3:2D:210:GLY:CA | 2.47 | 0.45 |
| 1:2A:2335:A:C8 | 1:2A:2337:G:C5 | 3.04 | 0.45 |
| 1:2A:2812:G:H2' | 1:2A:2813:A:C8 | 2.52 | 0.45 |
| 1:2A:2823:A:OP1 | 4:2E:159:HIS:NE2 | 2.37 | 0.45 |
| 2:2B:54:G:H21 | 6:2G:29:TRP:HE1 | 1.65 | 0.45 |
| 6:2G:16:ARG:O | 6:2G:20:ILE:HG13 | 2.16 | 0.45 |
| 7:2H:109:PHE:C | 7:2H:111:HIS:H | 2.24 | 0.45 |
| 13:2R:73:VAL:HG23 | 13:2R:74:LYS:N | 2.31 | 0.45 |
| 20:2Y:97:ARG:HD3 | 20:2Y:107:ASP:O | 2.17 | 0.45 |
| 26:24:41:PRO:HA | 26:24:44:THR:HG22 | 1.98 | 0.45 |
| 44:2m:13:LYS:C | 44:2m:44:ARG:HD2 | 2.41 | 0.45 |
| 47:2p:21:VAL:HG23 | 47:2p:33:ILE:HB | 1.98 | 0.45 |
| 1:1A:234:C:H2' | 1:1A:235:U:C6 | 2.51 | 0.45 |
| 1:1A:392:C:OP1 | 62:1A:4251:HOH:O | 2.21 | 0.45 |
| 1:1A:783:A:O2' | 1:1A:785:G:OP1 | 2.31 | 0.45 |
| 1:1A:2119:A:N1 | 1:1A:2170:A:H2' | 2.32 | 0.45 |
| 1:1A:2218:U:O4' | 23:11:52:ARG:NH2 | 2.49 | 0.45 |
| 1:1A:2774:C:H2' | 1:1A:2775:A:O4' | 2.16 | 0.45 |
| 5:1F:132:VAL:HA | 5:1F:138:GLU:HB3 | 1.99 | 0.45 |
| 32:1a:41:G:H2' | 32:1a:42:G:C8 | 2.52 | 0.45 |
| 32:1a:134:A:H61 | 47:1p:25:ARG:HH12 | 1.65 | 0.45 |
| 32:1a:765:G:H5'' | 32:1a:766:A:OP1 | 2.17 | 0.45 |
| 32:1a:1111:A:N1 | 34:1c:177:THR:OG1 | 2.38 | 0.45 |
| 32:1a:1260:C:O5' | 32:1a:1284:C:H4' | 2.17 | 0.45 |
| 32:1a:1286:A:H2 | 52:1u:18:TYR:OH | 1.99 | 0.45 |
| 33:1b:195:ASP:O | 39:1h:68:ARG:NH2 | 2.45 | 0.45 |
| 34:1c:132:ARG:HD3 | 34:1c:136:GLN:NE2 | 2.31 | 0.45 |
| 35:1d:107:ARG:NH2 | 35:1d:194:LEU:HD11 | 2.32 | 0.45 |
| 38:1g:20:ASP:OD2 | 38:1g:63:LYS:HE3 | 2.17 | 0.45 |
| 41:1j:16:LEU:HD23 | 41:1j:70:ARG:HG2 | 1.99 | 0.45 |
| 1:2A:885:C:H2' | 1:2A:886:C:H4' | 1.98 | 0.45 |
| 1:2A:1288:U:C2 | 1:2A:1327:C:O2 | 2.70 | 0.45 |
| 32:2a:662:G:O2' | 32:2a:836:G:OP1 | 2.34 | 0.45 |
| 33:2b:95:GLN:HG3 | 33:2b:147:LYS:HD3 | 1.98 | 0.45 |
| 34:2c:20:SER:HA | 34:2c:57:ILE:O | 2.17 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:2d:25:ARG:NH2 | 35:2d:30:LYS:HB3 | 2.32 | 0.45 |
| 35:2d:121:VAL:O | 35:2d:134:ASP:HA | 2.17 | 0.45 |
| 45:2n:3:ARG:HH21 | 45:2n:3:ARG:HA | 1.82 | 0.45 |
| 48:2q:50:LYS:O | 48:2q:50:LYS:HG2 | 2.17 | 0.45 |
| 1:1A:236:C:H2' | 1:1A:237:C:C6 | 2.52 | 0.45 |
| 1:1A:459:U:H5'' | 29:17:40:TRP:CD2 | 2.51 | 0.45 |
| 1:1A:657:U:H2' | 1:1A:658:C:H6 | 1.82 | 0.45 |
| 1:1A:1095:A:C8 | 1:1A:1096:A:C8 | 3.04 | 0.45 |
| 1:1A:2065:C:H2' | 1:1A:2066:C:C6 | 2.52 | 0.45 |
| 1:1A:2573:C:H3' | 62:1A:4342:HOH:O | 2.17 | 0.45 |
| 7:1H:144:VAL:O | 7:1H:148:ILE:HG12 | 2.16 | 0.45 |
| 11:1P:101:VAL:HA | 11:1P:106:LEU:O | 2.17 | 0.45 |
| 19:1X:57:LEU:HD11 | 19:1X:78:LYS:HE3 | 1.98 | 0.45 |
| 20:1Y:55:TYR:CE1 | 20:1Y:61:ILE:HG21 | 2.51 | 0.45 |
| 26:14:50:VAL:HG21 | 44:1m:64:TRP:C | 2.42 | 0.45 |
| 32:1a:657:G:H2' | 32:1a:658:G:C8 | 2.51 | 0.45 |
| 32:1a:977:A:O2' | 32:1a:981:U:N3 | 2.47 | 0.45 |
| 32:1a:1073:U:O2' | 33:1b:104:ASN:OD1 | 2.26 | 0.45 |
| 1:2A:27:G:C2 | 1:2A:512:G:N3 | 2.85 | 0.45 |
| 1:2A:1359:A:C2 | 1:2A:1360:A:C8 | 3.04 | 0.45 |
| 1:2A:1541:G:H3' | 1:2A:1542:A:H2' | 1.99 | 0.45 |
| 1:2A:1754:C:OP1 | 15:2T:96:ARG:NH1 | 2.50 | 0.45 |
| 1:2A:1826:G:H4' | 3:2D:242:ARG:CZ | 2.47 | 0.45 |
| 2:2B:110:G:C2' | 2:2B:111:G:H5' | 2.46 | 0.45 |
| 6:2G:107:LEU:HD13 | 6:2G:177:GLY:O | 2.17 | 0.45 |
| 11:2P:71:VAL:HG23 | 11:2P:72:PRO:HA | 1.99 | 0.45 |
| 12:2Q:22:LYS:HB3 | 12:2Q:22:LYS:HE2 | 1.61 | 0.45 |
| 32:2a:7:G:O2' | 36:2e:120:THR:O | 2.35 | 0.45 |
| 32:2a:1171:G:H2' | 32:2a:1172:C:C6 | 2.52 | 0.45 |
| 34:2c:3:ASN:N | 34:2c:3:ASN:OD1 | 2.50 | 0.45 |
| 34:2c:138:VAL:HG12 | 34:2c:151:VAL:HG23 | 1.97 | 0.45 |
| 38:2g:79:ARG:H | 38:2g:79:ARG:HG3 | 1.67 | 0.45 |
| 1:1A:365:C:OP2 | 62:1A:4252:HOH:O | 2.21 | 0.45 |
| 1:1A:428:A:H8 | 1:1A:428:A:OP2 | 2.00 | 0.45 |
| 1:1A:880:G:H1 | 1:1A:898:C:N4 | 2.15 | 0.45 |
| 1:1A:2160:G:N1 | 1:1A:2161:C:N3 | 2.65 | 0.45 |
| 1:1A:2314:C:H2' | 1:1A:2315:G:C8 | 2.51 | 0.45 |
| 3:1D:206:LEU:HA | 3:1D:211:ARG:HH11 | 1.82 | 0.45 |
| 6:1G:60:LEU:HA | 6:1G:60:LEU:HD12 | 1.71 | 0.45 |
| 11:1P:99:LEU:HD12 | 11:1P:102:ARG:HH21 | 1.82 | 0.45 |
| 24:12:3:LEU:HD23 | 24:12:3:LEU:HA | 1.83 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 32:1a:954:G:C6 | 32:1a:955:U:C4 | 3.05 | 0.45 |
| 32:1a:1035:A:C2 | 32:1a:1036:G:N2 | 2.84 | 0.45 |
| 32:1a:1182:G:H4' | 32:1a:1183:A:H5'' | 1.98 | 0.45 |
| 35:1d:173:TRP:HB3 | 35:1d:187:ARG:HG3 | 1.98 | 0.45 |
| 40:1i:25:LYS:HE3 | 40:1i:32:ASP:OD2 | 2.17 | 0.45 |
| 40:1i:85:LEU:O | 40:1i:88:TYR:HB3 | 2.16 | 0.45 |
| 42:1k:73:MET:C | 42:1k:75:TYR:H | 2.23 | 0.45 |
| 43:1l:88:GLY:O | 43:1l:99:HIS:HD2 | 2.00 | 0.45 |
| 54:1w:1:G:H2' | 54:1w:2:C:H6 | 1.79 | 0.45 |
| 1:2A:2190:G:H2' | 1:2A:2191:G:O4' | 2.16 | 0.45 |
| 1:2A:2406:U:C4 | 11:2P:72:PRO:HD2 | 2.52 | 0.45 |
| 17:2V:76:LYS:HD2 | 17:2V:81:TYR:CD2 | 2.51 | 0.45 |
| 19:2X:66:LEU:HD12 | 19:2X:66:LEU:HA | 1.69 | 0.45 |
| 23:21:32:LYS:O | 62:21:201:HOH:O | 2.21 | 0.45 |
| 32:2a:283:C:H2' | 32:2a:284:G:O4' | 2.17 | 0.45 |
| 32:2a:519:C:H2' | 32:2a:520:A:O4' | 2.17 | 0.45 |
| 32:2a:939:G:H2' | 32:2a:940:C:C6 | 2.52 | 0.45 |
| 32:2a:1305:G:O2' | 32:2a:1306:A:OP2 | 2.35 | 0.45 |
| 34:2c:39:ILE:HG22 | 34:2c:43:LEU:HD12 | 1.98 | 0.45 |
| 40:2i:81:ILE:O | 40:2i:85:LEU:HD23 | 2.17 | 0.45 |
| 44:2m:82:MET:CE | 44:2m:92:HIS:HB3 | 2.44 | 0.45 |
| 44:2m:117:VAL:HG22 | 44:2m:118:ALA:H | 1.80 | 0.45 |
| 46:2o:5:LYS:O | 46:2o:9:GLN:HG2 | 2.17 | 0.45 |
| 1:1A:1919:A:O2' | 32:1a:1517:G:N3 | 2.45 | 0.44 |
| 1:1A:2820:A:OP2 | 13:1R:2:ARG:NH2 | 2.50 | 0.44 |
| 5:1F:117:ARG:HH12 | 11:1P:1:MET:N | 2.15 | 0.44 |
| 12:1Q:85:LYS:N | 12:1Q:85:LYS:HD2 | 2.32 | 0.44 |
| 32:1a:159:G:N2 | 32:1a:161:A:O5' | 2.50 | 0.44 |
| 32:1a:189(D):C:H2' | 32:1a:189(E):U:O4' | 2.17 | 0.44 |
| 32:1a:358:U:H2' | 32:1a:359:U:H6 | 1.80 | 0.44 |
| 32:1a:1315:U:H2' | 32:1a:1316:G:O4' | 2.17 | 0.44 |
| 34:1c:22:TRP:CZ2 | 45:1n:54:PRO:HG2 | 2.53 | 0.44 |
| 44:1m:37:THR:OG1 | 44:1m:39:ILE:HD12 | 2.17 | 0.44 |
| 1:2A:1782:C:H1' | 1:2A:2609:U:H5'' | 1.99 | 0.44 |
| 1:2A:2151:G:H2' | 1:2A:2152:G:H8 | 1.82 | 0.44 |
| 1:2A:2359:C:H2' | 1:2A:2360:A:O4' | 2.18 | 0.44 |
| 1:2A:2409:G:H2' | 1:2A:2410:G:O4' | 2.17 | 0.44 |
| 1:2A:2732:G:H3' | 1:2A:2733:A:O4' | 2.17 | 0.44 |
| 2:2B:83:G:H1 | 2:2B:94:C:H42 | 1.63 | 0.44 |
| 4:2E:84:PHE:CZ | 4:2E:86:PRO:HB3 | 2.51 | 0.44 |
| 9:2N:58:ASP:OD1 | 9:2N:58:ASP:N | 2.40 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 9:2N:72:TYR:O | 9:2N:85:ILE:N | 2.41 | 0.44 |
| 27:25:33:CYS:HB2 | 27:25:40:LYS:HD3 | 1.99 | 0.44 |
| 27:25:41:PRO:O | 27:25:44:THR:OG1 | 2.29 | 0.44 |
| 32:2a:562:C:O2' | 43:2l:16:GLU:O | 2.34 | 0.44 |
| 32:2a:614:A:C6 | 32:2a:615:C:C4 | 3.04 | 0.44 |
| 32:2a:620:C:C2 | 35:2d:135:LEU:HG | 2.52 | 0.44 |
| 32:2a:1060:C:H4' | 41:2j:52:GLY:N | 2.32 | 0.44 |
| 32:2a:1104:G:H4' | 33:2b:111:ARG:NH2 | 2.31 | 0.44 |
| 38:2g:32:ARG:C | 38:2g:34:GLY:N | 2.75 | 0.44 |
| 1:1A:2078:C:C4 | 1:1A:2079:U:C4 | 3.04 | 0.44 |
| 1:1A:2359:C:H2' | 1:1A:2360:A:O4' | 2.17 | 0.44 |
| 4:1E:10:GLY:HA2 | 4:1E:192:ASN:OD1 | 2.17 | 0.44 |
| 7:1H:124:GLU:HG3 | 7:1H:132:ARG:HB3 | 2.00 | 0.44 |
| 26:14:56:VAL:HG23 | 26:14:60:GLN:HG3 | 1.99 | 0.44 |
| 32:1a:371:G:O2' | 32:1a:373:A:N7 | 2.44 | 0.44 |
| 32:1a:868:C:H2' | 32:1a:869:G:O4' | 2.17 | 0.44 |
| 32:1a:977:A:C8 | 32:1a:1223:C:C2 | 3.05 | 0.44 |
| 36:1e:74:GLY:HA3 | 36:1e:116:THR:HG22 | 2.00 | 0.44 |
| 40:1i:70:LYS:O | 40:1i:74:ILE:HG13 | 2.16 | 0.44 |
| 56:1y:34:G:H2' | 56:1y:35:A:O4' | 2.16 | 0.44 |
| 1:2A:1359:A:C2 | 1:2A:1372:U:O4 | 2.70 | 0.44 |
| 13:2R:107:ASP:OD1 | 13:2R:107:ASP:N | 2.47 | 0.44 |
| 14:2S:18:ILE:O | 14:2S:21:THR:HG23 | 2.17 | 0.44 |
| 21:2Z:67:LEU:HD23 | 21:2Z:67:LEU:HA | 1.78 | 0.44 |
| 32:2a:434:U:H2' | 32:2a:435:C:H6 | 1.82 | 0.44 |
| 32:2a:964:A:N3 | 32:2a:969:A:O2' | 2.48 | 0.44 |
| 32:2a:1346:A:H61 | 32:2a:1374:A:H3' | 1.83 | 0.44 |
| 34:2c:111:LEU:HD23 | 34:2c:111:LEU:HA | 1.84 | 0.44 |
| 36:2e:78:HIS:HB3 | 39:2h:107:LEU:HD13 | 1.99 | 0.44 |
| 37:2f:44:GLY:HA2 | 37:2f:59:TYR:CZ | 2.52 | 0.44 |
| 44:2m:20:THR:HG22 | 44:2m:26:GLY:C | 2.42 | 0.44 |
| 46:2o:63:ARG:HE | 46:2o:63:ARG:HB3 | 1.56 | 0.44 |
| 57:2z:6:PRO:O | 57:2z:15:VAL:HG22 | 2.17 | 0.44 |
| 1:1A:1388:G:O2' | 1:1A:1389:G:H5' | 2.17 | 0.44 |
| 1:1A:1401:G:H2' | 1:1A:1402:C:O4' | 2.17 | 0.44 |
| 1:1A:1800:C:OP1 | 3:1D:260:ARG:NH2 | 2.50 | 0.44 |
| 2:1B:66:A:H61 | 2:1B:109:C:H5' | 1.82 | 0.44 |
| 11:1P:3:LEU:HD23 | 11:1P:3:LEU:HA | 1.78 | 0.44 |
| 15:1T:128:GLU:O | 15:1T:128:GLU:HG3 | 2.17 | 0.44 |
| 21:1Z:104:PHE:CD1 | 21:1Z:139:VAL:HB | 2.52 | 0.44 |
| 22:10:10:THR:CG2 | 22:10:12:ASN:HB2 | 2.47 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 26:14:24:THR:OG1 | 26:14:25:TYR:N | 2.49 | 0.44 |
| 26:14:59:PHE:CE2 | 50:1s:64:GLU:HB3 | 2.52 | 0.44 |
| 32:1a:158:G:H2' | 32:1a:159:G:H8 | 1.82 | 0.44 |
| 32:1a:542:G:O3' | 35:1d:14:ARG:NH2 | 2.47 | 0.44 |
| 32:1a:1152:A:C5' | 41:1j:13:HIS:ND1 | 2.80 | 0.44 |
| 32:1a:1304:G:C6 | 32:1a:1305:G:N1 | 2.86 | 0.44 |
| 33:1b:162:ILE:O | 33:1b:185:ILE:HG12 | 2.17 | 0.44 |
| 34:1c:44:GLU:HA | 34:1c:52:LEU:HD23 | 1.98 | 0.44 |
| 44:1m:97:PRO:N | 44:1m:110:ARG:HG2 | 2.33 | 0.44 |
| 52:1u:3:LYS:HD3 | 52:1u:14:TRP:CD1 | 2.53 | 0.44 |
| 53:1v:14:A:C2 | 56:1y:34:G:N1 | 2.86 | 0.44 |
| 1:2A:660:G:C6 | 1:2A:661:C:C4 | 3.05 | 0.44 |
| 1:2A:673:C:OP1 | 5:2F:54:ARG:NH1 | 2.42 | 0.44 |
| 1:2A:764:A:H5'' | 3:2D:210:GLY:HA2 | 1.98 | 0.44 |
| 1:2A:2516:G:O6 | 1:2A:2517:C:N4 | 2.51 | 0.44 |
| 1:2A:2752:C:H2' | 1:2A:2753:A:O4' | 2.17 | 0.44 |
| 3:2D:118:VAL:HG22 | 3:2D:119:ALA:H | 1.83 | 0.44 |
| 6:2G:43:LEU:HD13 | 6:2G:43:LEU:HA | 1.67 | 0.44 |
| 7:2H:88:LEU:H | 7:2H:88:LEU:HD12 | 1.82 | 0.44 |
| 8:2I:139:GLN:OE1 | 8:2I:139:GLN:N | 2.49 | 0.44 |
| 14:2S:14:VAL:O | 14:2S:18:ILE:HG12 | 2.18 | 0.44 |
| 32:2a:1381:U:H1' | 38:2g:79:ARG:HD3 | 1.99 | 0.44 |
| 37:2f:41:GLU:HG3 | 37:2f:62:TRP:CE3 | 2.53 | 0.44 |
| 1:1A:362:U:H6 | 1:1A:362:U:H2' | 1.58 | 0.44 |
| 1:1A:667:U:O2 | 30:18:2:PRO:HD2 | 2.17 | 0.44 |
| 1:1A:898:C:N3 | 1:1A:899:A:N7 | 2.66 | 0.44 |
| 1:1A:1044:G:H5' | 1:1A:1045:A:OP2 | 2.16 | 0.44 |
| 1:1A:1321:A:H2' | 1:1A:1322:A:O4' | 2.18 | 0.44 |
| 1:1A:1548:C:H2' | 1:1A:1549:C:C6 | 2.52 | 0.44 |
| 8:1I:86:THR:O | 8:1I:123:LEU:HG | 2.17 | 0.44 |
| 8:1I:125:GLU:OE2 | 8:1I:143:SER:HB2 | 2.18 | 0.44 |
| 9:1N:75:TYR:CE2 | 9:1N:77:GLY:HA2 | 2.52 | 0.44 |
| 32:1a:49:U:C2 | 32:1a:361:G:N2 | 2.86 | 0.44 |
| 32:1a:972:C:OP2 | 41:1j:57:LYS:NZ | 2.50 | 0.44 |
| 32:1a:1038:C:H2' | 32:1a:1039:C:C6 | 2.53 | 0.44 |
| 32:1a:1470:G:N7 | 62:1a:1947:HOH:O | 2.36 | 0.44 |
| 39:1h:14:ARG:O | 39:1h:18:ARG:HD2 | 2.17 | 0.44 |
| 1:2A:27:G:N2 | 1:2A:512:G:H1' | 2.32 | 0.44 |
| 1:2A:72:U:OP1 | 62:2A:3957:HOH:O | 2.21 | 0.44 |
| 1:2A:793:A:OP2 | 1:2A:2071:A:O2' | 2.33 | 0.44 |
| 1:2A:1721:G:C2 | 1:2A:1739:U:OP2 | 2.71 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:2A:1857:G:C6 | 1:2A:1858:G:N1 | 2.86 | 0.44 |
| 1:2A:2189:U:H2' | 1:2A:2190:G:C8 | 2.52 | 0.44 |
| 6:2G:53:LEU:HA | 6:2G:53:LEU:HD13 | 1.69 | 0.44 |
| 8:2I:38:LEU:HB2 | 8:2I:40:THR:HG23 | 1.99 | 0.44 |
| 15:2T:53:ARG:HH11 | 15:2T:53:ARG:HG3 | 1.81 | 0.44 |
| 21:2Z:23:LYS:HD3 | 21:2Z:23:LYS:HA | 1.71 | 0.44 |
| 21:2Z:39:VAL:HG21 | 21:2Z:44:PHE:HB2 | 1.98 | 0.44 |
| 32:2a:189(L):G:H2' | 32:2a:190:U:C6 | 2.52 | 0.44 |
| 32:2a:266:G:H2' | 32:2a:266:G:N3 | 2.32 | 0.44 |
| 32:2a:458:C:H2' | 32:2a:460:G:O4' | 2.17 | 0.44 |
| 32:2a:593:G:C6 | 32:2a:594:G:C5 | 3.06 | 0.44 |
| 34:2c:108:ASN:OD1 | 34:2c:109:PRO:HD2 | 2.17 | 0.44 |
| 35:2d:10:ARG:HG3 | 35:2d:11:LEU:HD12 | 1.98 | 0.44 |
| 37:2f:82:ARG:HE | 37:2f:82:ARG:HB3 | 1.70 | 0.44 |
| 38:2g:113:GLU:CG | 38:2g:119:ARG:HG2 | 2.46 | 0.44 |
| 40:2i:56:LEU:HG | 40:2i:57:GLY:N | 2.33 | 0.44 |
| 44:2m:106:ASN:O | 44:2m:108:ARG:N | 2.49 | 0.44 |
| 1:1A:586:A:N1 | 1:1A:809:G:O2' | 2.45 | 0.44 |
| 1:1A:748:G:P | 18:1W:88:ARG:HH21 | 2.41 | 0.44 |
| 1:1A:1827:C:C2' | 1:1A:1828:G:H5' | 2.47 | 0.44 |
| 1:1A:2591:C:P | 3:1D:239:ARG:HG3 | 2.57 | 0.44 |
| 2:1B:41:U:H5 | 6:1G:70:VAL:N | 2.16 | 0.44 |
| 6:1G:138:GLN:HB3 | 6:1G:153:ARG:O | 2.17 | 0.44 |
| 7:1H:3:ARG:HH11 | 7:1H:4:ILE:H | 1.65 | 0.44 |
| 16:1U:105:VAL:HG22 | 17:1V:45:THR:HG22 | 1.98 | 0.44 |
| 25:13:59:VAL:O | 25:13:60:GLU:HG2 | 2.18 | 0.44 |
| 32:1a:109:A:H2' | 32:1a:326:G:N2 | 2.33 | 0.44 |
| 32:1a:376:G:H5'' | 47:1p:5:ARG:HG3 | 1.99 | 0.44 |
| 32:1a:524:G:H2' | 32:1a:525:C:C6 | 2.53 | 0.44 |
| 32:1a:626:U:H2' | 32:1a:627:G:H8 | 1.83 | 0.44 |
| 32:1a:1095:U:H2' | 32:1a:1096:C:O4' | 2.17 | 0.44 |
| 34:1c:181:ASN:ND2 | 34:1c:204:LEU:HB2 | 2.33 | 0.44 |
| 35:1d:31:CYS:CB | 61:1d:302:SF4:S3 | 3.06 | 0.44 |
| 1:2A:56:A:H2' | 1:2A:57:C:O4' | 2.18 | 0.44 |
| 12:2Q:18:LYS:O | 12:2Q:98:LYS:HE2 | 2.18 | 0.44 |
| 12:2Q:26:TYR:HD1 | 12:2Q:27:VAL:O | 1.99 | 0.44 |
| 20:2Y:8:LYS:HD3 | 20:2Y:97:ARG:NH1 | 2.33 | 0.44 |
| 32:2a:986:A:C4 | 32:2a:1220:G:N2 | 2.86 | 0.44 |
| 32:2a:1018:C:H2' | 32:2a:1019:C:O4' | 2.16 | 0.44 |
| 34:2c:188:LEU:HD12 | 34:2c:188:LEU:HA | 1.76 | 0.44 |
| 37:2f:76:ALA:O | 37:2f:80:ARG:HD2 | 2.18 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 38:2g:26:PHE:CD2 | 38:2g:62:PHE:HE1 | 2.35 | 0.44 |
| 38:2g:144:MET:HE2 | 38:2g:144:MET:HB3 | 1.72 | 0.44 |
| 51:2t:92:LEU:HD23 | 51:2t:92:LEU:HA | 1.75 | 0.44 |
| 1:1A:1449:A:N3 | 1:1A:1529:G:H1' | 2.32 | 0.44 |
| 1:1A:1540:U:C2' | 1:1A:1541:G:H5' | 2.47 | 0.44 |
| 1:1A:2040:C:H2' | 1:1A:2041:U:O4' | 2.18 | 0.44 |
| 26:14:14:ILE:C | 26:14:15:ILE:HD13 | 2.42 | 0.44 |
| 26:14:28:LYS:HA | 26:14:29:PRO:HD3 | 1.87 | 0.44 |
| 30:18:42:ARG:HD2 | 62:18:202:HOH:O | 2.17 | 0.44 |
| 32:1a:983:A:H3' | 32:1a:983:A:N3 | 2.33 | 0.44 |
| 32:1a:1359:C:O5' | 32:1a:1359:C:H6 | 2.00 | 0.44 |
| 32:1a:1458:G:OP1 | 51:1t:35:THR:OG1 | 2.33 | 0.44 |
| 33:1b:178:ARG:HH22 | 39:1h:74:PRO:HB3 | 1.82 | 0.44 |
| 34:1c:18:TRP:H | 34:1c:18:TRP:HE3 | 1.64 | 0.44 |
| 35:1d:162:LEU:CD1 | 35:1d:181:MET:HG2 | 2.48 | 0.44 |
| 42:1k:82:VAL:HG22 | 42:1k:98:LEU:HD12 | 1.99 | 0.44 |
| 44:1m:20:THR:C | 44:1m:22:ILE:H | 2.26 | 0.44 |
| 52:1u:14:TRP:HE3 | 52:1u:15:ARG:HG2 | 1.83 | 0.44 |
| 1:2A:224:G:H2' | 1:2A:225:A:O4' | 2.17 | 0.44 |
| 1:2A:391:G:H1' | 1:2A:411:G:O4' | 2.17 | 0.44 |
| 1:2A:1815:A:H8 | 1:2A:1815:A:OP1 | 2.00 | 0.44 |
| 1:2A:2276:G:H2' | 1:2A:2277:G:H5' | 1.99 | 0.44 |
| 3:2D:146:GLU:HB2 | 3:2D:189:CYS:HB3 | 2.00 | 0.44 |
| 21:2Z:77:ASP:OD2 | 21:2Z:80:ARG:NH1 | 2.51 | 0.44 |
| 24:22:13:ALA:HA | 24:22:16:LEU:HD12 | 1.98 | 0.44 |
| 28:26:38:LYS:HB3 | 28:26:38:LYS:HE3 | 1.70 | 0.44 |
| 32:2a:41:G:H2' | 32:2a:42:G:H8 | 1.83 | 0.44 |
| 32:2a:153:C:H2' | 32:2a:154:C:C6 | 2.52 | 0.44 |
| 32:2a:1030(A):G:N2 | 32:2a:1030(C):G:H3' | 2.33 | 0.44 |
| 32:2a:1318:A:H5'' | 50:2s:3:ARG:NH2 | 2.33 | 0.44 |
| 35:2d:150:GLU:N | 35:2d:150:GLU:CD | 2.75 | 0.44 |
| 39:2h:28:ALA:HB3 | 39:2h:57:PRO:HB2 | 1.99 | 0.44 |
| 43:2l:54:LYS:N | 43:2l:54:LYS:HD2 | 2.33 | 0.44 |
| 45:2n:24:CYS:HB2 | 45:2n:40:CYS:HB3 | 2.00 | 0.44 |
| 54:2w:21:A:H61 | 54:2w:46:G7M:H2' | 1.82 | 0.44 |
| 1:1A:881:G:C2 | 1:1A:882:G:H1' | 2.53 | 0.44 |
| 1:1A:2646:C:H2' | 1:1A:2647:U:O4' | 2.18 | 0.44 |
| 1:1A:2695:C:H2' | 1:1A:2696:U:H6 | 1.83 | 0.44 |
| 3:1D:3:VAL:HG22 | 3:1D:17:THR:HB | 1.98 | 0.44 |
| 6:1G:179:PRO:HB2 | 26:14:42:PHE:HE2 | 1.83 | 0.44 |
| 12:1Q:115:MET:HB3 | 12:1Q:115:MET:HE3 | 1.56 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 32:1a:93:G:O2' | 32:1a:96:U:H5' | 2.18 | 0.44 |
| 32:1a:636:U:H2' | 32:1a:637:G:C8 | 2.53 | 0.44 |
| 32:1a:1070:U:H2' | 32:1a:1071:C:H6 | 1.83 | 0.44 |
| 32:1a:1243:C:H2' | 32:1a:1244:C:C6 | 2.53 | 0.44 |
| 36:1e:51:VAL:O | 36:1e:55:VAL:HG23 | 2.18 | 0.44 |
| 36:1e:68:GLU:HG3 | 36:1e:69:VAL:N | 2.33 | 0.44 |
| 40:1i:20:ARG:O | 40:1i:60:ASP:N | 2.24 | 0.44 |
| 40:1i:25:LYS:HB3 | 40:1i:60:ASP:OD2 | 2.17 | 0.44 |
| 41:1j:49:VAL:HG22 | 45:1n:41:ARG:HB2 | 1.99 | 0.44 |
| 45:1n:58:LYS:HE3 | 45:1n:58:LYS:HB3 | 1.74 | 0.44 |
| 1:2A:7:G:H2' | 1:2A:8:A:C8 | 2.51 | 0.44 |
| 1:2A:854:G:O2' | 1:2A:855:G:H5' | 2.18 | 0.44 |
| 1:2A:868:U:C4 | 1:2A:869:G:N7 | 2.85 | 0.44 |
| 7:2H:25:LYS:HD3 | 7:2H:27:LYS:HE3 | 1.99 | 0.44 |
| 8:2I:69:LYS:HD3 | 8:2I:136:VAL:HG13 | 1.99 | 0.44 |
| 11:2P:121:LYS:CB | 11:2P:123:LEU:HD13 | 2.48 | 0.44 |
| 19:2X:30:VAL:HG22 | 19:2X:77:LYS:HG2 | 1.99 | 0.44 |
| 26:24:48:ARG:HD2 | 26:24:48:ARG:HA | 1.81 | 0.44 |
| 32:2a:627:G:H2' | 32:2a:628:G:C8 | 2.53 | 0.44 |
| 32:2a:1168:A:C6 | 32:2a:1169:A:C6 | 3.05 | 0.44 |
| 32:2a:1204:A:OP2 | 62:2a:1915:HOH:O | 2.21 | 0.44 |
| 34:2c:123:GLN:O | 34:2c:128:PHE:HB2 | 2.18 | 0.44 |
| 42:2k:110:ASP:HB3 | 49:2r:85:LEU:HB3 | 1.98 | 0.44 |
| 1:1A:534:U:H2' | 1:1A:535:C:C6 | 2.53 | 0.44 |
| 1:1A:630:G:OP1 | 30:18:47:LYS:NZ | 2.41 | 0.44 |
| 1:1A:1028:A:H61 | 1:1A:1125:G:H2' | 1.82 | 0.44 |
| 1:1A:1094:U:H1' | 1:1A:1097:U:C4 | 2.53 | 0.44 |
| 1:1A:2156:G:OP2 | 1:1A:2156:G:C8 | 2.69 | 0.44 |
| 2:1B:96:U:H2' | 2:1B:97:G:H8 | 1.81 | 0.44 |
| 10:1O:16:ALA:HB2 | 10:1O:52:VAL:CG2 | 2.48 | 0.44 |
| 15:1T:27:THR:HB | 15:1T:90:GLN:HB3 | 2.00 | 0.44 |
| 16:1U:74:LEU:HD12 | 16:1U:74:LEU:H | 1.83 | 0.44 |
| 21:1Z:53:ILE:HG22 | 21:1Z:71:VAL:HG12 | 1.99 | 0.44 |
| 32:1a:70:G:H2' | 32:1a:71:C:H6 | 1.83 | 0.44 |
| 32:1a:475:G:N3 | 32:1a:475:G:H2' | 2.33 | 0.44 |
| 32:1a:1030(C):G:H2' | 32:1a:1030(D):A:C8 | 2.53 | 0.44 |
| 32:1a:1146:A:H5' | 32:1a:1146:A:H8 | 1.83 | 0.44 |
| 32:1a:1347:G:H5'' | 40:1i:107:ARG:HB3 | 1.98 | 0.44 |
| 33:1b:121:LEU:HD23 | 33:1b:122:PHE:CD1 | 2.53 | 0.44 |
| 33:1b:124:SER:HA | 33:1b:125:PRO:HA | 1.49 | 0.44 |
| 35:1d:64:LEU:HB2 | 35:1d:198:VAL:HG11 | 2.00 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 37:1f:39:LYS:HE3 | 37:1f:39:LYS:HB3 | 1.69 | 0.44 |
| 37:1f:99:ALA:HB1 | 49:1r:23:LYS:NZ | 2.33 | 0.44 |
| 41:1j:13:HIS:O | 41:1j:16:LEU:N | 2.51 | 0.44 |
| 49:1r:31:LEU:O | 49:1r:69:THR:HG21 | 2.17 | 0.44 |
| 1:2A:191:A:H2' | 1:2A:192:C:C6 | 2.52 | 0.44 |
| 1:2A:1169:G:N1 | 1:2A:1170:G:N7 | 2.65 | 0.44 |
| 1:2A:1297:C:OP1 | 1:2A:2710:C:H4' | 2.18 | 0.44 |
| 1:2A:1449:A:O2' | 1:2A:1529:G:N2 | 2.32 | 0.44 |
| 15:2T:77:PRO:HB2 | 15:2T:80:SER:HB2 | 2.00 | 0.44 |
| 15:2T:125:ARG:NH1 | 32:2a:1442(B):A:H4' | 2.33 | 0.44 |
| 21:2Z:40:ASP:OD1 | 21:2Z:42:VAL:HG13 | 2.17 | 0.44 |
| 32:2a:646:U:C2 | 32:2a:647:C:C5 | 3.05 | 0.44 |
| 33:2b:8:LYS:O | 33:2b:9:GLU:HB2 | 2.17 | 0.44 |
| 39:2h:104:ARG:HG2 | 39:2h:138:TRP:CE3 | 2.52 | 0.44 |
| 1:1A:218:A:C2 | 1:1A:235:U:H4' | 2.53 | 0.44 |
| 1:1A:816:C:H2' | 1:1A:817:C:H6 | 1.83 | 0.44 |
| 1:1A:2577:A:H5'' | 1:1A:2578:G:H5' | 2.00 | 0.44 |
| 6:1G:110:ALA:O | 6:1G:111:LEU:C | 2.60 | 0.44 |
| 7:1H:13:LYS:HA | 7:1H:14:GLY:HA2 | 1.74 | 0.44 |
| 11:1P:79:ARG:HD2 | 11:1P:110:TYR:CZ | 2.53 | 0.44 |
| 18:1W:11:ARG:NH1 | 18:1W:99:ARG:O | 2.48 | 0.44 |
| 28:16:6:ARG:NH2 | 28:16:26:ASN:HB2 | 2.33 | 0.44 |
| 32:1a:197:A:N6 | 32:1a:221:C:H5' | 2.33 | 0.44 |
| 34:1c:70:VAL:O | 34:1c:106:VAL:HG13 | 2.17 | 0.44 |
| 34:1c:130:VAL:HG12 | 34:1c:134:ILE:HD11 | 1.99 | 0.44 |
| 38:1g:144:MET:HE2 | 38:1g:144:MET:HB3 | 1.75 | 0.44 |
| 56:1y:5:G:N1 | 56:1y:6:G:C5 | 2.86 | 0.44 |
| 1:2A:271(D):G:H2' | 1:2A:271(E):U:C6 | 2.53 | 0.44 |
| 1:2A:1331:A:O2' | 1:2A:1332:G:H5' | 2.17 | 0.44 |
| 1:2A:1703:G:H2' | 1:2A:1704:G:C8 | 2.53 | 0.44 |
| 1:2A:2197:U:O2' | 1:2A:2198:A:H2' | 2.18 | 0.44 |
| 1:2A:2336:A:H61 | 22:20:43:THR:CG2 | 2.31 | 0.44 |
| 1:2A:2747:G:O6 | 1:2A:2755:C:H5'' | 2.18 | 0.44 |
| 23:21:73:LEU:HD23 | 23:21:73:LEU:HA | 1.74 | 0.44 |
| 32:2a:321:A:C2 | 32:2a:333:G:C2 | 3.06 | 0.44 |
| 32:2a:942:G:C2 | 32:2a:1342:C:C2 | 3.06 | 0.44 |
| 32:2a:1013:G:O2' | 32:2a:1015:A:N7 | 2.48 | 0.44 |
| 32:2a:1176:A:H2' | 32:2a:1177:G:H8 | 1.81 | 0.44 |
| 32:2a:1239:A:H62 | 32:2a:1299:A:N6 | 2.15 | 0.44 |
| 33:2b:15:VAL:O | 33:2b:17:PHE:N | 2.49 | 0.44 |
| 33:2b:192:SER:O | 33:2b:194:PRO:HD3 | 2.17 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 34:2c:195:VAL:C | 34:2c:196:LEU:HD23 | 2.43 | 0.44 |
| 35:2d:96:LEU:HD12 | 35:2d:139:ARG:CZ | 2.48 | 0.44 |
| 36:2e:34:VAL:HG12 | 36:2e:62:ALA:HB1 | 1.99 | 0.44 |
| 36:2e:36:ASP:OD1 | 36:2e:38:GLN:HB2 | 2.17 | 0.44 |
| 38:2g:78:ARG:NH1 | 38:2g:156:TRP:HE3 | 2.14 | 0.44 |
| 47:2p:39:TYR:HA | 47:2p:48:TRP:O | 2.17 | 0.44 |
| 47:2p:70:ALA:HA | 47:2p:73:LEU:HD12 | 1.99 | 0.44 |
| 1:1A:182:A:H2' | 1:1A:183:C:O4' | 2.18 | 0.43 |
| 1:1A:185:U:H2' | 1:1A:186:G:C8 | 2.53 | 0.43 |
| 1:1A:338:G:OP1 | 20:1Y:4:LYS:HE3 | 2.18 | 0.43 |
| 1:1A:483:A:O4' | 20:1Y:48:ALA:HB1 | 2.17 | 0.43 |
| 1:1A:659:C:H4' | 5:1F:100:THR:O | 2.18 | 0.43 |
| 1:1A:1176:G:OP2 | 1:1A:1176:G:H4' | 2.17 | 0.43 |
| 1:1A:1581:G:C5 | 1:1A:1582:C:C4 | 3.06 | 0.43 |
| 3:1D:24:ILE:HD13 | 3:1D:84:TYR:HB2 | 2.00 | 0.43 |
| 3:1D:35:LYS:HB2 | 3:1D:36:PRO:HD2 | 2.00 | 0.43 |
| 4:1E:21:VAL:O | 4:1E:23:VAL:HG13 | 2.17 | 0.43 |
| 9:1N:46:VAL:HG23 | 9:1N:48:MET:HG2 | 1.99 | 0.43 |
| 18:1W:11:ARG:HA | 18:1W:11:ARG:HD2 | 1.81 | 0.43 |
| 21:1Z:103:ARG:O | 21:1Z:139:VAL:N | 2.50 | 0.43 |
| 32:1a:1005:A:C2 | 32:1a:1025:U:H1' | 2.53 | 0.43 |
| 33:1b:108:ILE:O | 33:1b:111:ARG:HB2 | 2.18 | 0.43 |
| 1:2A:857:C:H1' | 22:20:26:TYR:CE1 | 2.53 | 0.43 |
| 1:2A:1504:C:O2' | 1:2A:1505:C:H5' | 2.18 | 0.43 |
| 1:2A:2635:C:H5'' | 4:2E:78:LEU:O | 2.18 | 0.43 |
| 1:2A:2723:C:O3' | 13:2R:1:MET:HE1 | 2.18 | 0.43 |
| 3:2D:245:PRO:HA | 3:2D:246:PRO:HD3 | 1.91 | 0.43 |
| 7:2H:73:ALA:O | 7:2H:76:VAL:HG22 | 2.18 | 0.43 |
| 11:2P:132:LYS:O | 11:2P:135:LEU:N | 2.49 | 0.43 |
| 14:2S:10:ARG:HG2 | 14:2S:91:PRO:HA | 1.98 | 0.43 |
| 15:2T:99:LEU:O | 15:2T:102:ILE:HG23 | 2.18 | 0.43 |
| 20:2Y:7:VAL:HG13 | 20:2Y:27:VAL:HG21 | 1.99 | 0.43 |
| 20:2Y:87:LYS:HD2 | 20:2Y:95:LYS:HD2 | 2.00 | 0.43 |
| 27:25:20:ARG:HG2 | 27:25:23:HIS:ND1 | 2.33 | 0.43 |
| 32:2a:979:C:H2' | 32:2a:980:C:H5' | 2.00 | 0.43 |
| 32:2a:1320:C:C2 | 50:2s:72:GLY:HA3 | 2.52 | 0.43 |
| 36:2e:148:VAL:HG13 | 36:2e:152:ARG:CZ | 2.48 | 0.43 |
| 39:2h:9:MET:HG3 | 39:2h:26:VAL:HG11 | 2.00 | 0.43 |
| 1:1A:476:G:N1 | 1:1A:479:A:OP2 | 2.49 | 0.43 |
| 1:1A:588:U:H2' | 1:1A:589:C:C6 | 2.53 | 0.43 |
| 1:1A:1068:G:H2' | 1:1A:1096:A:H1' | 2.00 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:1B:74:U:H2' | 2:1B:75:G:O4' | 2.18 | 0.43 |
| 4:1E:98:PRO:HA | 4:1E:172:VAL:HG12 | 2.00 | 0.43 |
| 7:1H:11:VAL:HG13 | 7:1H:15:VAL:HG23 | 2.00 | 0.43 |
| 8:1I:30:LEU:HD23 | 8:1I:30:LEU:HA | 1.65 | 0.43 |
| 54:1w:19:G:H4' | 54:1w:20:U:OP1 | 2.18 | 0.43 |
| 1:2A:265:A:H8 | 1:2A:266:G:H1' | 1.82 | 0.43 |
| 1:2A:1464:C:C2 | 1:2A:1465:G:C8 | 3.06 | 0.43 |
| 1:2A:2218:U:O2 | 23:21:52:ARG:HD3 | 2.18 | 0.43 |
| 6:2G:20:ILE:O | 6:2G:24:GLY:HA2 | 2.17 | 0.43 |
| 8:2I:83:ALA:HB1 | 8:2I:87:LYS:O | 2.18 | 0.43 |
| 11:2P:86:LYS:HG3 | 11:2P:87:ASP:OD1 | 2.18 | 0.43 |
| 11:2P:126:VAL:HG12 | 11:2P:148:LEU:CD2 | 2.48 | 0.43 |
| 14:2S:84:GLN:HA | 14:2S:111:GLU:HB2 | 2.00 | 0.43 |
| 19:2X:2:LYS:NZ | 19:2X:38:GLU:OE2 | 2.47 | 0.43 |
| 21:2Z:27:VAL:HG12 | 21:2Z:85:HIS:HE1 | 1.83 | 0.43 |
| 25:23:31:LEU:HD22 | 25:23:31:LEU:HA | 1.74 | 0.43 |
| 32:2a:141:A:H1' | 32:2a:182:U:O2 | 2.17 | 0.43 |
| 32:2a:350:G:H5' | 32:2a:351:G:OP2 | 2.18 | 0.43 |
| 32:2a:376:G:H5'' | 47:2p:5:ARG:HB2 | 1.99 | 0.43 |
| 32:2a:1305:G:C2 | 32:2a:1331:G:N3 | 2.86 | 0.43 |
| 35:2d:92:VAL:O | 35:2d:96:LEU:HD23 | 2.18 | 0.43 |
| 36:2e:43:LEU:O | 36:2e:65:ASN:ND2 | 2.51 | 0.43 |
| 42:2k:17:GLY:O | 42:2k:80:VAL:HA | 2.18 | 0.43 |
| 45:2n:53:LEU:HD12 | 45:2n:53:LEU:HA | 1.76 | 0.43 |
| 54:2w:19:G:H8 | 54:2w:19:G:OP2 | 2.01 | 0.43 |
| 54:2w:73:A:H3' | 54:2w:73:A:OP2 | 2.18 | 0.43 |
| 1:1A:1057:A:N7 | 1:1A:1086:A:H2' | 2.34 | 0.43 |
| 1:1A:1710:C:H4' | 1:1A:2858:C:O2 | 2.18 | 0.43 |
| 1:1A:2515:C:O2' | 1:1A:2516:G:H5' | 2.19 | 0.43 |
| 5:1F:170:LEU:HD13 | 5:1F:172:TRP:CZ2 | 2.52 | 0.43 |
| 6:1G:15:VAL:HG21 | 6:1G:176:LEU:HD23 | 2.01 | 0.43 |
| 7:1H:154:PRO:HB3 | 7:1H:163:TYR:CE1 | 2.53 | 0.43 |
| 7:1H:174:GLY:O | 7:1H:175:LYS:HG3 | 2.18 | 0.43 |
| 8:1I:7:GLU:O | 8:1I:9:LEU:HG | 2.18 | 0.43 |
| 15:1T:112:ARG:HG3 | 15:1T:115:ARG:HH21 | 1.83 | 0.43 |
| 32:1a:358:U:H2' | 32:1a:359:U:C6 | 2.52 | 0.43 |
| 32:1a:405:U:H3' | 32:1a:406:G:H5' | 2.00 | 0.43 |
| 32:1a:418:C:H1' | 32:1a:540:G:O2' | 2.18 | 0.43 |
| 32:1a:679:C:H2' | 32:1a:680:C:C6 | 2.53 | 0.43 |
| 32:1a:935:A:C2 | 32:1a:936:C:C2 | 3.06 | 0.43 |
| 32:1a:1003:G:C4 | 32:1a:1004:A:H2 | 2.37 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 32:1a:1151:A:O4' | 41:1j:39:PRO:HB2 | 2.18 | 0.43 |
| 36:1e:142:LEU:O | 36:1e:143:ARG:NH1 | 2.47 | 0.43 |
| 1:2A:600:G:H2' | 1:2A:601:C:C6 | 2.53 | 0.43 |
| 1:2A:601:C:O2 | 1:2A:605:C:H4' | 2.18 | 0.43 |
| 1:2A:862:G:H2' | 1:2A:863:A:O4' | 2.19 | 0.43 |
| 1:2A:878:A:N6 | 1:2A:900:A:N7 | 2.66 | 0.43 |
| 1:2A:945:A:C4 | 1:2A:2448:A:C2 | 3.07 | 0.43 |
| 1:2A:1651:G:OP1 | 13:2R:40:LYS:NZ | 2.49 | 0.43 |
| 1:2A:2203:U:O4' | 3:2D:151:LYS:HE2 | 2.17 | 0.43 |
| 1:2A:2769:C:H2' | 1:2A:2770:G:O4' | 2.18 | 0.43 |
| 2:2B:11:C:OP2 | 2:2B:12:C:H5 | 2.02 | 0.43 |
| 9:2N:14:VAL:HG11 | 9:2N:138:LEU:HD12 | 2.00 | 0.43 |
| 21:2Z:27:VAL:HG12 | 21:2Z:85:HIS:CE1 | 2.53 | 0.43 |
| 26:24:64:GLY:C | 26:24:66:SER:H | 2.26 | 0.43 |
| 30:28:56:GLU:HA | 30:28:59:LYS:HE3 | 1.99 | 0.43 |
| 32:2a:49:U:C2 | 32:2a:361:G:N2 | 2.86 | 0.43 |
| 32:2a:352:C:OP2 | 62:2a:1916:HOH:O | 2.21 | 0.43 |
| 33:2b:77:ALA:HB2 | 33:2b:211:ILE:HD13 | 2.00 | 0.43 |
| 36:2e:11:ILE:HB | 36:2e:31:LEU:HB3 | 2.00 | 0.43 |
| 39:2h:13:ILE:O | 39:2h:17:THR:OG1 | 2.31 | 0.43 |
| 44:2m:97:PRO:N | 44:2m:110:ARG:HG2 | 2.33 | 0.43 |
| 1:1A:271(H):G:H4' | 23:11:81:LYS:HG2 | 2.00 | 0.43 |
| 1:1A:484:C:H2' | 1:1A:485:C:C6 | 2.53 | 0.43 |
| 1:1A:515:A:H2 | 1:1A:1260:G:N3 | 2.16 | 0.43 |
| 1:1A:656:G:H2' | 1:1A:657:U:O4' | 2.19 | 0.43 |
| 1:1A:2846:G:H2' | 1:1A:2847:U:O4' | 2.17 | 0.43 |
| 16:1U:11:ARG:NH1 | 62:1U:302:HOH:O | 2.49 | 0.43 |
| 23:11:52:ARG:HG3 | 23:11:56:GLN:O | 2.19 | 0.43 |
| 32:1a:110:C:O2' | 47:1p:25:ARG:O | 2.33 | 0.43 |
| 32:1a:450:G:OP1 | 47:1p:43:LYS:NZ | 2.51 | 0.43 |
| 32:1a:1465:C:H2' | 32:1a:1466:C:O4' | 2.19 | 0.43 |
| 33:1b:80:ILE:HD11 | 33:1b:211:ILE:HG22 | 2.00 | 0.43 |
| 33:1b:139:LYS:O | 33:1b:143:GLU:HG3 | 2.19 | 0.43 |
| 35:1d:178:VAL:O | 35:1d:179:GLU:HB2 | 2.18 | 0.43 |
| 40:1i:98:PRO:O | 40:1i:99:LEU:HD13 | 2.17 | 0.43 |
| 44:1m:90:LEU:HB3 | 44:1m:94:ARG:NH2 | 2.32 | 0.43 |
| 45:1n:53:LEU:HD12 | 45:1n:53:LEU:HA | 1.66 | 0.43 |
| 49:1r:53:ARG:O | 49:1r:55:ARG:N | 2.51 | 0.43 |
| 1:2A:31:C:H5'' | 1:2A:1239:G:OP1 | 2.18 | 0.43 |
| 1:2A:1537:G:H2' | 1:2A:1538:G:H8 | 1.82 | 0.43 |
| 1:2A:1755:A:P | 15:2T:113:LYS:HZ1 | 2.40 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 2:2B:17:C:H2' | 2:2B:18:G:O4' | 2.17 | 0.43 |
| 8:2I:4:ILE:HG12 | 8:2I:18:VAL:CG2 | 2.48 | 0.43 |
| 8:2I:5:LEU:HD13 | 8:2I:17:GLN:HB3 | 2.00 | 0.43 |
| 10:2O:36:GLY:HA2 | 10:2O:106:LEU:HD23 | 1.99 | 0.43 |
| 12:2Q:134:ARG:HA | 12:2Q:138:ASP:OD2 | 2.19 | 0.43 |
| 32:2a:955:U:O2' | 50:2s:83:HIS:CD2 | 2.72 | 0.43 |
| 32:2a:1030(D):A:H62 | 32:2a:1031:G:N2 | 2.16 | 0.43 |
| 33:2b:178:ARG:NH1 | 33:2b:198:ASP:OD1 | 2.51 | 0.43 |
| 34:2c:6:HIS:CD2 | 34:2c:8:ILE:H | 2.36 | 0.43 |
| 42:2k:66:LEU:O | 42:2k:69:ALA:N | 2.50 | 0.43 |
| 42:2k:73:MET:HA | 42:2k:77:MET:H | 1.84 | 0.43 |
| 1:1A:226:G:N2 | 1:1A:228:A:H62 | 2.17 | 0.43 |
| 1:1A:548:A:N1 | 17:1V:18:LEU:HD12 | 2.34 | 0.43 |
| 1:1A:1180:C:H2' | 1:1A:1181:C:C6 | 2.53 | 0.43 |
| 1:1A:1824:G:O3' | 3:1D:249:PRO:HD3 | 2.19 | 0.43 |
| 1:1A:2160:G:N2 | 1:1A:2161:C:O2 | 2.51 | 0.43 |
| 21:1Z:93:ASP:CB | 21:1Z:131:ARG:HH12 | 2.30 | 0.43 |
| 26:14:34:GLU:HG2 | 26:14:35:VAL:HG12 | 2.00 | 0.43 |
| 32:1a:461:A:H8 | 32:1a:461:A:O5' | 2.01 | 0.43 |
| 32:1a:783:C:OP1 | 32:1a:1515:C:O2' | 2.34 | 0.43 |
| 32:1a:1349:A:C2 | 32:1a:1374:A:C4 | 3.07 | 0.43 |
| 33:1b:80:ILE:HD11 | 33:1b:215:LEU:HD22 | 1.98 | 0.43 |
| 41:1j:13:HIS:CD2 | 41:1j:13:HIS:N | 2.84 | 0.43 |
| 41:1j:40:LEU:HB2 | 41:1j:69:ASN:HB2 | 2.00 | 0.43 |
| 52:1u:10:ARG:HA | 52:1u:10:ARG:HD3 | 1.78 | 0.43 |
| 1:2A:894:C:C2 | 1:2A:895:U:C5 | 3.06 | 0.43 |
| 1:2A:1540:U:O2' | 1:2A:1541:G:H5' | 2.17 | 0.43 |
| 1:2A:1657:C:H2' | 1:2A:1658:C:C6 | 2.53 | 0.43 |
| 8:2I:87:LYS:H | 8:2I:87:LYS:HD3 | 1.84 | 0.43 |
| 19:2X:92:LEU:O | 19:2X:95:LEU:HB2 | 2.18 | 0.43 |
| 32:2a:982:U:O2 | 32:2a:1222:G:N1 | 2.40 | 0.43 |
| 32:2a:1055:A:N7 | 32:2a:1200:C:N4 | 2.65 | 0.43 |
| 32:2a:1346:A:N6 | 32:2a:1375:A:OP2 | 2.43 | 0.43 |
| 36:2e:36:ASP:OD2 | 36:2e:40:ARG:HB2 | 2.18 | 0.43 |
| 38:2g:78:ARG:HH21 | 38:2g:79:ARG:HE | 1.66 | 0.43 |
| 38:2g:78:ARG:NH2 | 38:2g:79:ARG:HE | 2.16 | 0.43 |
| 51:2t:39:LYS:HB2 | 51:2t:39:LYS:HE2 | 1.80 | 0.43 |
| 56:2y:73:A:H2' | 56:2y:74:C:O4' | 2.19 | 0.43 |
| 1:1A:957:A:H5' | 12:1Q:76:LYS:HD2 | 2.00 | 0.43 |
| 1:1A:1181:C:H2' | 1:1A:1182:A:O4' | 2.18 | 0.43 |
| 1:1A:1972:A:H2' | 1:1A:1973:G:H8 | 1.84 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 6:1G:171:ALA:O | 6:1G:175:LEU:HG | 2.18 | 0.43 |
| 8:1I:12:LEU:HD12 | 8:1I:12:LEU:HA | 1.84 | 0.43 |
| 18:1W:19:LEU:HB3 | 27:15:25:LEU:HD11 | 1.99 | 0.43 |
| 21:1Z:94:GLU:H | 21:1Z:94:GLU:HG2 | 1.62 | 0.43 |
| 25:13:24:LYS:HB2 | 25:13:24:LYS:HE2 | 1.69 | 0.43 |
| 28:16:17:LYS:HB3 | 28:16:17:LYS:HE3 | 1.72 | 0.43 |
| 30:18:23:VAL:HG21 | 30:18:47:LYS:HD3 | 1.99 | 0.43 |
| 32:1a:159:G:H2' | 32:1a:161:A:OP2 | 2.19 | 0.43 |
| 32:1a:984:C:H4' | 57:1z:16:LYS:HD2 | 2.00 | 0.43 |
| 32:1a:1280:A:O2' | 32:1a:1281:U:H5' | 2.19 | 0.43 |
| 32:1a:1321:C:OP2 | 32:1a:1322:C:O2' | 2.33 | 0.43 |
| 32:1a:1326:C:H2' | 32:1a:1327:C:C6 | 2.53 | 0.43 |
| 33:1b:46:LYS:HA | 33:1b:49:GLU:HB2 | 2.00 | 0.43 |
| 33:1b:53:ARG:HA | 33:1b:56:ARG:NH1 | 2.34 | 0.43 |
| 33:1b:163:PHE:CD1 | 33:1b:185:ILE:HG13 | 2.54 | 0.43 |
| 35:1d:106:TYR:HA | 35:1d:111:ALA:HB3 | 2.00 | 0.43 |
| 35:1d:140:VAL:HG11 | 35:1d:146:ILE:HD11 | 2.00 | 0.43 |
| 38:1g:115:ARG:O | 38:1g:118:VAL:HG12 | 2.19 | 0.43 |
| 51:1t:26:ASN:O | 51:1t:30:LYS:HG3 | 2.18 | 0.43 |
| 51:1t:89:ARG:HA | 51:1t:89:ARG:HD2 | 1.81 | 0.43 |
| 1:2A:370:G:O5' | 1:2A:423:A:N6 | 2.52 | 0.43 |
| 1:2A:894:C:O2' | 1:2A:895:U:H5'' | 2.18 | 0.43 |
| 1:2A:1037:G:H2' | 1:2A:1038:C:O4' | 2.18 | 0.43 |
| 1:2A:1163:G:N2 | 1:2A:1164:G:C4 | 2.86 | 0.43 |
| 1:2A:2506:U:C2 | 1:2A:2585:U:O4 | 2.71 | 0.43 |
| 1:2A:2785:C:OP1 | 4:2E:41:LYS:HE3 | 2.19 | 0.43 |
| 1:2A:2812:G:H2' | 1:2A:2813:A:H8 | 1.84 | 0.43 |
| 4:2E:96:PHE:O | 4:2E:175:VAL:HG21 | 2.18 | 0.43 |
| 5:2F:129:PHE:CD2 | 5:2F:163:VAL:HG21 | 2.53 | 0.43 |
| 6:2G:98:ARG:NE | 26:24:1:MET:HE3 | 2.33 | 0.43 |
| 11:2P:20:GLY:O | 11:2P:21:ARG:HD3 | 2.19 | 0.43 |
| 11:2P:81:GLN:NE2 | 11:2P:106:LEU:HA | 2.33 | 0.43 |
| 12:2Q:50:ALA:HB1 | 12:2Q:121:ALA:HB1 | 2.00 | 0.43 |
| 16:2U:76:TYR:HH | 16:2U:92:ARG:HE | 1.62 | 0.43 |
| 28:26:35:GLU:HG2 | 28:26:50:ARG:HD3 | 2.01 | 0.43 |
| 30:28:26:LYS:HG2 | 30:28:46:ARG:O | 2.18 | 0.43 |
| 32:2a:1366:C:H2' | 32:2a:1367:C:C6 | 2.54 | 0.43 |
| 32:2a:1376:U:H2' | 32:2a:1377:A:C8 | 2.53 | 0.43 |
| 34:2c:52:LEU:HD12 | 34:2c:53:ALA:H | 1.84 | 0.43 |
| 44:2m:13:LYS:HA | 44:2m:44:ARG:HD2 | 2.01 | 0.43 |
| 1:1A:298:G:H5'' | 1:1A:299:A:OP1 | 2.18 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 1:1A:652(D):C:N4 | 1:1A:652(U):G:H1 | 2.16 | 0.43 |
| 1:1A:723:G:H2' | 1:1A:724:U:O4' | 2.19 | 0.43 |
| 1:1A:1005:C:H5'' | 62:1A:4225:HOH:O | 2.18 | 0.43 |
| 1:1A:1038:C:H6 | 1:1A:1038:C:H5'' | 1.83 | 0.43 |
| 1:1A:1073:A:C6 | 1:1A:1074:G:C8 | 3.06 | 0.43 |
| 1:1A:1268:A:C2 | 1:1A:2013:A:C4 | 3.07 | 0.43 |
| 1:1A:1315:C:H2' | 1:1A:1316:U:H6 | 1.84 | 0.43 |
| 1:1A:1430:C:H2' | 1:1A:1431:U:C6 | 2.53 | 0.43 |
| 1:1A:1741:A:H2' | 1:1A:1742:G:O4' | 2.17 | 0.43 |
| 1:1A:1769:G:O2' | 1:1A:1958:C:OP1 | 2.34 | 0.43 |
| 1:1A:2127:G:H2' | 1:1A:2128:C:H6 | 1.82 | 0.43 |
| 6:1G:3:LEU:CD1 | 6:1G:5:VAL:HG12 | 2.49 | 0.43 |
| 10:1O:19:ILE:HB | 10:1O:41:ALA:HB1 | 2.00 | 0.43 |
| 11:1P:89:ALA:HA | 11:1P:121:LYS:HD3 | 2.00 | 0.43 |
| 32:1a:828:A:H2' | 32:1a:829:G:O4' | 2.18 | 0.43 |
| 32:1a:1030(A):G:H4' | 32:1a:1030(C):G:C6 | 2.54 | 0.43 |
| 33:1b:16:HIS:C | 33:1b:18:GLY:N | 2.76 | 0.43 |
| 35:1d:158:ILE:HD12 | 35:1d:159:ARG:N | 2.34 | 0.43 |
| 43:1l:117:ARG:NH2 | 43:1l:124:LYS:HB2 | 2.33 | 0.43 |
| 54:1w:73:A:C8 | 54:1w:73:A:H3' | 2.53 | 0.43 |
| 56:1y:5:G:C2 | 56:1y:69:G:C4 | 3.07 | 0.43 |
| 1:2A:821:A:H2' | 1:2A:946:G:H5'' | 1.99 | 0.43 |
| 1:2A:980:A:N3 | 1:2A:2037:G:O2' | 2.42 | 0.43 |
| 1:2A:2102:U:C4 | 1:2A:2103:C:N4 | 2.86 | 0.43 |
| 1:2A:2809:A:N6 | 1:2A:2892:A:O4' | 2.52 | 0.43 |
| 2:2B:53:A:OP2 | 62:2B:302:HOH:O | 2.21 | 0.43 |
| 7:2H:3:ARG:HA | 7:2H:3:ARG:HD2 | 1.65 | 0.43 |
| 8:2I:90:GLY:O | 8:2I:121:LYS:HE3 | 2.19 | 0.43 |
| 19:2X:72:LYS:HE2 | 19:2X:73:ARG:O | 2.19 | 0.43 |
| 23:21:53:VAL:HG22 | 23:21:74:VAL:HG13 | 2.01 | 0.43 |
| 29:27:46:VAL:HG22 | 29:27:48:LYS:HD2 | 2.01 | 0.43 |
| 32:2a:109:A:C6 | 32:2a:326:G:C6 | 3.07 | 0.43 |
| 32:2a:273:A:N6 | 32:2a:274:A:C6 | 2.87 | 0.43 |
| 32:2a:560:U:H4' | 32:2a:561:U:H5'' | 2.01 | 0.43 |
| 32:2a:986:A:H2' | 32:2a:987:G:O4' | 2.18 | 0.43 |
| 32:2a:1002:G:C2 | 32:2a:1003:G:C8 | 3.06 | 0.43 |
| 32:2a:1513:A:H2' | 32:2a:1514:C:C6 | 2.54 | 0.43 |
| 36:2e:91:LEU:HD23 | 36:2e:91:LEU:HA | 1.76 | 0.43 |
| 40:2i:28:VAL:HA | 40:2i:63:ILE:O | 2.17 | 0.43 |
| 49:2r:33:ASP:OD2 | 49:2r:36:ASN:HB2 | 2.17 | 0.43 |
| 56:2y:30:G:H2' | 56:2y:31:A:H8 | 1.83 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:1A:86:C:O2' | 1:1A:104:U:O2' | 2.27 | 0.43 |
| 1:1A:548:A:H1' | 1:1A:549:G:OP1 | 2.19 | 0.43 |
| 1:1A:894:C:H2' | 1:1A:895:U:O4' | 2.18 | 0.43 |
| 1:1A:1268:A:H2' | 1:1A:1269:A:O4' | 2.19 | 0.43 |
| 2:1B:87:G:N2 | 2:1B:90:A:OP2 | 2.41 | 0.43 |
| 6:1G:82:LEU:HD21 | 6:1G:88:ILE:HG21 | 1.99 | 0.43 |
| 8:1I:95:LYS:O | 8:1I:99:GLU:HG3 | 2.19 | 0.43 |
| 15:1T:74:ARG:HG2 | 15:1T:76:PHE:CZ | 2.54 | 0.43 |
| 25:13:54:VAL:HG13 | 25:13:55:ARG:N | 2.33 | 0.43 |
| 28:16:38:LYS:HE3 | 28:16:38:LYS:HB3 | 1.67 | 0.43 |
| 32:1a:300:A:H1' | 32:1a:565:U:O2 | 2.19 | 0.43 |
| 32:1a:1133:G:H2' | 32:1a:1134:G:H8 | 1.83 | 0.43 |
| 34:1c:130:VAL:HG21 | 34:1c:157:ILE:HG23 | 2.01 | 0.43 |
| 36:1e:144:THR:C | 39:1h:107:LEU:HD21 | 2.43 | 0.43 |
| 38:1g:51:GLN:O | 38:1g:55:GLY:HA2 | 2.19 | 0.43 |
| 39:1h:51:VAL:CG2 | 39:1h:60:ARG:HB2 | 2.49 | 0.43 |
| 42:1k:16:SER:O | 42:1k:35:PRO:HD3 | 2.18 | 0.43 |
| 1:2A:597:U:H2' | 1:2A:598:G:C8 | 2.54 | 0.43 |
| 1:2A:1509(A):A:H3' | 1:2A:1509(B):A:H8 | 1.83 | 0.43 |
| 1:2A:2023:G:H5' | 1:2A:2617:C:H4' | 2.01 | 0.43 |
| 1:2A:2526:G:C6 | 1:2A:2527:C:C4 | 3.06 | 0.43 |
| 4:2E:34:VAL:HG21 | 4:2E:78:LEU:HD11 | 2.01 | 0.43 |
| 7:2H:11:VAL:CG2 | 7:2H:50:VAL:HG23 | 2.49 | 0.43 |
| 19:2X:5:TYR:CZ | 24:22:30:ARG:HB2 | 2.54 | 0.43 |
| 32:2a:1124:G:N7 | 32:2a:1145:C:O2' | 2.52 | 0.43 |
| 33:2b:71:VAL:HA | 33:2b:93:VAL:HG12 | 2.01 | 0.43 |
| 40:2i:48:GLU:HG3 | 40:2i:101:PHE:CZ | 2.54 | 0.43 |
| 42:2k:59:TYR:CZ | 42:2k:63:LEU:HD11 | 2.54 | 0.43 |
| 1:1A:529:A:OP2 | 9:1N:114:ARG:NH2 | 2.52 | 0.43 |
| 1:1A:655:A:H2' | 1:1A:656:G:O4' | 2.18 | 0.43 |
| 1:1A:890:A:C6 | 1:1A:892:G:H1' | 2.53 | 0.43 |
| 1:1A:1065:U:H3' | 1:1A:1066:U:H6 | 1.84 | 0.43 |
| 1:1A:1171:G:H3' | 1:1A:1173:G:H5' | 2.00 | 0.43 |
| 1:1A:1359:A:N3 | 1:1A:1359:A:H5' | 2.34 | 0.43 |
| 1:1A:1709:U:H2' | 1:1A:1710:C:C6 | 2.54 | 0.43 |
| 1:1A:2136:C:C2 | 1:1A:2155:G:N2 | 2.85 | 0.43 |
| 1:1A:2335:A:C8 | 1:1A:2337:G:C5 | 3.07 | 0.43 |
| 1:1A:2506:U:C2 | 1:1A:2585:U:O4 | 2.72 | 0.43 |
| 4:1E:67:PHE:CE1 | 4:1E:75:VAL:HG22 | 2.54 | 0.43 |
| 11:1P:94:GLU:OE2 | 11:1P:124:LYS:HE2 | 2.19 | 0.43 |
| 13:1R:61:HIS:O | 13:1R:65:LEU:HG | 2.19 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 21:1Z:72:ARG:HA | 21:1Z:72:ARG:HD3 | 1.81 | 0.43 |
| 24:12:41:ILE:HG13 | 24:12:43:GLN:CG | 2.44 | 0.43 |
| 29:17:33:ARG:HH11 | 29:17:33:ARG:HD2 | 1.63 | 0.43 |
| 32:1a:189:G:C6 | 32:1a:189(L):G:N1 | 2.87 | 0.43 |
| 32:1a:976:G:H5' | 32:1a:1358:U:O2' | 2.18 | 0.43 |
| 32:1a:977:A:H1' | 32:1a:982:U:O4 | 2.18 | 0.43 |
| 32:1a:1347:G:C6 | 40:1i:107:ARG:NH2 | 2.87 | 0.43 |
| 33:1b:16:HIS:ND1 | 33:1b:17:PHE:N | 2.65 | 0.43 |
| 34:1c:3:ASN:OD1 | 34:1c:3:ASN:N | 2.51 | 0.43 |
| 35:1d:19:LEU:O | 35:1d:21:LEU:HG | 2.18 | 0.43 |
| 40:1i:3:GLN:HG2 | 40:1i:20:ARG:HE | 1.83 | 0.43 |
| 46:1o:82:ILE:O | 46:1o:86:GLY:N | 2.51 | 0.43 |
| 48:1q:66:SER:O | 48:1q:70:ARG:NH1 | 2.51 | 0.43 |
| 54:1w:72:C:H2' | 54:1w:73:A:C5 | 2.53 | 0.43 |
| 1:2A:411:G:OP2 | 1:2A:2406:U:O2' | 2.36 | 0.43 |
| 1:2A:775:G:O3' | 62:2A:3958:HOH:O | 2.21 | 0.43 |
| 1:2A:1198:U:H2' | 1:2A:1199:U:C6 | 2.54 | 0.43 |
| 1:2A:1614:A:N6 | 18:2W:92:ARG:O | 2.50 | 0.43 |
| 1:2A:2029:G:H2' | 1:2A:2031:A:OP1 | 2.19 | 0.43 |
| 1:2A:2336:A:N3 | 1:2A:2385:C:H1' | 2.33 | 0.43 |
| 2:2B:83:G:H1 | 2:2B:94:C:N4 | 2.17 | 0.43 |
| 3:2D:73:VAL:O | 3:2D:75:ILE:N | 2.52 | 0.43 |
| 3:2D:112:GLN:N | 3:2D:115:GLN:OE1 | 2.45 | 0.43 |
| 3:2D:260:ARG:NH2 | 3:2D:266:SER:OG | 2.52 | 0.43 |
| 6:2G:115:ARG:CZ | 6:2G:115:ARG:HB2 | 2.47 | 0.43 |
| 7:2H:33:LEU:HD11 | 7:2H:136:ILE:HG22 | 2.01 | 0.43 |
| 9:2N:24:GLY:O | 9:2N:28:THR:HG23 | 2.19 | 0.43 |
| 21:2Z:104:PHE:CD2 | 21:2Z:139:VAL:HG11 | 2.54 | 0.43 |
| 23:21:67:ILE:N | 23:21:68:PRO:HD2 | 2.34 | 0.43 |
| 32:2a:38:G:C2 | 32:2a:397:A:C2 | 3.07 | 0.43 |
| 32:2a:203:U:H2' | 32:2a:203:U:OP2 | 2.19 | 0.43 |
| 32:2a:237:C:H5'' | 48:2q:25:ARG:CZ | 2.48 | 0.43 |
| 33:2b:160:ASP:O | 33:2b:183:PRO:HD2 | 2.19 | 0.43 |
| 41:2j:6:ILE:HG12 | 41:2j:98:ILE:HG22 | 2.00 | 0.43 |
| 1:1A:436:C:H2' | 1:1A:437:G:C8 | 2.54 | 0.43 |
| 1:1A:1070:A:N6 | 1:1A:1096:A:C2 | 2.87 | 0.43 |
| 1:1A:1108:U:H2' | 1:1A:1109:C:O4' | 2.19 | 0.43 |
| 1:1A:1379:A:H8 | 1:1A:1379:A:O5' | 2.01 | 0.43 |
| 2:1B:14:U:O2 | 2:1B:108:U:H4' | 2.18 | 0.43 |
| 9:1N:62:VAL:HG22 | 9:1N:66:LYS:HD2 | 2.00 | 0.43 |
| 19:1X:44:GLU:HG2 | 19:1X:49:VAL:O | 2.18 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 23:11:52:ARG:HA | 23:11:56:GLN:O | 2.18 | 0.43 |
| 32:1a:186:C:H2' | 32:1a:187:C:C6 | 2.53 | 0.43 |
| 32:1a:473:G:OP2 | 47:1p:75:ARG:NH1 | 2.51 | 0.43 |
| 32:1a:585:G:N3 | 32:1a:879:C:H4' | 2.34 | 0.43 |
| 32:1a:1358:U:OP1 | 45:1n:35:ARG:HG3 | 2.19 | 0.43 |
| 32:1a:1529:G:H4' | 32:1a:1530:G:OP2 | 2.19 | 0.43 |
| 35:1d:140:VAL:HG12 | 35:1d:144:ASP:OD2 | 2.19 | 0.43 |
| 1:2A:8:A:H2' | 1:2A:9:U:C6 | 2.54 | 0.43 |
| 1:2A:18:C:H2' | 1:2A:19:C:C6 | 2.53 | 0.43 |
| 1:2A:1041:C:H6 | 1:2A:1041:C:O5' | 2.02 | 0.43 |
| 1:2A:1436:G:O2' | 1:2A:1477:A:H4' | 2.18 | 0.43 |
| 1:2A:1510:G:H2' | 1:2A:1511:C:O4' | 2.19 | 0.43 |
| 1:2A:2328:A:H2' | 1:2A:2329:G:C8 | 2.54 | 0.43 |
| 1:2A:2552:OMU:H2' | 1:2A:2554:U:OP2 | 2.19 | 0.43 |
| 1:2A:2895:U:H2' | 1:2A:2896:C:O4' | 2.19 | 0.43 |
| 2:2B:110:G:O2' | 2:2B:111:G:H5' | 2.19 | 0.43 |
| 7:2H:3:ARG:NH1 | 7:2H:4:ILE:H | 2.17 | 0.43 |
| 21:2Z:31:ARG:HD3 | 21:2Z:94:GLU:OE2 | 2.18 | 0.43 |
| 26:24:16:CYS:HA | 26:24:33:VAL:HG12 | 2.01 | 0.43 |
| 31:29:29:ASN:HD22 | 31:29:32:HIS:CE1 | 2.37 | 0.43 |
| 32:2a:1212:U:H4' | 32:2a:1213:A:C8 | 2.54 | 0.43 |
| 32:2a:1412:C:H2' | 32:2a:1413:A:C8 | 2.54 | 0.43 |
| 33:2b:150:SER:O | 33:2b:153:ARG:HG2 | 2.19 | 0.43 |
| 33:2b:167:PRO:HD3 | 33:2b:187:LEU:O | 2.19 | 0.43 |
| 36:2e:95:ALA:O | 36:2e:97:GLY:N | 2.51 | 0.43 |
| 44:2m:70:LEU:O | 44:2m:74:VAL:HG23 | 2.19 | 0.43 |
| 44:2m:115:LYS:HE2 | 44:2m:115:LYS:HB2 | 1.74 | 0.43 |
| 56:2y:68:C:H3' | 56:2y:69:G:H5'' | 2.01 | 0.43 |
| 1:1A:887:A:N1 | 1:1A:890:A:H8 | 2.17 | 0.42 |
| 1:1A:1584:C:O2' | 1:1A:1586:A:H5' | 2.19 | 0.42 |
| 1:1A:2259:G:C8 | 1:1A:2427:C:C4 | 3.07 | 0.42 |
| 4:1E:24:THR:O | 4:1E:184:VAL:HG12 | 2.19 | 0.42 |
| 6:1G:66:GLN:NE2 | 6:1G:94:LEU:HD23 | 2.33 | 0.42 |
| 7:1H:84:SER:OG | 7:1H:132:ARG:NH1 | 2.52 | 0.42 |
| 8:1I:133:HIS:HA | 62:1I:301:HOH:O | 2.19 | 0.42 |
| 9:1N:68:GLU:HG3 | 9:1N:88:GLU:OE2 | 2.19 | 0.42 |
| 10:1O:104:ARG:NE | 15:1T:36:GLU:OE2 | 2.44 | 0.42 |
| 27:15:11:THR:HG23 | 27:15:15:ARG:HB3 | 2.01 | 0.42 |
| 32:1a:245:C:O2 | 32:1a:283:C:N3 | 2.52 | 0.42 |
| 32:1a:990:C:C2' | 32:1a:991:U:H5' | 2.48 | 0.42 |
| 32:1a:1273:G:C6 | 32:1a:1274:G:C4 | 3.07 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 35:1d:67:ILE:HD13 | 35:1d:196:LEU:HD22 | 2.01 | 0.42 |
| 39:1h:87:SER:HB2 | 39:1h:93:VAL:HB | 2.01 | 0.42 |
| 44:1m:126:LYS:H | 44:1m:126:LYS:HG3 | 1.34 | 0.42 |
| 1:2A:443:A:C5 | 5:2F:45:ARG:HD2 | 2.54 | 0.42 |
| 1:2A:1664:A:H61 | 1:2A:1996:C:N4 | 2.16 | 0.42 |
| 1:2A:1790:C:H2' | 1:2A:1791:A:C5 | 2.54 | 0.42 |
| 1:2A:2850:A:C2 | 1:2A:2851:A:C4 | 3.07 | 0.42 |
| 32:2a:1141:C:C2 | 32:2a:1142:G:C8 | 3.07 | 0.42 |
| 32:2a:1268:A:H2' | 32:2a:1269:A:C8 | 2.54 | 0.42 |
| 32:2a:1271:G:N2 | 32:2a:1272:G:N7 | 2.66 | 0.42 |
| 33:2b:84:GLU:OE1 | 33:2b:84:GLU:HA | 2.19 | 0.42 |
| 33:2b:217:ARG:HA | 33:2b:217:ARG:HD3 | 1.92 | 0.42 |
| 35:2d:5:ILE:HA | 35:2d:115:ARG:HH11 | 1.83 | 0.42 |
| 39:2h:6:ILE:O | 39:2h:10:LEU:HG | 2.18 | 0.42 |
| 40:2i:40:LEU:C | 40:2i:42:ARG:N | 2.77 | 0.42 |
| 40:2i:93:ARG:O | 40:2i:97:LYS:N | 2.42 | 0.42 |
| 46:2o:48:LYS:HD3 | 46:2o:48:LYS:HA | 1.78 | 0.42 |
| 47:2p:60:LEU:HA | 47:2p:60:LEU:HD13 | 1.74 | 0.42 |
| 56:2y:48:C:H2' | 56:2y:59:U:H1' | 2.00 | 0.42 |
| 1:1A:877:U:H3 | 1:1A:899:A:H2 | 1.67 | 0.42 |
| 1:1A:911:A:H2' | 12:1Q:9:TYR:OH | 2.19 | 0.42 |
| 4:1E:60:ASN:O | 4:1E:64:LYS:HG3 | 2.19 | 0.42 |
| 5:1F:110:LEU:HD12 | 5:1F:110:LEU:HA | 1.74 | 0.42 |
| 6:1G:131:TYR:HB3 | 6:1G:159:VAL:HG13 | 2.00 | 0.42 |
| 8:1I:66:GLU:HA | 8:1I:69:LYS:HB3 | 2.01 | 0.42 |
| 15:1T:90:GLN:HG3 | 15:1T:91:ARG:N | 2.34 | 0.42 |
| 28:16:9:LEU:HD21 | 28:16:25:LYS:HB3 | 2.00 | 0.42 |
| 32:1a:255:G:H1' | 48:1q:16:GLN:OE1 | 2.19 | 0.42 |
| 32:1a:580:U:H2' | 32:1a:581:G:O4' | 2.19 | 0.42 |
| 32:1a:691:G:OP2 | 42:1k:26:ASN:ND2 | 2.51 | 0.42 |
| 32:1a:1172:C:H2' | 32:1a:1173:G:H8 | 1.84 | 0.42 |
| 32:1a:1312:G:H5' | 50:1s:5:LEU:HD21 | 2.01 | 0.42 |
| 32:1a:1316:G:H2' | 32:1a:1318:A:OP2 | 2.19 | 0.42 |
| 33:1b:63:MET:HG2 | 33:1b:225:ALA:HB1 | 2.00 | 0.42 |
| 38:1g:23:VAL:HG13 | 38:1g:43:PHE:CE2 | 2.54 | 0.42 |
| 44:1m:102:ARG:HE | 44:1m:102:ARG:HB2 | 1.45 | 0.42 |
| 46:1o:17:ARG:HG3 | 46:1o:17:ARG:NH1 | 2.34 | 0.42 |
| 47:1p:49:LEU:HD12 | 47:1p:50:LYS:N | 2.34 | 0.42 |
| 50:1s:20:LEU:HD23 | 50:1s:20:LEU:HA | 1.87 | 0.42 |
| 1:2A:68:G:H2' | 1:2A:69:C:C6 | 2.54 | 0.42 |
| 1:2A:466:A:N1 | 1:2A:795:C:O2' | 2.47 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:2A:570:G:H2' | 1:2A:2030:A:C5 | 2.54 | 0.42 |
| 1:2A:1503:U:H2' | 1:2A:1504:C:C6 | 2.54 | 0.42 |
| 1:2A:2853:C:H2' | 1:2A:2854:G:C8 | 2.54 | 0.42 |
| 5:2F:117:ARG:NH2 | 5:2F:189:THR:O | 2.52 | 0.42 |
| 16:2U:27:LEU:HD23 | 16:2U:27:LEU:HA | 1.65 | 0.42 |
| 32:2a:827:U:C2 | 32:2a:874:G:N2 | 2.87 | 0.42 |
| 32:2a:1141:C:H2' | 32:2a:1142:G:O4' | 2.18 | 0.42 |
| 32:2a:1238:A:C2 | 32:2a:1241:G:N3 | 2.83 | 0.42 |
| 32:2a:1366:C:H2' | 32:2a:1367:C:H6 | 1.83 | 0.42 |
| 40:2i:40:LEU:O | 40:2i:42:ARG:N | 2.52 | 0.42 |
| 46:2o:6:GLU:OE1 | 46:2o:6:GLU:N | 2.46 | 0.42 |
| 57:2z:7:GLY:HA2 | 57:2z:14:GLY:HA2 | 2.01 | 0.42 |
| 1:1A:524:U:H2' | 1:1A:525:U:C6 | 2.54 | 0.42 |
| 1:1A:811:U:H2' | 11:1P:21:ARG:HA | 2.01 | 0.42 |
| 1:1A:1359:A:N3 | 1:1A:1359:A:O4' | 2.51 | 0.42 |
| 1:1A:1767:C:O2' | 1:1A:1768:U:H5' | 2.19 | 0.42 |
| 3:1D:130:ALA:C | 3:1D:131:LEU:HD12 | 2.44 | 0.42 |
| 9:1N:41:ASP:O | 9:1N:48:MET:HE1 | 2.19 | 0.42 |
| 15:1T:19:LEU:HD22 | 15:1T:86:ILE:HG13 | 2.02 | 0.42 |
| 18:1W:58:ALA:HB1 | 18:1W:64:MET:HB2 | 2.01 | 0.42 |
| 21:1Z:54:HIS:HD2 | 21:1Z:99:TYR:O | 2.02 | 0.42 |
| 32:1a:244:U:OP2 | 48:1q:100:LYS:NZ | 2.52 | 0.42 |
| 32:1a:627:G:O2' | 32:1a:628:G:H5' | 2.19 | 0.42 |
| 32:1a:966:M2G:CM1 | 40:1i:127:LYS:HE2 | 2.50 | 0.42 |
| 32:1a:1095:U:OP1 | 32:1a:1108:G:N2 | 2.50 | 0.42 |
| 32:1a:1118:C:OP1 | 40:1i:9:ARG:HD2 | 2.19 | 0.42 |
| 33:1b:12:GLU:HB2 | 33:1b:213:LEU:HD21 | 2.00 | 0.42 |
| 33:1b:55:PHE:O | 33:1b:59:GLU:HB2 | 2.19 | 0.42 |
| 33:1b:207:ALA:HB3 | 33:1b:210:SER:HB2 | 2.01 | 0.42 |
| 36:1e:41:VAL:O | 36:1e:66:MET:HA | 2.19 | 0.42 |
| 50:1s:6:LYS:HE3 | 50:1s:6:LYS:HB3 | 1.76 | 0.42 |
| 51:1t:74:LYS:HE2 | 51:1t:74:LYS:HB3 | 1.86 | 0.42 |
| 1:2A:478:A:N1 | 1:2A:500:G:H4' | 2.35 | 0.42 |
| 1:2A:2513:G:N2 | 4:2E:143:ASN:HD21 | 2.16 | 0.42 |
| 6:2G:50:ALA:O | 6:2G:52:ILE:N | 2.52 | 0.42 |
| 9:2N:71:ILE:CG2 | 9:2N:84:LYS:HB3 | 2.47 | 0.42 |
| 17:2V:71:LEU:N | 17:2V:71:LEU:HD23 | 2.34 | 0.42 |
| 20:2Y:67:LEU:HA | 20:2Y:67:LEU:HD23 | 1.72 | 0.42 |
| 32:2a:429:U:O3' | 35:2d:22:LYS:NZ | 2.51 | 0.42 |
| 32:2a:737:A:H2' | 32:2a:738:C:C6 | 2.55 | 0.42 |
| 45:2n:23:ARG:C | 45:2n:33:VAL:HG11 | 2.44 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 54:2w:8:4SU:S4 | 54:2w:13:C:O2' | 2.66 | 0.42 |
| 1:1A:34:C:H5'' | 1:1A:35:G:OP2 | 2.19 | 0.42 |
| 1:1A:189:G:O6 | 1:1A:205:G:O2' | 2.36 | 0.42 |
| 1:1A:271(E):U:C2 | 1:1A:271(F):C:C5 | 3.08 | 0.42 |
| 1:1A:862:G:H2' | 1:1A:863:A:O4' | 2.19 | 0.42 |
| 1:1A:1096:A:N6 | 1:1A:1097:U:O2 | 2.45 | 0.42 |
| 1:1A:2470:G:OP1 | 12:1Q:56:ARG:NH2 | 2.52 | 0.42 |
| 1:1A:2687:U:H2' | 1:1A:2688:U:O4' | 2.18 | 0.42 |
| 6:1G:99:MET:HE2 | 6:1G:99:MET:HB3 | 1.79 | 0.42 |
| 6:1G:170:ARG:NH2 | 6:1G:182:LYS:O | 2.50 | 0.42 |
| 13:1R:67:LEU:HD21 | 13:1R:73:VAL:HG12 | 2.02 | 0.42 |
| 20:1Y:9:LYS:HA | 20:1Y:10:GLY:HA2 | 1.58 | 0.42 |
| 23:11:19:GLN:HB2 | 23:11:35:THR:HG22 | 2.00 | 0.42 |
| 32:1a:144:G:C6 | 32:1a:145:G:C5 | 3.07 | 0.42 |
| 32:1a:487:A:H2' | 32:1a:488:C:O4' | 2.19 | 0.42 |
| 32:1a:932:C:O2' | 32:1a:933:G:H5' | 2.19 | 0.42 |
| 32:1a:997:U:H3 | 32:1a:1044:A:H61 | 1.67 | 0.42 |
| 32:1a:1035:A:N3 | 32:1a:1036:G:N2 | 2.68 | 0.42 |
| 32:1a:1314:C:H2' | 32:1a:1315:U:C6 | 2.54 | 0.42 |
| 1:2A:10:G:C1' | 1:2A:2801(A):A:H62 | 2.27 | 0.42 |
| 1:2A:70:G:H5'' | 1:2A:112:U:O2 | 2.18 | 0.42 |
| 1:2A:874:G:N2 | 1:2A:904:C:C2 | 2.87 | 0.42 |
| 1:2A:1024:G:O2' | 1:2A:1144:G:O2' | 2.38 | 0.42 |
| 1:2A:1171:G:H8 | 1:2A:1171:G:O5' | 2.02 | 0.42 |
| 1:2A:1786:A:H1' | 1:2A:1938:A:N6 | 2.33 | 0.42 |
| 1:2A:1952:A:OP1 | 10:2O:42:SER:OG | 2.35 | 0.42 |
| 2:2B:33:G:C2 | 2:2B:50:G:C2 | 3.07 | 0.42 |
| 2:2B:54:G:H2' | 2:2B:55:U:H6 | 1.84 | 0.42 |
| 3:2D:182:LEU:HB2 | 3:2D:272:ALA:HB3 | 2.02 | 0.42 |
| 5:2F:117:ARG:HH12 | 11:2P:1:MET:H3 | 1.66 | 0.42 |
| 5:2F:185:ASP:HA | 5:2F:188:ARG:HB2 | 2.01 | 0.42 |
| 17:2V:32:THR:HA | 17:2V:59:ALA:O | 2.19 | 0.42 |
| 19:2X:92:LEU:O | 19:2X:94:GLY:N | 2.52 | 0.42 |
| 32:2a:23:C:OP2 | 32:2a:561:U:N3 | 2.39 | 0.42 |
| 32:2a:67:C:H4' | 32:2a:172:A:O4' | 2.20 | 0.42 |
| 32:2a:93:G:C6 | 32:2a:96:U:C4 | 3.08 | 0.42 |
| 32:2a:413:G:N2 | 32:2a:428:G:H1' | 2.35 | 0.42 |
| 32:2a:540:G:C4 | 32:2a:541:G:C8 | 3.07 | 0.42 |
| 32:2a:1004:A:N6 | 32:2a:1037:C:O2 | 2.48 | 0.42 |
| 32:2a:1315:U:H2' | 32:2a:1316:G:O4' | 2.19 | 0.42 |
| 39:2h:38:ILE:HD12 | 39:2h:118:VAL:HG12 | 2.00 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 41:2j:33:GLN:HE21 | 41:2j:33:GLN:HB3 | 1.62 | 0.42 |
| 42:2k:91:ARG:HE | 42:2k:91:ARG:HB3 | 1.57 | 0.42 |
| 51:2t:73:HIS:ND1 | 51:2t:75:ASN:HB2 | 2.35 | 0.42 |
| 1:1A:1680:U:H2' | 1:1A:1681:G:O4' | 2.20 | 0.42 |
| 1:1A:2579:C:O5' | 1:1A:2579:C:H6 | 2.02 | 0.42 |
| 26:14:55:ARG:H | 26:14:56:VAL:HA | 1.78 | 0.42 |
| 32:1a:352:C:H4' | 32:1a:354:G:OP1 | 2.20 | 0.42 |
| 32:1a:1152:A:H2' | 32:1a:1153:C:C6 | 2.54 | 0.42 |
| 35:1d:194:LEU:HD12 | 35:1d:195:ALA:H | 1.84 | 0.42 |
| 39:1h:86:ILE:HG22 | 39:1h:87:SER:N | 2.33 | 0.42 |
| 40:1i:128:ARG:NH1 | 55:1x:35:A:OP2 | 2.53 | 0.42 |
| 47:1p:62:VAL:O | 47:1p:62:VAL:HG13 | 2.20 | 0.42 |
| 1:2A:754:C:H2' | 1:2A:755:C:C6 | 2.54 | 0.42 |
| 1:2A:852:G:H2' | 1:2A:853:G:C8 | 2.55 | 0.42 |
| 1:2A:2222:G:O2' | 3:2D:148:GLU:HG2 | 2.19 | 0.42 |
| 11:2P:81:GLN:HE22 | 11:2P:106:LEU:HA | 1.84 | 0.42 |
| 25:23:12:PRO:HB2 | 25:23:20:LYS:HE3 | 2.01 | 0.42 |
| 27:25:33:CYS:HB2 | 27:25:40:LYS:CD | 2.50 | 0.42 |
| 32:2a:179:A:C2 | 32:2a:180:U:C2 | 3.07 | 0.42 |
| 32:2a:356:A:N3 | 32:2a:368:U:O2' | 2.46 | 0.42 |
| 32:2a:1253:G:H2' | 32:2a:1254:C:C6 | 2.54 | 0.42 |
| 37:2f:86:ARG:O | 37:2f:87:ARG:HG2 | 2.18 | 0.42 |
| 40:2i:3:GLN:HA | 40:2i:20:ARG:HG2 | 1.99 | 0.42 |
| 45:2n:48:ALA:HB2 | 45:2n:53:LEU:HD23 | 2.02 | 0.42 |
| 1:1A:236:C:H2' | 1:1A:237:C:H6 | 1.84 | 0.42 |
| 1:1A:1179:C:O2' | 1:1A:1180:C:H5' | 2.20 | 0.42 |
| 1:1A:1419:A:C8 | 1:1A:1421:G:C6 | 3.08 | 0.42 |
| 5:1F:8:GLN:HE22 | 5:1F:21:ALA:HB2 | 1.85 | 0.42 |
| 5:1F:117:ARG:HH12 | 11:1P:1:MET:H2 | 1.66 | 0.42 |
| 7:1H:78:GLY:O | 7:1H:136:ILE:HG22 | 2.19 | 0.42 |
| 10:1O:7:TYR:C | 10:1O:8:LEU:HD12 | 2.44 | 0.42 |
| 10:1O:17:ARG:O | 10:1O:18:LYS:HG2 | 2.19 | 0.42 |
| 10:1O:24:VAL:HG13 | 10:1O:33:ALA:HB2 | 2.02 | 0.42 |
| 12:1Q:16:ARG:C | 12:1Q:17:LEU:HD23 | 2.45 | 0.42 |
| 14:1S:11:LYS:HD3 | 14:1S:91:PRO:HD3 | 2.01 | 0.42 |
| 26:14:58:ARG:O | 26:14:60:GLN:N | 2.52 | 0.42 |
| 32:1a:160:A:H1' | 32:1a:344:A:C4 | 2.53 | 0.42 |
| 32:1a:899:C:H6 | 32:1a:899:C:O5' | 2.03 | 0.42 |
| 32:1a:912:C:O2' | 32:1a:913:A:H5' | 2.19 | 0.42 |
| 32:1a:1026:G:H3' | 32:1a:1027:C:C6 | 2.54 | 0.42 |
| 32:1a:1367:C:H4' | 41:1j:48:THR:HG21 | 2.01 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 33:1b:122:PHE:HE2 | 33:1b:139:LYS:HB2 | 1.85 | 0.42 |
| 37:1f:19:LEU:HD21 | 37:1f:59:TYR:CE2 | 2.55 | 0.42 |
| 1:2A:141:A:C8 | 1:2A:1408:C:O2' | 2.63 | 0.42 |
| 1:2A:234:C:H2' | 1:2A:235:U:C6 | 2.54 | 0.42 |
| 1:2A:1021:A:C8 | 1:2A:1022:G:H5'' | 2.54 | 0.42 |
| 1:2A:1372:U:H2' | 1:2A:1373:A:O4' | 2.19 | 0.42 |
| 1:2A:1703:G:H2' | 1:2A:1704:G:H8 | 1.85 | 0.42 |
| 1:2A:2331:G:O2' | 22:20:43:THR:HG22 | 2.20 | 0.42 |
| 1:2A:2576:G:O2' | 1:2A:2579:C:OP2 | 2.30 | 0.42 |
| 1:2A:2615:U:H2' | 1:2A:2616:C:H6 | 1.85 | 0.42 |
| 1:2A:2741:A:H2' | 1:2A:2742:C:O4' | 2.20 | 0.42 |
| 2:2B:75:G:H8 | 2:2B:75:G:C5' | 2.32 | 0.42 |
| 5:2F:43:LYS:HG2 | 5:2F:43:LYS:O | 2.20 | 0.42 |
| 6:2G:39:ILE:O | 6:2G:91:ARG:HA | 2.19 | 0.42 |
| 8:2I:82:ARG:HH11 | 8:2I:82:ARG:HD3 | 1.63 | 0.42 |
| 16:2U:68:ALA:O | 16:2U:71:GLN:HB2 | 2.20 | 0.42 |
| 19:2X:5:TYR:CE1 | 24:22:30:ARG:HB2 | 2.54 | 0.42 |
| 32:2a:50:A:H4' | 32:2a:52:G:OP1 | 2.19 | 0.42 |
| 32:2a:62:U:H2' | 32:2a:63:C:C6 | 2.55 | 0.42 |
| 32:2a:350:G:C6 | 32:2a:351:G:O6 | 2.72 | 0.42 |
| 32:2a:790:A:H2' | 32:2a:791:G:C8 | 2.55 | 0.42 |
| 32:2a:1091:U:C2 | 32:2a:1095:U:C4 | 3.06 | 0.42 |
| 36:2e:28:PHE:O | 36:2e:47:LYS:HA | 2.20 | 0.42 |
| 37:2f:99:ALA:HB1 | 49:2r:23:LYS:HZ3 | 1.82 | 0.42 |
| 38:2g:32:ARG:C | 38:2g:34:GLY:H | 2.26 | 0.42 |
| 1:1A:721:C:H2' | 1:1A:722:A:C8 | 2.55 | 0.42 |
| 1:1A:2164:C:H2' | 1:1A:2165:G:H5' | 2.01 | 0.42 |
| 5:1F:120:GLU:HB2 | 5:1F:122:LYS:HG2 | 2.01 | 0.42 |
| 6:1G:17:PRO:HA | 6:1G:20:ILE:HD12 | 2.01 | 0.42 |
| 9:1N:1:MET:O | 9:1N:2:LYS:HB2 | 2.20 | 0.42 |
| 11:1P:1:MET:HE2 | 11:1P:1:MET:HB2 | 1.84 | 0.42 |
| 21:1Z:59:LEU:HB3 | 21:1Z:61:LEU:CD2 | 2.47 | 0.42 |
| 24:12:63:VAL:O | 24:12:67:LYS:HG2 | 2.19 | 0.42 |
| 32:1a:193:C:H2' | 32:1a:194:C:C6 | 2.55 | 0.42 |
| 32:1a:391:G:C6 | 32:1a:392:G:C5 | 3.08 | 0.42 |
| 32:1a:734:G:H21 | 49:1r:75:ILE:HD11 | 1.85 | 0.42 |
| 32:1a:975:A:N6 | 41:1j:60:ARG:HH12 | 2.18 | 0.42 |
| 33:1b:16:HIS:HB2 | 33:1b:204:ASN:CB | 2.49 | 0.42 |
| 50:1s:22:LEU:O | 50:1s:23:ASN:C | 2.63 | 0.42 |
| 51:1t:60:GLU:HG3 | 51:1t:81:LYS:HD2 | 2.02 | 0.42 |
| 1:2A:852:G:H2' | 1:2A:853:G:H8 | 1.85 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 1:2A:893:C:H6 | 1:2A:894:C:N4 | 2.18 | 0.42 |
| 1:2A:1022:G:N2 | 1:2A:1023:U:O4 | 2.52 | 0.42 |
| 1:2A:1754:C:P | 15:2T:96:ARG:HH12 | 2.42 | 0.42 |
| 1:2A:2183:C:H2' | 1:2A:2184:G:C8 | 2.50 | 0.42 |
| 1:2A:2507:C:H2' | 1:2A:2508:G:O4' | 2.20 | 0.42 |
| 1:2A:2819:G:H2' | 1:2A:2821:A:N7 | 2.35 | 0.42 |
| 2:2B:1:U:O2' | 2:2B:2:C:O5' | 2.35 | 0.42 |
| 5:2F:202:PHE:CZ | 5:2F:206:ILE:HD13 | 2.55 | 0.42 |
| 8:2I:86:THR:O | 8:2I:123:LEU:HD12 | 2.20 | 0.42 |
| 10:2O:88:ASN:OD1 | 10:2O:90:GLN:N | 2.52 | 0.42 |
| 29:27:1:MET:HE3 | 29:27:3:ARG:NH2 | 2.34 | 0.42 |
| 32:2a:1363(A):A:H1' | 32:2a:1365:G:N7 | 2.34 | 0.42 |
| 37:2f:30:LEU:HD23 | 37:2f:30:LEU:HA | 1.73 | 0.42 |
| 42:2k:53:SER:O | 42:2k:55:LYS:N | 2.53 | 0.42 |
| 51:2t:53:LEU:HD23 | 51:2t:53:LEU:HA | 1.81 | 0.42 |
| 1:1A:271(D):G:H2' | 1:1A:271(E):U:O4' | 2.20 | 0.42 |
| 1:1A:754:C:H2' | 1:1A:755:C:C6 | 2.54 | 0.42 |
| 1:1A:1721:G:H1' | 1:1A:1741:A:H61 | 1.85 | 0.42 |
| 4:1E:101:ARG:HA | 4:1E:170:LEU:O | 2.19 | 0.42 |
| 11:1P:97:PRO:HD3 | 11:1P:126:VAL:O | 2.19 | 0.42 |
| 26:14:48:ARG:HA | 26:14:48:ARG:HD3 | 1.78 | 0.42 |
| 32:1a:93:G:H2' | 32:1a:96:U:H6 | 1.84 | 0.42 |
| 32:1a:190:U:C5 | 32:1a:191:G:N7 | 2.87 | 0.42 |
| 32:1a:191:G:N3 | 51:1t:103:GLY:HA2 | 2.34 | 0.42 |
| 32:1a:439:A:C8 | 32:1a:496:A:C6 | 3.07 | 0.42 |
| 32:1a:1516:G:H2' | 32:1a:1518:MA6:OP2 | 2.19 | 0.42 |
| 35:1d:157:LEU:HD22 | 35:1d:161:ASN:ND2 | 2.34 | 0.42 |
| 36:1e:91:LEU:HB3 | 36:1e:118:ILE:HD11 | 2.01 | 0.42 |
| 44:1m:22:ILE:HB | 44:1m:25:ILE:HD12 | 2.01 | 0.42 |
| 1:2A:763:G:H1' | 1:2A:765:G:O4' | 2.20 | 0.42 |
| 1:2A:969:U:H2' | 1:2A:970:C:C6 | 2.55 | 0.42 |
| 1:2A:1425:G:C6 | 1:2A:1426:G:C6 | 3.08 | 0.42 |
| 1:2A:1429:G:H1' | 1:2A:1568:G:H1' | 2.02 | 0.42 |
| 4:2E:16:ARG:NH1 | 4:2E:173:VAL:HG22 | 2.35 | 0.42 |
| 6:2G:22:ARG:NH1 | 6:2G:175:LEU:HD21 | 2.35 | 0.42 |
| 10:2O:12:ASP:C | 10:2O:12:ASP:OD1 | 2.63 | 0.42 |
| 10:2O:64:ARG:HB3 | 10:2O:79:PHE:CG | 2.54 | 0.42 |
| 10:2O:66:LYS:HA | 10:2O:79:PHE:O | 2.20 | 0.42 |
| 31:29:13:LYS:HD3 | 31:29:13:LYS:HA | 1.80 | 0.42 |
| 32:2a:542:G:H5' | 35:2d:41:GLY:HA3 | 2.02 | 0.42 |
| 32:2a:687:A:H4' | 32:2a:688:G:O5' | 2.20 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 32:2a:1014:A:C2 | 32:2a:1219:U:H1' | 2.54 | 0.42 |
| 32:2a:1179:A:C5 | 32:2a:1180:A:C5 | 3.08 | 0.42 |
| 32:2a:1183:A:HO2' | 32:2a:1184:G:P | 2.43 | 0.42 |
| 32:2a:1218:C:P | 45:2n:9:LYS:HE2 | 2.60 | 0.42 |
| 32:2a:1263:C:N3 | 32:2a:1272:G:O6 | 2.53 | 0.42 |
| 32:2a:1411:C:H2' | 32:2a:1412:C:C6 | 2.54 | 0.42 |
| 38:2g:104:LEU:HD23 | 38:2g:104:LEU:HA | 1.86 | 0.42 |
| 54:2w:59:U:C4 | 54:2w:60:U:C4 | 3.07 | 0.42 |
| 1:1A:489:G:H2' | 1:1A:491:G:O4' | 2.20 | 0.42 |
| 1:1A:775:G:C5 | 1:1A:794:G:C8 | 3.08 | 0.42 |
| 1:1A:1058:G:C2' | 1:1A:1059:G:H5' | 2.49 | 0.42 |
| 1:1A:1116:C:H5' | 1:1A:1117:G:OP2 | 2.19 | 0.42 |
| 1:1A:1170:G:H1 | 1:1A:1179:C:N4 | 2.17 | 0.42 |
| 8:1I:88:ILE:HD12 | 8:1I:122:GLU:N | 2.35 | 0.42 |
| 11:1P:140:ALA:C | 11:1P:142:GLY:H | 2.28 | 0.42 |
| 32:1a:184:G:O2' | 32:1a:185:A:H5' | 2.20 | 0.42 |
| 32:1a:509:A:C8 | 32:1a:509:A:H3' | 2.54 | 0.42 |
| 32:1a:731:G:O2' | 32:1a:732:C:H5' | 2.19 | 0.42 |
| 32:1a:785:G:O2' | 32:1a:786:G:H5' | 2.20 | 0.42 |
| 32:1a:872:A:C4 | 32:1a:874:G:N7 | 2.88 | 0.42 |
| 32:1a:1238:A:C2 | 32:1a:1241:G:N3 | 2.88 | 0.42 |
| 32:1a:1262:C:H2' | 32:1a:1263:C:C6 | 2.55 | 0.42 |
| 35:1d:149:ALA:HB3 | 35:1d:152:SER:CB | 2.50 | 0.42 |
| 35:1d:172:PRO:C | 35:1d:174:LEU:N | 2.78 | 0.42 |
| 38:1g:93:PRO:O | 38:1g:96:GLN:HB2 | 2.20 | 0.42 |
| 42:1k:46:GLY:HA2 | 42:1k:50:TYR:O | 2.20 | 0.42 |
| 47:1p:38:TYR:CD1 | 47:1p:38:TYR:C | 2.98 | 0.42 |
| 57:1z:2:LYS:HB3 | 57:1z:3:LYS:H | 1.62 | 0.42 |
| 1:2A:36:G:N3 | 1:2A:450:G:O2' | 2.53 | 0.42 |
| 1:2A:1131:G:C2 | 1:2A:1132:A:C4 | 3.07 | 0.42 |
| 1:2A:2671:A:H2' | 1:2A:2672:G:O4' | 2.20 | 0.42 |
| 4:2E:68:ALA:O | 4:2E:71:GLY:N | 2.42 | 0.42 |
| 5:2F:114:VAL:HG21 | 5:2F:202:PHE:CZ | 2.55 | 0.42 |
| 8:2I:5:LEU:HD12 | 8:2I:5:LEU:H | 1.85 | 0.42 |
| 8:2I:37:VAL:HG13 | 8:2I:38:LEU:HD12 | 2.01 | 0.42 |
| 10:2O:122:LEU:HD23 | 10:2O:122:LEU:HA | 1.81 | 0.42 |
| 12:2Q:79:LEU:HA | 12:2Q:79:LEU:HD23 | 1.74 | 0.42 |
| 13:2R:18:LEU:HD21 | 13:2R:22:ARG:CZ | 2.50 | 0.42 |
| 20:2Y:9:LYS:HA | 20:2Y:10:GLY:HA2 | 1.46 | 0.42 |
| 24:22:64:LEU:O | 24:22:68:ARG:HG3 | 2.20 | 0.42 |
| 32:2a:37:U:H2' | 32:2a:38:G:O4' | 2.19 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 32:2a:473:G:H2' | 32:2a:474:G:H8 | 1.85 | 0.42 |
| 32:2a:1101:A:H62 | 33:2b:175:ARG:HH21 | 1.67 | 0.42 |
| 32:2a:1263:C:O2 | 32:2a:1273:G:C2 | 2.72 | 0.42 |
| 34:2c:164:ARG:NH1 | 34:2c:166:GLU:OE1 | 2.52 | 0.42 |
| 44:2m:39:ILE:HG22 | 44:2m:40:ASN:O | 2.19 | 0.42 |
| 44:2m:67:GLU:HG3 | 44:2m:71:ARG:HH21 | 1.85 | 0.42 |
| 47:2p:1:MET:HE2 | 47:2p:1:MET:N | 2.35 | 0.42 |
| 47:2p:43:LYS:HG2 | 47:2p:48:TRP:CD1 | 2.55 | 0.42 |
| 56:2y:53:G:H2' | 56:2y:53:G:N3 | 2.35 | 0.42 |
| 1:1A:2404:C:O3' | 11:1P:77:ARG:NH2 | 2.53 | 0.42 |
| 1:1A:2406:U:H2' | 1:1A:2406:U:H6 | 1.59 | 0.42 |
| 1:1A:2552:OMU:C2 | 1:1A:2554:U:H5' | 2.50 | 0.42 |
| 5:1F:63:LYS:NZ | 5:1F:75:HIS:O | 2.47 | 0.42 |
| 13:1R:2:ARG:HA | 13:1R:5:LYS:HD2 | 2.02 | 0.42 |
| 15:1T:31:SER:OG | 15:1T:44:ASP:OD2 | 2.22 | 0.42 |
| 18:1W:65:LEU:HD23 | 18:1W:65:LEU:HA | 1.82 | 0.42 |
| 18:1W:82:LEU:HB2 | 18:1W:98:LYS:HB2 | 2.02 | 0.42 |
| 32:1a:192:U:H2' | 32:1a:193:C:H6 | 1.85 | 0.42 |
| 32:1a:254:G:OP1 | 48:1q:67:LYS:O | 2.38 | 0.42 |
| 32:1a:451:A:H61 | 32:1a:481:G:H5' | 1.85 | 0.42 |
| 32:1a:1255:G:C2 | 32:1a:1283:G:C2 | 3.08 | 0.42 |
| 33:1b:72:GLY:HA2 | 33:1b:165:VAL:HG12 | 2.01 | 0.42 |
| 36:1e:92:LYS:HB3 | 36:1e:119:LEU:HB2 | 2.01 | 0.42 |
| 41:1j:8:LEU:HD22 | 41:1j:96:ILE:HG22 | 2.00 | 0.42 |
| 1:2A:71:A:N7 | 19:2X:31:HIS:HE1 | 2.17 | 0.42 |
| 1:2A:280:C:C2 | 1:2A:361:G:C2 | 3.07 | 0.42 |
| 1:2A:1187:G:H5' | 17:2V:81:TYR:CE1 | 2.54 | 0.42 |
| 1:2A:1354:A:H2' | 1:2A:1355:G:O4' | 2.19 | 0.42 |
| 1:2A:2309:A:C6 | 1:2A:2310:A:C6 | 3.07 | 0.42 |
| 62:2A:4232:HOH:O | 11:2P:39:LYS:HD3 | 2.19 | 0.42 |
| 2:2B:4:C:H42 | 2:2B:117:G:H1 | 1.68 | 0.42 |
| 4:2E:63:LEU:HD23 | 4:2E:63:LEU:HA | 1.95 | 0.42 |
| 8:2I:134:PRO:C | 8:2I:136:VAL:H | 2.28 | 0.42 |
| 11:2P:1:MET:HE3 | 11:2P:1:MET:HB2 | 1.95 | 0.42 |
| 21:2Z:158:PRO:O | 21:2Z:161:VAL:HG12 | 2.18 | 0.42 |
| 28:26:34:LEU:HD23 | 28:26:34:LEU:HA | 1.86 | 0.42 |
| 32:2a:302:G:N3 | 32:2a:556:C:H4' | 2.34 | 0.42 |
| 32:2a:529:G:O6 | 43:2l:49:ASN:HA | 2.20 | 0.42 |
| 32:2a:656:C:H2' | 32:2a:657:G:O4' | 2.20 | 0.42 |
| 33:2b:118:LEU:HD11 | 33:2b:138:LEU:HB3 | 2.01 | 0.42 |
| 35:2d:122:ARG:O | 35:2d:134:ASP:HB2 | 2.20 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 36:2e:76:ILE:O | 36:2e:93:PRO:HB3 | 2.19 | 0.42 |
| 50:2s:53:ASN:OD1 | 50:2s:54:GLY:N | 2.52 | 0.42 |
| 51:2t:73:HIS:O | 51:2t:76:ALA:N | 2.48 | 0.42 |
| 54:2w:73:A:OP2 | 54:2w:73:A:H8 | 2.02 | 0.42 |
| 1:1A:226:G:H21 | 1:1A:228:A:H62 | 1.68 | 0.41 |
| 1:1A:1274:A:N3 | 1:1A:1297:C:H1' | 2.34 | 0.41 |
| 1:1A:1394:U:H6 | 1:1A:1394:U:H3' | 1.85 | 0.41 |
| 1:1A:2099:U:O4 | 1:1A:2190:G:O6 | 2.37 | 0.41 |
| 10:1O:60:ALA:HB1 | 10:1O:84:ALA:HB1 | 2.02 | 0.41 |
| 14:1S:39:ILE:HB | 14:1S:49:VAL:CG1 | 2.50 | 0.41 |
| 25:13:7:LYS:HA | 25:13:33:GLN:O | 2.19 | 0.41 |
| 32:1a:392:G:H2' | 32:1a:393:A:C8 | 2.55 | 0.41 |
| 32:1a:995:C:O2' | 32:1a:996:A:H5' | 2.20 | 0.41 |
| 32:1a:1366:C:H2' | 32:1a:1367:C:C6 | 2.55 | 0.41 |
| 33:1b:73:THR:O | 33:1b:78:GLN:NE2 | 2.51 | 0.41 |
| 38:1g:78:ARG:NH1 | 38:1g:156:TRP:HB3 | 2.35 | 0.41 |
| 39:1h:25:ASP:OD2 | 39:1h:60:ARG:HG3 | 2.19 | 0.41 |
| 44:1m:106:ASN:HB3 | 44:1m:107:ALA:H | 1.62 | 0.41 |
| 1:2A:730:C:O2' | 1:2A:731:C:H5' | 2.20 | 0.41 |
| 1:2A:1463:C:O2' | 1:2A:1464:C:H5' | 2.20 | 0.41 |
| 2:2B:28:C:N3 | 2:2B:56:G:N1 | 2.44 | 0.41 |
| 11:2P:36:LYS:HB3 | 11:2P:37:GLY:H | 1.60 | 0.41 |
| 11:2P:89:ALA:HA | 11:2P:121:LYS:HD3 | 2.02 | 0.41 |
| 11:2P:90:ARG:HB3 | 11:2P:91:PHE:CD2 | 2.54 | 0.41 |
| 12:2Q:75:THR:HG21 | 12:2Q:87:LYS:HE3 | 2.02 | 0.41 |
| 21:2Z:51:ALA:O | 21:2Z:55:HIS:HD2 | 2.03 | 0.41 |
| 32:2a:160:A:H2' | 32:2a:161:A:O4' | 2.19 | 0.41 |
| 32:2a:352:C:O2' | 32:2a:354:G:OP1 | 2.27 | 0.41 |
| 32:2a:828:A:H2' | 32:2a:829:G:O4' | 2.19 | 0.41 |
| 32:2a:874:G:O2' | 32:2a:875:C:H5' | 2.20 | 0.41 |
| 32:2a:957:U:H1' | 32:2a:960:U:C4 | 2.55 | 0.41 |
| 32:2a:1149:C:O2' | 32:2a:1280:A:N1 | 2.53 | 0.41 |
| 32:2a:1246:C:O2' | 32:2a:1247:U:H5' | 2.20 | 0.41 |
| 34:2c:20:SER:HB3 | 45:2n:54:PRO:HG3 | 2.01 | 0.41 |
| 34:2c:83:ARG:C | 34:2c:85:ARG:N | 2.76 | 0.41 |
| 35:2d:126:ILE:HD13 | 35:2d:126:ILE:HA | 1.93 | 0.41 |
| 38:2g:10:ARG:HE | 38:2g:10:ARG:HB3 | 1.58 | 0.41 |
| 40:2i:85:LEU:HD12 | 40:2i:92:TYR:CD2 | 2.55 | 0.41 |
| 45:2n:6:LEU:HB3 | 45:2n:23:ARG:HH21 | 1.85 | 0.41 |
| 56:2y:57:G:H2' | 56:2y:58:A:C5' | 2.50 | 0.41 |
| 1:1A:829:A:N7 | 1:1A:2248:C:H5' | 2.36 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:1A:876:C:H42 | 1:1A:901:A:H61 | 1.67 | 0.41 |
| 1:1A:1825:A:OP1 | 3:1D:249:PRO:HD3 | 2.19 | 0.41 |
| 1:1A:1951:U:O4 | 62:1A:4254:HOH:O | 2.21 | 0.41 |
| 1:1A:2093:G:C6 | 1:1A:2225:A:C8 | 3.08 | 0.41 |
| 1:1A:2206:G:H5' | 1:1A:2207:G:C5 | 2.54 | 0.41 |
| 1:1A:2251:OMG:HM23 | 1:1A:2251:OMG:H1' | 1.67 | 0.41 |
| 1:1A:2283:C:H2' | 1:1A:2284:C:O4' | 2.20 | 0.41 |
| 3:1D:20:ASP:OD1 | 3:1D:21:PHE:N | 2.54 | 0.41 |
| 3:1D:145:VAL:HG12 | 3:1D:146:GLU:O | 2.20 | 0.41 |
| 4:1E:56:PRO:C | 4:1E:58:ARG:H | 2.27 | 0.41 |
| 6:1G:34:LEU:HD23 | 6:1G:34:LEU:HA | 1.80 | 0.41 |
| 15:1T:35:LYS:HA | 15:1T:40:THR:HG22 | 2.01 | 0.41 |
| 32:1a:55:A:C5 | 32:1a:56:U:C5 | 3.08 | 0.41 |
| 32:1a:219:C:H2' | 32:1a:220:G:O4' | 2.19 | 0.41 |
| 32:1a:920:U:H2' | 32:1a:921:U:C6 | 2.55 | 0.41 |
| 33:1b:43:ASP:OD2 | 33:1b:46:LYS:N | 2.44 | 0.41 |
| 34:1c:15:THR:HG21 | 34:1c:181:ASN:HA | 2.02 | 0.41 |
| 34:1c:124:ILE:CG2 | 34:1c:130:VAL:HG22 | 2.50 | 0.41 |
| 36:1e:11:ILE:HG22 | 36:1e:12:LEU:HB2 | 2.02 | 0.41 |
| 54:1w:18:G:HO2' | 54:1w:57:G:H22 | 1.62 | 0.41 |
| 1:2A:1488:G:C6 | 1:2A:1489:U:N3 | 2.88 | 0.41 |
| 1:2A:2130:U:H3' | 1:2A:2130:U:H6 | 1.84 | 0.41 |
| 1:2A:2131:G:H4' | 1:2A:2132:U:H3' | 2.02 | 0.41 |
| 1:2A:2788:C:H5' | 4:2E:61:ARG:HH21 | 1.85 | 0.41 |
| 7:2H:167:GLU:HA | 7:2H:168:PRO:HD3 | 1.94 | 0.41 |
| 11:2P:63:PRO:HD3 | 30:28:27:THR:HG22 | 2.03 | 0.41 |
| 32:2a:20:U:H2' | 32:2a:21:G:O4' | 2.19 | 0.41 |
| 32:2a:687:A:O2' | 32:2a:701:C:N4 | 2.53 | 0.41 |
| 32:2a:807:A:H2' | 32:2a:808:C:O4' | 2.20 | 0.41 |
| 32:2a:1048:G:H1' | 32:2a:1215:G:H5' | 2.02 | 0.41 |
| 32:2a:1218:C:OP1 | 45:2n:9:LYS:HE2 | 2.20 | 0.41 |
| 32:2a:1232:U:H6 | 32:2a:1232:U:O5' | 2.03 | 0.41 |
| 33:2b:74:LYS:HE3 | 33:2b:74:LYS:HB3 | 1.55 | 0.41 |
| 41:2j:38:ILE:HG12 | 41:2j:71:LEU:O | 2.20 | 0.41 |
| 50:2s:49:ILE:H | 50:2s:62:ILE:HD11 | 1.85 | 0.41 |
| 51:2t:33:ILE:HD11 | 51:2t:62:LEU:O | 2.20 | 0.41 |
| 55:2x:53:G:H2' | 55:2x:54:5MU:C6 | 2.56 | 0.41 |
| 1:1A:211:A:H2' | 1:1A:212:G:O4' | 2.20 | 0.41 |
| 1:1A:311:A:C6 | 1:1A:328:U:C4 | 3.08 | 0.41 |
| 1:1A:556:G:H2' | 1:1A:557:U:C6 | 2.55 | 0.41 |
| 1:1A:1006:C:C2 | 1:1A:1138:G:N2 | 2.88 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1A:1142(A):A:C4 | 1:1A:1144:G:N7 | 2.87 | 0.41 |
| 1:1A:1230:C:H2' | 1:1A:1231:G:C8 | 2.55 | 0.41 |
| 1:1A:1359:A:N1 | 1:1A:1372:U:C4 | 2.88 | 0.41 |
| 1:1A:1439:A:C2 | 1:1A:1553:A:C4 | 3.09 | 0.41 |
| 1:1A:1669:A:H5'' | 1:1A:2550:G:OP1 | 2.20 | 0.41 |
| 1:1A:1946:U:H2' | 1:1A:1947:C:C6 | 2.56 | 0.41 |
| 1:1A:2072:G:H2' | 1:1A:2073:C:O4' | 2.20 | 0.41 |
| 1:1A:2112:G:N3 | 56:1y:19:G:H1' | 2.36 | 0.41 |
| 1:1A:2600:A:H2' | 1:1A:2601:C:C6 | 2.55 | 0.41 |
| 1:1A:2846:G:C6 | 1:1A:2847:U:N3 | 2.88 | 0.41 |
| 32:1a:877:C:OP1 | 39:1h:88:LYS:HE2 | 2.20 | 0.41 |
| 32:1a:1267:C:O2 | 52:1u:20:LYS:NZ | 2.50 | 0.41 |
| 36:1e:48:ALA:HB3 | 36:1e:54:ALA:HB2 | 2.02 | 0.41 |
| 36:1e:90:VAL:O | 36:1e:91:LEU:HD23 | 2.20 | 0.41 |
| 41:1j:31:GLY:HA3 | 41:1j:32:ALA:HA | 1.79 | 0.41 |
| 42:1k:72:ALA:O | 42:1k:75:TYR:HB2 | 2.20 | 0.41 |
| 1:2A:171:G:H2' | 1:2A:172:C:C6 | 2.55 | 0.41 |
| 1:2A:880:G:N2 | 1:2A:898:C:H1' | 2.31 | 0.41 |
| 1:2A:1002:G:C6 | 1:2A:1003:G:C5 | 3.08 | 0.41 |
| 1:2A:1512:U:H2' | 1:2A:1513:C:C6 | 2.55 | 0.41 |
| 1:2A:2199:A:H5'' | 23:21:50:ARG:HH21 | 1.85 | 0.41 |
| 1:2A:2406:U:C2 | 11:2P:72:PRO:HG2 | 2.56 | 0.41 |
| 1:2A:2558:C:H2' | 1:2A:2559:C:O4' | 2.20 | 0.41 |
| 4:2E:12:THR:HG22 | 4:2E:13:ARG:H | 1.86 | 0.41 |
| 15:2T:119:LYS:HD3 | 15:2T:123:GLN:NE2 | 2.34 | 0.41 |
| 24:22:70:GLN:CD | 24:22:70:GLN:C | 2.87 | 0.41 |
| 29:27:22:MET:SD | 29:27:31:LEU:HD12 | 2.60 | 0.41 |
| 32:2a:202:U:H3' | 32:2a:203:U:H6 | 1.85 | 0.41 |
| 32:2a:1024:G:N2 | 32:2a:1025:U:C5 | 2.88 | 0.41 |
| 32:2a:1039:C:C5 | 32:2a:1040:U:C6 | 3.08 | 0.41 |
| 33:2b:28:PHE:O | 33:2b:32:ILE:HG13 | 2.20 | 0.41 |
| 36:2e:40:ARG:HA | 36:2e:40:ARG:HD2 | 1.74 | 0.41 |
| 38:2g:11:GLN:OE1 | 38:2g:11:GLN:HA | 2.17 | 0.41 |
| 40:2i:114:TYR:C | 40:2i:116:LYS:H | 2.27 | 0.41 |
| 48:2q:27:PHE:CE1 | 48:2q:36:ILE:HD11 | 2.55 | 0.41 |
| 51:2t:54:LYS:HB3 | 51:2t:54:LYS:HE2 | 1.57 | 0.41 |
| 56:2y:8:4SU:C2 | 56:2y:14:A:H62 | 2.33 | 0.41 |
| 1:1A:652(D):C:H2' | 1:1A:652(E):G:O4' | 2.21 | 0.41 |
| 1:1A:2147:G:H3' | 1:1A:2147:G:N3 | 2.36 | 0.41 |
| 1:1A:2356:C:H2' | 1:1A:2357:U:O4' | 2.21 | 0.41 |
| 1:1A:2512:C:H5'' | 1:1A:2513:G:OP2 | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:1I:109:ILE:HA | 8:1I:109:ILE:HD13 | 1.70 | 0.41 |
| 11:1P:39:LYS:HB2 | 11:1P:45:LEU:CG | 2.47 | 0.41 |
| 26:14:5:ILE:H | 26:14:5:ILE:HG12 | 1.73 | 0.41 |
| 26:14:69:LYS:HA | 26:14:69:LYS:HD2 | 1.76 | 0.41 |
| 32:1a:108:G:OP2 | 62:1a:1924:HOH:O | 2.22 | 0.41 |
| 32:1a:135:C:N3 | 47:1p:1:MET:N | 2.64 | 0.41 |
| 32:1a:542:G:H5' | 35:1d:41:GLY:HA3 | 2.03 | 0.41 |
| 32:1a:625:G:H4' | 47:1p:16:HIS:CG | 2.55 | 0.41 |
| 32:1a:966:M2G:HM11 | 40:1i:127:LYS:HE2 | 2.01 | 0.41 |
| 32:1a:1004:A:H5'' | 32:1a:1025:U:C5 | 2.55 | 0.41 |
| 40:1i:97:LYS:HB3 | 40:1i:97:LYS:HE2 | 1.88 | 0.41 |
| 51:1t:33:ILE:HG12 | 51:1t:62:LEU:HB3 | 2.02 | 0.41 |
| 1:2A:125:G:O2' | 29:27:48:LYS:NZ | 2.49 | 0.41 |
| 1:2A:146:G:H2' | 1:2A:147:U:C6 | 2.55 | 0.41 |
| 1:2A:784:A:H5' | 1:2A:785:G:OP1 | 2.20 | 0.41 |
| 1:2A:1446:C:H42 | 1:2A:1465:G:H1 | 1.66 | 0.41 |
| 1:2A:1589:C:H2' | 1:2A:1590:U:C6 | 2.56 | 0.41 |
| 1:2A:2291:U:O2' | 1:2A:2374:C:O2 | 2.33 | 0.41 |
| 2:2B:7:G:H5' | 14:2S:29:PHE:CE2 | 2.56 | 0.41 |
| 2:2B:22:U:H3 | 2:2B:61:G:H1 | 1.68 | 0.41 |
| 4:2E:32:PRO:HD2 | 4:2E:50:GLY:O | 2.20 | 0.41 |
| 5:2F:167:ALA:HB1 | 5:2F:173:VAL:HG11 | 2.02 | 0.41 |
| 8:2I:83:ALA:HB3 | 8:2I:123:LEU:HD11 | 2.01 | 0.41 |
| 25:23:4:LEU:O | 25:23:36:VAL:HA | 2.20 | 0.41 |
| 29:27:21:ARG:HH11 | 29:27:21:ARG:HD3 | 1.72 | 0.41 |
| 31:29:28:GLU:H | 31:29:28:GLU:HG3 | 1.59 | 0.41 |
| 32:2a:9:G:C2 | 32:2a:10:A:C4 | 3.09 | 0.41 |
| 32:2a:406:G:C2 | 32:2a:407:G:C8 | 3.09 | 0.41 |
| 32:2a:1076:C:OP1 | 33:2b:179:LYS:NZ | 2.53 | 0.41 |
| 32:2a:1179:A:H2' | 32:2a:1180:A:C8 | 2.55 | 0.41 |
| 32:2a:1264:C:N4 | 32:2a:1272:G:O6 | 2.53 | 0.41 |
| 32:2a:1265:G:C6 | 32:2a:1266:G:C5 | 3.09 | 0.41 |
| 38:2g:101:LEU:O | 38:2g:105:VAL:HG23 | 2.21 | 0.41 |
| 42:2k:34:ASP:OD2 | 42:2k:38:ASN:HB2 | 2.21 | 0.41 |
| 43:2l:8:ASN:O | 43:2l:12:ARG:HG3 | 2.20 | 0.41 |
| 49:2r:31:LEU:O | 49:2r:65:ILE:HG22 | 2.21 | 0.41 |
| 1:1A:127:A:H5'' | 1:1A:128:C:C6 | 2.56 | 0.41 |
| 1:1A:271(C):C:H42 | 1:1A:271(U):G:H1 | 1.68 | 0.41 |
| 1:1A:335:C:O2' | 1:1A:336:C:H5' | 2.20 | 0.41 |
| 1:1A:381:G:O2' | 1:1A:382:G:H5' | 2.21 | 0.41 |
| 1:1A:817:C:H4' | 1:1A:932:G:C5 | 2.56 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:1A:1427:A:H4' | 1:1A:1428:C:O4' | 2.21 | 0.41 |
| 1:1A:2150:U:H2' | 1:1A:2151:G:C8 | 2.55 | 0.41 |
| 12:1Q:34:LEU:HD21 | 12:1Q:129:THR:HG21 | 2.01 | 0.41 |
| 13:1R:2:ARG:HD2 | 62:1R:307:HOH:O | 2.21 | 0.41 |
| 26:14:58:ARG:HD2 | 44:1m:80:ARG:HH12 | 1.84 | 0.41 |
| 32:1a:1202:G:H1' | 45:1n:29:ARG:HD2 | 2.03 | 0.41 |
| 35:1d:107:ARG:HH21 | 35:1d:194:LEU:CD2 | 2.33 | 0.41 |
| 44:1m:107:ALA:O | 44:1m:111:LYS:N | 2.45 | 0.41 |
| 48:1q:32:TYR:O | 48:1q:34:LYS:N | 2.49 | 0.41 |
| 54:1w:66:U:C4 | 54:1w:67:C:N4 | 2.89 | 0.41 |
| 1:2A:704:G:N3 | 1:2A:726:G:C2 | 2.88 | 0.41 |
| 1:2A:909:A:H2' | 1:2A:912:C:H5 | 1.85 | 0.41 |
| 1:2A:1473:G:C6 | 1:2A:1474:C:C4 | 3.08 | 0.41 |
| 1:2A:2065:C:H2' | 1:2A:2066:C:C6 | 2.55 | 0.41 |
| 1:2A:2464:C:C2 | 1:2A:2487:G:C2 | 3.08 | 0.41 |
| 1:2A:2792:G:C2 | 1:2A:2805:G:C2 | 3.09 | 0.41 |
| 2:2B:11:C:OP2 | 22:20:72:ARG:NH2 | 2.52 | 0.41 |
| 6:2G:127:GLY:HA2 | 6:2G:166:ASP:OD1 | 2.20 | 0.41 |
| 9:2N:30:ILE:O | 9:2N:34:LEU:HG | 2.20 | 0.41 |
| 28:26:6:ARG:NH1 | 28:26:24:GLU:OE2 | 2.42 | 0.41 |
| 32:2a:119:A:C5 | 32:2a:288:A:C2 | 3.08 | 0.41 |
| 32:2a:565:U:OP2 | 32:2a:566:G:O2' | 2.36 | 0.41 |
| 32:2a:722:A:N6 | 32:2a:724:G:C2 | 2.88 | 0.41 |
| 33:2b:229:VAL:O | 33:2b:230:VAL:HG23 | 2.20 | 0.41 |
| 34:2c:121:ALA:HB1 | 34:2c:188:LEU:O | 2.20 | 0.41 |
| 36:2e:28:PHE:CD1 | 36:2e:51:VAL:HG13 | 2.56 | 0.41 |
| 38:2g:109:ASN:OD1 | 38:2g:119:ARG:NH2 | 2.46 | 0.41 |
| 44:2m:37:THR:O | 44:2m:55:ARG:NH1 | 2.46 | 0.41 |
| 47:2p:8:ARG:HB3 | 47:2p:28:ARG:NH1 | 2.35 | 0.41 |
| 48:2q:22:LEU:HD11 | 48:2q:39:SER:HB3 | 2.03 | 0.41 |
| 51:2t:9:ASN:HB2 | 51:2t:10:LEU:H | 1.68 | 0.41 |
| 54:2w:39:PSU:H2' | 54:2w:40:C:H6 | 1.84 | 0.41 |
| 1:1A:323:G:C8 | 5:1F:171:PRO:HG3 | 2.56 | 0.41 |
| 1:1A:1039:G:H1 | 1:1A:1116:C:N4 | 2.10 | 0.41 |
| 1:1A:1174:A:H1' | 1:1A:1175:U:C5' | 2.50 | 0.41 |
| 1:1A:1184:G:H5' | 25:13:29:ARG:NH2 | 2.26 | 0.41 |
| 1:1A:1658:C:OP1 | 4:1E:135:HIS:NE2 | 2.53 | 0.41 |
| 1:1A:1864:U:OP1 | 1:1A:2410:G:O2' | 2.37 | 0.41 |
| 1:1A:2147:G:H2' | 1:1A:2148:G:O4' | 2.21 | 0.41 |
| 1:1A:2756:U:H1' | 1:1A:2757:A:H5'' | 2.02 | 0.41 |
| 1:1A:2848:G:H3' | 15:1T:95:ARG:O | 2.21 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 3:1D:175:LEU:HD12 | 3:1D:185:VAL:HG21 | 2.01 | 0.41 |
| 5:1F:89:VAL:O | 62:1F:401:HOH:O | 2.21 | 0.41 |
| 7:1H:24:VAL:HG11 | 7:1H:72:ILE:HD13 | 2.02 | 0.41 |
| 10:1O:17:ARG:HB2 | 10:1O:45:GLU:HG2 | 2.02 | 0.41 |
| 14:1S:36:TYR:CD1 | 14:1S:52:SER:HB2 | 2.55 | 0.41 |
| 18:1W:82:LEU:HD23 | 18:1W:82:LEU:HA | 1.78 | 0.41 |
| 19:1X:11:PRO:HB3 | 19:1X:92:LEU:HD11 | 2.01 | 0.41 |
| 24:12:30:ARG:O | 24:12:34:GLU:HG3 | 2.21 | 0.41 |
| 32:1a:159:G:N2 | 32:1a:161:A:H3' | 2.36 | 0.41 |
| 34:1c:115:LEU:HD23 | 34:1c:115:LEU:HA | 1.85 | 0.41 |
| 34:1c:121:ALA:HB1 | 34:1c:189:ALA:HB2 | 2.02 | 0.41 |
| 34:1c:139:GLN:O | 34:1c:143:GLU:HG3 | 2.19 | 0.41 |
| 35:1d:65:ARG:HD2 | 35:1d:72:GLU:HA | 2.02 | 0.41 |
| 40:1i:89:ASN:HD22 | 40:1i:91:ASP:H | 1.69 | 0.41 |
| 44:1m:96:LEU:C | 44:1m:110:ARG:HG2 | 2.46 | 0.41 |
| 48:1q:53:LEU:HB3 | 48:1q:82:MET:HE1 | 2.03 | 0.41 |
| 54:1w:8:4SU:H6 | 54:1w:8:4SU:O5' | 2.21 | 0.41 |
| 57:1z:17:ARG:HE | 57:1z:17:ARG:HB3 | 1.34 | 0.41 |
| 1:2A:1221(A):C:C2 | 1:2A:1229:G:C2 | 3.08 | 0.41 |
| 1:2A:1810:A:H2' | 1:2A:1811:G:O4' | 2.19 | 0.41 |
| 1:2A:2156:G:H2' | 1:2A:2157:G:C2 | 2.55 | 0.41 |
| 1:2A:2166:G:C8 | 1:2A:2167:U:H5'' | 2.55 | 0.41 |
| 4:2E:23:VAL:HA | 4:2E:184:VAL:O | 2.21 | 0.41 |
| 5:2F:148:LEU:HD13 | 5:2F:154:VAL:HG21 | 2.02 | 0.41 |
| 7:2H:11:VAL:CG1 | 7:2H:15:VAL:HG23 | 2.51 | 0.41 |
| 9:2N:15:LEU:HD12 | 9:2N:53:VAL:HB | 2.03 | 0.41 |
| 12:2Q:7:MET:HB3 | 12:2Q:7:MET:HE2 | 1.65 | 0.41 |
| 13:2R:75:LEU:HD12 | 13:2R:75:LEU:HA | 1.82 | 0.41 |
| 13:2R:87:TYR:OH | 13:2R:116:LEU:HB3 | 2.19 | 0.41 |
| 23:21:85:LEU:HD23 | 23:21:89:GLU:OE1 | 2.21 | 0.41 |
| 26:24:46:GLN:O | 26:24:48:ARG:N | 2.54 | 0.41 |
| 32:2a:32:A:H2' | 32:2a:33:A:C8 | 2.56 | 0.41 |
| 32:2a:1142:G:H2' | 32:2a:1143:G:O4' | 2.20 | 0.41 |
| 32:2a:1298:C:N4 | 38:2g:114:ARG:HB3 | 2.36 | 0.41 |
| 32:2a:1305:G:C2 | 32:2a:1331:G:H1' | 2.55 | 0.41 |
| 32:2a:1356:G:H2' | 32:2a:1357:A:C8 | 2.55 | 0.41 |
| 37:2f:91:VAL:HG12 | 37:2f:92:LYS:O | 2.21 | 0.41 |
| 39:2h:2:LEU:HD12 | 39:2h:2:LEU:HA | 1.67 | 0.41 |
| 40:2i:89:ASN:O | 40:2i:92:TYR:HB2 | 2.20 | 0.41 |
| 50:2s:27:GLU:HA | 50:2s:28:LYS:O | 2.20 | 0.41 |
| 55:2x:54:5MU:H6 | 55:2x:54:5MU:O5' | 2.04 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 56:2y:61:C:H2' | 56:2y:62:C:H6 | 1.81 | 0.41 |
| 1:1A:396:G:H1' | 23:11:42:GLN:HB3 | 2.01 | 0.41 |
| 1:1A:1062:G:N2 | 1:1A:1077:A:H61 | 2.18 | 0.41 |
| 1:1A:1063:G:N2 | 1:1A:1076:C:C2 | 2.87 | 0.41 |
| 1:1A:1298:C:N4 | 1:1A:1299:G:C6 | 2.88 | 0.41 |
| 1:1A:1364:G:P | 23:11:3:LYS:HG3 | 2.60 | 0.41 |
| 1:1A:2086:U:H2' | 1:1A:2087:G:H8 | 1.86 | 0.41 |
| 1:1A:2104:G:H2' | 1:1A:2105:C:H6 | 1.86 | 0.41 |
| 8:1I:61:ARG:N | 8:1I:61:ARG:HD2 | 2.35 | 0.41 |
| 13:1R:38:VAL:H | 13:1R:38:VAL:HG23 | 1.67 | 0.41 |
| 21:1Z:34:ASN:O | 21:1Z:35:ARG:HD2 | 2.21 | 0.41 |
| 24:12:63:VAL:O | 24:12:66:GLU:HB2 | 2.21 | 0.41 |
| 28:16:47:THR:HG22 | 28:16:48:VAL:O | 2.21 | 0.41 |
| 29:17:25:PRO:HD2 | 62:17:205:HOH:O | 2.21 | 0.41 |
| 32:1a:344:A:O2' | 32:1a:346:G:O6 | 2.28 | 0.41 |
| 32:1a:375:U:OP1 | 47:1p:69:THR:OG1 | 2.15 | 0.41 |
| 32:1a:614:A:C5 | 32:1a:615:C:C5 | 3.09 | 0.41 |
| 33:1b:44:LEU:O | 33:1b:47:THR:HB | 2.21 | 0.41 |
| 34:1c:11:ARG:NH2 | 34:1c:177:THR:O | 2.40 | 0.41 |
| 38:1g:76:ARG:HG3 | 38:1g:156:TRP:CH2 | 2.55 | 0.41 |
| 38:1g:93:PRO:HA | 38:1g:96:GLN:HB2 | 2.03 | 0.41 |
| 39:1h:110:ALA:HB3 | 39:1h:121:ASP:HB3 | 2.02 | 0.41 |
| 41:1j:27:ALA:O | 41:1j:31:GLY:HA2 | 2.21 | 0.41 |
| 1:2A:221:A:C4 | 1:2A:266:G:N7 | 2.89 | 0.41 |
| 1:2A:307:G:H21 | 1:2A:330:A:H62 | 1.66 | 0.41 |
| 1:2A:531:C:C5 | 1:2A:2035:G:C2 | 3.09 | 0.41 |
| 1:2A:643:A:C8 | 28:26:44:ARG:NH1 | 2.88 | 0.41 |
| 1:2A:844:C:C5 | 1:2A:845:G:C6 | 3.08 | 0.41 |
| 1:2A:886:C:H2' | 1:2A:887:A:O4' | 2.20 | 0.41 |
| 1:2A:1171:G:H1 | 1:2A:1178:C:H42 | 1.67 | 0.41 |
| 1:2A:1686:C:H2' | 1:2A:1687:G:O4' | 2.20 | 0.41 |
| 1:2A:2341:G:H2' | 1:2A:2342:C:C6 | 2.55 | 0.41 |
| 1:2A:2669:G:H2' | 1:2A:2670:A:H8 | 1.85 | 0.41 |
| 4:2E:9:VAL:HG23 | 4:2E:25:VAL:HB | 2.01 | 0.41 |
| 5:2F:31:HIS:HB2 | 11:2P:9:ASN:OD1 | 2.20 | 0.41 |
| 5:2F:64:ILE:HD12 | 5:2F:65:TRP:CZ3 | 2.55 | 0.41 |
| 8:2I:133:HIS:CD2 | 8:2I:134:PRO:HD2 | 2.55 | 0.41 |
| 12:2Q:103:MET:CE | 12:2Q:125:LEU:HD13 | 2.50 | 0.41 |
| 14:2S:64:GLU:H | 14:2S:64:GLU:HG3 | 1.47 | 0.41 |
| 19:2X:12:VAL:HG22 | 19:2X:29:TRP:CE2 | 2.56 | 0.41 |
| 20:2Y:43:ASN:HB3 | 20:2Y:65:ALA:O | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 21:2Z:131:ARG:H | 21:2Z:131:ARG:HG2 | 1.46 | 0.41 |
| 32:2a:491:G:C4 | 32:2a:492:G:C8 | 3.09 | 0.41 |
| 32:2a:523:A:H61 | 43:2l:92:0TD:CG | 2.34 | 0.41 |
| 32:2a:1121:U:H2' | 32:2a:1122:U:O4' | 2.20 | 0.41 |
| 32:2a:1148:U:H2' | 32:2a:1149:C:O4' | 2.20 | 0.41 |
| 33:2b:92:TYR:OH | 33:2b:150:SER:HB2 | 2.20 | 0.41 |
| 35:2d:4:TYR:OH | 35:2d:7:PRO:O | 2.25 | 0.41 |
| 40:2i:106:ALA:O | 40:2i:108:VAL:HG22 | 2.20 | 0.41 |
| 56:2y:68:C:C4 | 56:2y:69:G:N7 | 2.88 | 0.41 |
| 1:1A:491:G:H2' | 1:1A:492:A:C8 | 2.56 | 0.41 |
| 1:1A:1373:A:H2' | 1:1A:1374:G:O4' | 2.21 | 0.41 |
| 4:1E:9:VAL:HG22 | 4:1E:25:VAL:HB | 2.03 | 0.41 |
| 8:1I:72:LEU:C | 8:1I:74:ASN:N | 2.77 | 0.41 |
| 19:1X:53:LYS:HB3 | 19:1X:82:GLN:HB3 | 2.03 | 0.41 |
| 32:1a:911:U:H2' | 32:1a:912:C:C6 | 2.56 | 0.41 |
| 32:1a:1194:U:H4' | 36:1e:22:GLY:HA2 | 2.02 | 0.41 |
| 32:1a:1429:C:H2' | 32:1a:1430:C:H6 | 1.84 | 0.41 |
| 33:1b:93:VAL:HG11 | 33:1b:97:TRP:CD1 | 2.56 | 0.41 |
| 34:1c:143:GLU:C | 34:1c:145:GLY:N | 2.79 | 0.41 |
| 36:1e:18:ARG:HD3 | 36:1e:27:ARG:HH21 | 1.86 | 0.41 |
| 36:1e:33:VAL:HG22 | 36:1e:112:LEU:HD12 | 2.02 | 0.41 |
| 46:1o:84:LYS:HA | 46:1o:84:LYS:HD2 | 1.75 | 0.41 |
| 1:2A:493:G:H2' | 1:2A:494:G:O4' | 2.21 | 0.41 |
| 1:2A:1344:G:N2 | 1:2A:1404:C:H1' | 2.36 | 0.41 |
| 1:2A:1448:G:H4' | 1:2A:1542:A:OP1 | 2.21 | 0.41 |
| 1:2A:2203:U:H4' | 3:2D:151:LYS:HG2 | 2.02 | 0.41 |
| 1:2A:2530:A:O2' | 1:2A:2532:G:OP2 | 2.32 | 0.41 |
| 1:2A:2774:C:H2' | 1:2A:2775:A:O4' | 2.20 | 0.41 |
| 3:2D:149:PRO:O | 3:2D:151:LYS:N | 2.54 | 0.41 |
| 4:2E:36:ARG:NH2 | 4:2E:88:GLY:O | 2.54 | 0.41 |
| 6:2G:104:GLU:O | 6:2G:108:ASN:HB2 | 2.20 | 0.41 |
| 8:2I:26:ALA:O | 8:2I:31:LEU:HB2 | 2.21 | 0.41 |
| 11:2P:84:ASN:CG | 11:2P:117:GLU:HB3 | 2.46 | 0.41 |
| 11:2P:95:VAL:CG1 | 11:2P:125:VAL:HG12 | 2.51 | 0.41 |
| 19:2X:31:HIS:CD2 | 19:2X:33:LYS:H | 2.36 | 0.41 |
| 20:2Y:9:LYS:HD2 | 20:2Y:28:LYS:O | 2.21 | 0.41 |
| 23:21:80:LEU:HD23 | 23:21:80:LEU:HA | 1.69 | 0.41 |
| 26:24:61:ARG:HG2 | 26:24:61:ARG:HH11 | 1.85 | 0.41 |
| 32:2a:163:C:H2' | 32:2a:164:U:C6 | 2.55 | 0.41 |
| 32:2a:958:A:C6 | 32:2a:959:A:C6 | 3.09 | 0.41 |
| 32:2a:1274:G:H8 | 32:2a:1274:G:O5' | 2.04 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 33:2b:92:TYR:C | 33:2b:92:TYR:CD1 | 2.99 | 0.41 |
| 38:2g:65:ALA:O | 38:2g:69:VAL:HG23 | 2.20 | 0.41 |
| 1:1A:293:U:H5'' | 1:1A:294:A:OP2 | 2.20 | 0.41 |
| 1:1A:388:G:O2' | 1:1A:389:G:N7 | 2.53 | 0.41 |
| 1:1A:535:C:H6 | 1:1A:535:C:O5' | 2.04 | 0.41 |
| 1:1A:1252:G:O4' | 16:1U:33:ARG:HD2 | 2.21 | 0.41 |
| 1:1A:1453:U:O2' | 1:1A:1455:G:N7 | 2.51 | 0.41 |
| 1:1A:1660:C:H2' | 1:1A:1661:G:H8 | 1.86 | 0.41 |
| 1:1A:1767:C:C2' | 1:1A:1768:U:H5' | 2.51 | 0.41 |
| 1:1A:2160:G:C2 | 1:1A:2161:C:C2 | 3.09 | 0.41 |
| 1:1A:2630:G:H2' | 1:1A:2631:G:C8 | 2.56 | 0.41 |
| 1:1A:2836:U:C4 | 1:1A:2883:A:N6 | 2.89 | 0.41 |
| 1:1A:2849:U:O4 | 15:1T:23:ARG:NH2 | 2.46 | 0.41 |
| 1:1A:2850:A:C2 | 1:1A:2851:A:C4 | 3.09 | 0.41 |
| 2:1B:8:U:O3' | 14:1S:25:ARG:NH2 | 2.54 | 0.41 |
| 2:1B:66:A:N6 | 2:1B:108:U:H2' | 2.35 | 0.41 |
| 3:1D:218:ARG:HB3 | 3:1D:219:PRO:HD2 | 2.03 | 0.41 |
| 6:1G:64:THR:HB | 6:1G:94:LEU:HD11 | 2.03 | 0.41 |
| 11:1P:46:LYS:HE3 | 11:1P:46:LYS:HB3 | 1.81 | 0.41 |
| 14:1S:20:ARG:HD2 | 14:1S:20:ARG:HA | 1.90 | 0.41 |
| 16:1U:49:HIS:HA | 16:1U:52:ARG:HB2 | 2.02 | 0.41 |
| 17:1V:16:PRO:HA | 17:1V:96:ILE:HG22 | 2.03 | 0.41 |
| 19:1X:5:TYR:CZ | 24:12:30:ARG:HB2 | 2.56 | 0.41 |
| 22:10:10:THR:HG21 | 22:10:12:ASN:HB2 | 2.02 | 0.41 |
| 27:15:20:ARG:C | 27:15:22:HIS:H | 2.28 | 0.41 |
| 31:19:1:MET:HE2 | 31:19:1:MET:HB2 | 1.98 | 0.41 |
| 32:1a:22:G:H2' | 32:1a:23:C:C6 | 2.56 | 0.41 |
| 32:1a:112:G:H5' | 32:1a:389:A:O2' | 2.21 | 0.41 |
| 32:1a:152:A:N6 | 32:1a:170:U:C2 | 2.88 | 0.41 |
| 32:1a:161:A:H2' | 32:1a:162:A:O4' | 2.20 | 0.41 |
| 32:1a:399:G:H2' | 32:1a:400:C:C6 | 2.56 | 0.41 |
| 32:1a:418:C:H2' | 32:1a:419:C:C6 | 2.55 | 0.41 |
| 32:1a:431:A:H2' | 32:1a:432:A:O4' | 2.21 | 0.41 |
| 32:1a:486:U:H2' | 32:1a:487:A:C8 | 2.54 | 0.41 |
| 32:1a:741:G:H2' | 32:1a:742:G:O4' | 2.20 | 0.41 |
| 32:1a:865:A:H2 | 32:1a:918:A:H4' | 1.86 | 0.41 |
| 32:1a:933:G:OP2 | 38:1g:3:ARG:HB2 | 2.21 | 0.41 |
| 32:1a:1337:G:N7 | 62:1a:1948:HOH:O | 2.37 | 0.41 |
| 33:1b:230:VAL:CG1 | 33:1b:231:GLU:N | 2.83 | 0.41 |
| 34:1c:112:SER:HB3 | 34:1c:115:LEU:HD12 | 2.03 | 0.41 |
| 38:1g:95:ARG:O | 38:1g:99:LEU:HG | 2.21 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 43:1l:42:THR:HG21 | 43:1l:52:LEU:HB3 | 2.02 | 0.41 |
| 45:1n:24:CYS:SG | 45:1n:40:CYS:N | 2.87 | 0.41 |
| 47:1p:47:ASP:OD1 | 47:1p:47:ASP:N | 2.53 | 0.41 |
| 48:1q:67:LYS:HA | 48:1q:70:ARG:HH12 | 1.86 | 0.41 |
| 49:1r:46:GLU:OE2 | 49:1r:86:VAL:HG23 | 2.20 | 0.41 |
| 53:1v:16:A:H2' | 53:1v:17:U:O4' | 2.20 | 0.41 |
| 54:1w:46:G7M:O2' | 54:1w:47:U:H5' | 2.21 | 0.41 |
| 1:2A:395:U:O2' | 1:2A:396:G:N7 | 2.53 | 0.41 |
| 1:2A:625:G:O6 | 11:2P:107:LYS:NZ | 2.42 | 0.41 |
| 1:2A:797:C:H6 | 1:2A:797:C:O5' | 2.04 | 0.41 |
| 1:2A:820:A:H1' | 1:2A:943:U:H1' | 2.02 | 0.41 |
| 1:2A:848:G:O2' | 1:2A:849:A:H5' | 2.21 | 0.41 |
| 1:2A:868:U:N3 | 1:2A:869:G:N7 | 2.69 | 0.41 |
| 1:2A:1219:G:H1 | 1:2A:1230:C:H42 | 1.69 | 0.41 |
| 1:2A:1314:C:C2 | 1:2A:1339:G:N2 | 2.89 | 0.41 |
| 1:2A:1358:G:O2' | 1:2A:1359:A:H5'' | 2.20 | 0.41 |
| 1:2A:1418:G:O5' | 1:2A:1418:G:H8 | 2.04 | 0.41 |
| 1:2A:1813:G:H4' | 3:2D:43:ARG:O | 2.21 | 0.41 |
| 1:2A:1963:U:H4' | 1:2A:1964:G:OP1 | 2.20 | 0.41 |
| 1:2A:2074:U:H2' | 1:2A:2075:U:C6 | 2.56 | 0.41 |
| 1:2A:2134:A:H1' | 1:2A:2158:A:N6 | 2.36 | 0.41 |
| 1:2A:2571:C:H5'' | 1:2A:2572:A:H5'' | 2.02 | 0.41 |
| 1:2A:2654:A:H8 | 1:2A:2654:A:OP1 | 2.03 | 0.41 |
| 1:2A:2851:A:H2' | 1:2A:2852:G:O4' | 2.21 | 0.41 |
| 2:2B:106:G:H5' | 21:2Z:31:ARG:HG2 | 2.03 | 0.41 |
| 4:2E:145:LYS:HZ3 | 4:2E:145:LYS:HG3 | 1.68 | 0.41 |
| 5:2F:116:ASP:CG | 5:2F:119:ARG:HH21 | 2.28 | 0.41 |
| 5:2F:197:ASP:O | 5:2F:200:GLU:HB3 | 2.21 | 0.41 |
| 6:2G:81:LYS:O | 6:2G:86:MET:HE1 | 2.21 | 0.41 |
| 7:2H:11:VAL:HG12 | 7:2H:15:VAL:HG23 | 2.02 | 0.41 |
| 7:2H:90:LYS:HD2 | 7:2H:159:GLU:CD | 2.46 | 0.41 |
| 8:2I:29:TYR:C | 8:2I:32:PRO:HD2 | 2.46 | 0.41 |
| 8:2I:78:THR:HA | 8:2I:143:SER:HB3 | 2.02 | 0.41 |
| 9:2N:70:LYS:O | 9:2N:86:PRO:HA | 2.21 | 0.41 |
| 12:2Q:78:PRO:HD3 | 55:2x:1:C:N3 | 2.36 | 0.41 |
| 12:2Q:85:LYS:HG2 | 22:20:7:LEU:HB3 | 2.02 | 0.41 |
| 19:2X:2:LYS:HD2 | 19:2X:2:LYS:HA | 1.66 | 0.41 |
| 21:2Z:152:ALA:HB2 | 21:2Z:169:GLU:HB3 | 2.03 | 0.41 |
| 26:24:62:ARG:HB2 | 26:24:63:TYR:CD2 | 2.55 | 0.41 |
| 32:2a:50:A:N1 | 32:2a:360:A:O2' | 2.48 | 0.41 |
| 32:2a:300:A:O2' | 32:2a:564:C:N3 | 2.38 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 32:2a:599:C:C2 | 32:2a:640:A:C2 | 3.08 | 0.41 |
| 32:2a:909:A:H2' | 32:2a:910:C:O4' | 2.21 | 0.41 |
| 32:2a:985:C:C2 | 32:2a:1221:G:N2 | 2.89 | 0.41 |
| 32:2a:1135:U:H4' | 32:2a:1136:U:H5 | 1.85 | 0.41 |
| 32:2a:1309:G:N2 | 32:2a:1329:A:H1' | 2.36 | 0.41 |
| 32:2a:1370:G:O2' | 32:2a:1371:G:H5' | 2.21 | 0.41 |
| 32:2a:1400:5MC:N4 | 55:2x:34:C:H1' | 2.36 | 0.41 |
| 33:2b:149:LEU:HD23 | 33:2b:149:LEU:HA | 1.85 | 0.41 |
| 36:2e:35:GLY:HA2 | 36:2e:40:ARG:O | 2.21 | 0.41 |
| 37:2f:7:ASN:OD1 | 37:2f:62:TRP:HD1 | 2.04 | 0.41 |
| 37:2f:70:ASP:OD1 | 37:2f:70:ASP:N | 2.36 | 0.41 |
| 38:2g:78:ARG:O | 38:2g:84:ASN:HA | 2.21 | 0.41 |
| 40:2i:43:ALA:HA | 40:2i:74:ILE:HD13 | 2.02 | 0.41 |
| 40:2i:70:LYS:O | 40:2i:74:ILE:HG13 | 2.21 | 0.41 |
| 41:2j:5:ARG:O | 41:2j:98:ILE:HA | 2.20 | 0.41 |
| 43:2l:42:THR:HG21 | 43:2l:52:LEU:HB3 | 2.03 | 0.41 |
| 48:2q:78:GLU:OE2 | 48:2q:81:ARG:NH1 | 2.41 | 0.41 |
| 56:2y:15:G:H22 | 56:2y:48:C:H42 | 1.69 | 0.41 |
| 1:1A:512:G:OP1 | 1:1A:1234:U:O2' | 2.28 | 0.41 |
| 1:1A:851:U:O2' | 25:13:45:GLY:HA3 | 2.20 | 0.41 |
| 1:1A:857:C:N4 | 1:1A:858:U:O4 | 2.54 | 0.41 |
| 1:1A:1309:G:O6 | 62:1A:4249:HOH:O | 2.21 | 0.41 |
| 1:1A:1448:G:H4' | 1:1A:1542:A:OP1 | 2.21 | 0.41 |
| 1:1A:2126:A:C5 | 1:1A:2163:C:H1' | 2.54 | 0.41 |
| 1:1A:2142:C:H2' | 1:1A:2143:C:C6 | 2.56 | 0.41 |
| 22:10:7:LEU:O | 55:1x:2:G:H4' | 2.21 | 0.41 |
| 22:10:36:ILE:H | 22:10:36:ILE:HG12 | 1.71 | 0.41 |
| 25:13:23:LEU:HD12 | 25:13:23:LEU:HA | 1.89 | 0.41 |
| 32:1a:510:A:H5'' | 32:1a:511:C:OP2 | 2.21 | 0.41 |
| 32:1a:848:C:H2' | 32:1a:849:C:C6 | 2.56 | 0.41 |
| 32:1a:964:A:O2' | 41:1j:55:LYS:HE3 | 2.21 | 0.41 |
| 32:1a:993:G:H2' | 32:1a:993:G:N3 | 2.36 | 0.41 |
| 32:1a:1286:A:C8 | 32:1a:1287:A:H4' | 2.57 | 0.41 |
| 33:1b:211:ILE:HG13 | 33:1b:211:ILE:H | 1.66 | 0.41 |
| 36:1e:150:ARG:HB3 | 36:1e:150:ARG:NH1 | 2.36 | 0.41 |
| 40:1i:116:LYS:HD2 | 40:1i:122:ALA:HA | 2.01 | 0.41 |
| 42:1k:15:ALA:HA | 42:1k:77:MET:HA | 2.02 | 0.41 |
| 46:1o:3:ILE:HD12 | 46:1o:3:ILE:H | 1.86 | 0.41 |
| 46:1o:42:HIS:CE1 | 46:1o:46:HIS:CD2 | 3.08 | 0.41 |
| 51:1t:77:ALA:O | 51:1t:81:LYS:HG3 | 2.21 | 0.41 |
| 56:1y:5:G:C2 | 56:1y:6:G:C4 | 3.09 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:2A:2065:C:H2' | 1:2A:2066:C:H6 | 1.85 | 0.41 |
| 1:2A:2390:U:P | 30:28:35:GLN:HE22 | 2.43 | 0.41 |
| 3:2D:5:LYS:HG2 | 3:2D:17:THR:HG22 | 2.03 | 0.41 |
| 4:2E:48:GLN:NE2 | 4:2E:78:LEU:HG | 2.35 | 0.41 |
| 7:2H:123:PHE:O | 7:2H:124:GLU:HG2 | 2.21 | 0.41 |
| 25:23:30:ARG:HH12 | 25:23:33:GLN:HG3 | 1.85 | 0.41 |
| 26:24:24:THR:OG1 | 26:24:25:TYR:N | 2.40 | 0.41 |
| 28:26:9:LEU:HD11 | 28:26:34:LEU:HD12 | 2.03 | 0.41 |
| 30:28:63:PRO:HG2 | 30:28:64:TYR:CE2 | 2.56 | 0.41 |
| 32:2a:590:C:OP1 | 39:2h:30:ARG:N | 2.31 | 0.41 |
| 32:2a:622:A:C8 | 32:2a:623:C:C6 | 3.09 | 0.41 |
| 32:2a:663:A:H2' | 32:2a:664:G:O4' | 2.21 | 0.41 |
| 32:2a:1048:G:OP1 | 45:2n:4:LYS:HB2 | 2.21 | 0.41 |
| 32:2a:1313:U:O4 | 50:2s:2:PRO:HD2 | 2.20 | 0.41 |
| 32:2a:1376:U:H2' | 32:2a:1377:A:H8 | 1.86 | 0.41 |
| 33:2b:215:LEU:O | 33:2b:219:VAL:HG23 | 2.21 | 0.41 |
| 36:2e:72:GLN:O | 36:2e:74:GLY:N | 2.54 | 0.41 |
| 37:2f:44:GLY:HA2 | 37:2f:59:TYR:CE1 | 2.56 | 0.41 |
| 41:2j:16:LEU:HA | 41:2j:16:LEU:HD23 | 1.67 | 0.41 |
| 47:2p:43:LYS:HG2 | 47:2p:48:TRP:CG | 2.55 | 0.41 |
| 1:1A:279:C:H42 | 1:1A:361:G:H1 | 1.69 | 0.40 |
| 1:1A:748:G:OP1 | 1:1A:2612:C:N4 | 2.54 | 0.40 |
| 1:1A:862:G:H8 | 1:1A:862:G:O5' | 2.04 | 0.40 |
| 1:1A:1224:C:H2' | 1:1A:1225:G:O4' | 2.22 | 0.40 |
| 1:1A:1674:G:H1' | 1:1A:1676:A:N6 | 2.35 | 0.40 |
| 1:1A:1945:G:C2 | 1:1A:1946:U:C2 | 3.09 | 0.40 |
| 1:1A:2094:G:H5' | 8:1I:25:TYR:CD1 | 2.56 | 0.40 |
| 1:1A:2422:A:H5'' | 56:1y:76:A:H61 | 1.86 | 0.40 |
| 1:1A:2748:A:H5' | 7:1H:4:ILE:HD13 | 2.02 | 0.40 |
| 7:1H:3:ARG:NH1 | 7:1H:4:ILE:H | 2.19 | 0.40 |
| 11:1P:92:GLU:O | 11:1P:94:GLU:N | 2.54 | 0.40 |
| 14:1S:65:VAL:O | 14:1S:68:GLN:N | 2.54 | 0.40 |
| 18:1W:90:ARG:HE | 18:1W:90:ARG:HB3 | 1.75 | 0.40 |
| 26:14:14:ILE:HA | 26:14:31:ILE:O | 2.21 | 0.40 |
| 32:1a:261:U:O2' | 32:1a:263:A:N7 | 2.49 | 0.40 |
| 32:1a:453:A:C6 | 32:1a:454:C:C4 | 3.10 | 0.40 |
| 32:1a:1312:G:O6 | 50:1s:2:PRO:HD2 | 2.21 | 0.40 |
| 33:1b:15:VAL:HG13 | 33:1b:209:ARG:CG | 2.51 | 0.40 |
| 35:1d:128:VAL:O | 35:1d:129:ASN:C | 2.64 | 0.40 |
| 40:1i:77:ILE:O | 40:1i:81:ILE:HG22 | 2.20 | 0.40 |
| 41:1j:78:ASN:O | 41:1j:80:LYS:N | 2.54 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 44:1m:70:LEU:HD23 | 44:1m:70:LEU:HA | 1.54 | 0.40 |
| 49:1r:65:ILE:O | 49:1r:69:THR:HG23 | 2.21 | 0.40 |
| 54:1w:14:A:C5 | 54:1w:22:G:C2 | 3.09 | 0.40 |
| 1:2A:248:G:C2 | 1:2A:2431:U:H4' | 2.56 | 0.40 |
| 1:2A:304:G:H2' | 1:2A:305:U:H6 | 1.82 | 0.40 |
| 1:2A:627:A:N7 | 11:2P:84:ASN:ND2 | 2.60 | 0.40 |
| 1:2A:1204:A:N1 | 1:2A:1241:A:N7 | 2.69 | 0.40 |
| 1:2A:2138:C:C2 | 1:2A:2154:G:N2 | 2.89 | 0.40 |
| 1:2A:2274:A:C5 | 1:2A:2276:G:C8 | 3.10 | 0.40 |
| 1:2A:2401:U:H3' | 1:2A:2402:C:C6 | 2.57 | 0.40 |
| 1:2A:2572:A:OP1 | 1:2A:2574:G:O2' | 2.37 | 0.40 |
| 1:2A:2712:U:OP1 | 1:2A:2714:G:H4' | 2.21 | 0.40 |
| 2:2B:83:G:H5'' | 25:23:52:HIS:CD2 | 2.55 | 0.40 |
| 5:2F:187:VAL:HG11 | 11:2P:6:LEU:HD11 | 2.03 | 0.40 |
| 7:2H:26:VAL:O | 7:2H:79:VAL:HG11 | 2.21 | 0.40 |
| 11:2P:125:VAL:HG22 | 11:2P:138:LEU:HD21 | 2.03 | 0.40 |
| 12:2Q:30:GLY:HA2 | 12:2Q:107:ALA:HB2 | 2.03 | 0.40 |
| 26:24:60:GLN:C | 26:24:61:ARG:HG3 | 2.46 | 0.40 |
| 32:2a:974:A:OP2 | 45:2n:29:ARG:NH2 | 2.54 | 0.40 |
| 32:2a:996:A:N1 | 32:2a:1045:C:O2' | 2.48 | 0.40 |
| 32:2a:1399:C:H4' | 32:2a:1400:5MC:O5' | 2.21 | 0.40 |
| 32:2a:1445:C:O2' | 32:2a:1447:A:N6 | 2.54 | 0.40 |
| 33:2b:178:ARG:HE | 33:2b:178:ARG:HB3 | 1.75 | 0.40 |
| 34:2c:35:GLU:HG2 | 34:2c:59:ARG:HH22 | 1.85 | 0.40 |
| 34:2c:109:PRO:O | 34:2c:115:LEU:HD12 | 2.21 | 0.40 |
| 41:2j:35:SER:OG | 41:2j:73:ASP:HB2 | 2.21 | 0.40 |
| 48:2q:40:LYS:HD3 | 48:2q:42:TYR:OH | 2.21 | 0.40 |
| 54:2w:18:G:HO2' | 54:2w:57:G:H22 | 1.58 | 0.40 |
| 56:2y:24:G:C6 | 56:2y:25:C:C4 | 3.09 | 0.40 |
| 1:1A:1079:C:H2' | 1:1A:1080:C:O4' | 2.21 | 0.40 |
| 1:1A:1311:G:H2' | 29:17:47:ARG:HH22 | 1.87 | 0.40 |
| 1:1A:1786:A:C4 | 1:1A:1938:A:C6 | 3.10 | 0.40 |
| 1:1A:1826:G:H4' | 3:1D:242:ARG:CZ | 2.51 | 0.40 |
| 2:1B:37:C:H2' | 2:1B:38:C:O4' | 2.21 | 0.40 |
| 5:1F:114:VAL:HG22 | 5:1F:192:LEU:HD11 | 2.04 | 0.40 |
| 5:1F:197:ASP:O | 5:1F:201:VAL:HG13 | 2.21 | 0.40 |
| 8:1I:134:PRO:C | 8:1I:136:VAL:N | 2.78 | 0.40 |
| 10:1O:68:GLU:CB | 10:1O:78:ARG:HB2 | 2.50 | 0.40 |
| 23:11:12:PRO:HB2 | 23:11:41:ARG:HH21 | 1.87 | 0.40 |
| 29:17:8:ASN:OD1 | 29:17:8:ASN:C | 2.65 | 0.40 |
| 32:1a:194:C:C2' | 32:1a:195:A:H5'' | 2.52 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 32:1a:373:A:H2' | 32:1a:374:A:H8 | 1.87 | 0.40 |
| 33:1b:155:LEU:HD12 | 33:1b:155:LEU:HA | 1.75 | 0.40 |
| 36:1e:103:GLY:O | 36:1e:106:PRO:HD2 | 2.21 | 0.40 |
| 41:1j:13:HIS:CD2 | 41:1j:14:LYS:N | 2.89 | 0.40 |
| 47:1p:44:THR:OG1 | 47:1p:45:THR:N | 2.54 | 0.40 |
| 1:2A:394:A:C6 | 1:2A:395:U:C4 | 3.09 | 0.40 |
| 1:2A:652(U):G:H2' | 1:2A:652(V):C:C6 | 2.55 | 0.40 |
| 1:2A:699:A:H2' | 1:2A:700:G:O4' | 2.21 | 0.40 |
| 1:2A:1144:G:C5 | 1:2A:1145:C:C5 | 3.09 | 0.40 |
| 1:2A:1579:A:H2' | 1:2A:1580:A:C8 | 2.56 | 0.40 |
| 1:2A:2091:U:OP2 | 1:2A:2092:U:O2' | 2.34 | 0.40 |
| 1:2A:2164:C:C5 | 1:2A:2165:G:H1' | 2.56 | 0.40 |
| 1:2A:2199:A:H5'' | 23:21:50:ARG:NH2 | 2.36 | 0.40 |
| 1:2A:2400:G:O2' | 1:2A:2401:U:H5' | 2.21 | 0.40 |
| 1:2A:2577:A:C5' | 1:2A:2578:G:H5' | 2.48 | 0.40 |
| 7:2H:113:VAL:HG11 | 7:2H:151:ILE:HD13 | 2.02 | 0.40 |
| 7:2H:150:ALA:HA | 7:2H:153:LYS:HG3 | 2.02 | 0.40 |
| 19:2X:12:VAL:HG21 | 19:2X:27:THR:HG22 | 2.03 | 0.40 |
| 21:2Z:73:GLN:HB3 | 21:2Z:87:ASP:OD1 | 2.21 | 0.40 |
| 22:20:6:GLY:O | 22:20:7:LEU:HD23 | 2.21 | 0.40 |
| 24:22:1:MET:HE3 | 24:22:5:GLU:HB2 | 2.03 | 0.40 |
| 25:23:28:LEU:HD23 | 25:23:28:LEU:HA | 1.94 | 0.40 |
| 30:28:8:LYS:HD3 | 30:28:8:LYS:HA | 1.84 | 0.40 |
| 32:2a:583:A:H2' | 32:2a:584:G:O4' | 2.22 | 0.40 |
| 32:2a:1060:C:C5' | 41:2j:51:ARG:HB3 | 2.51 | 0.40 |
| 33:2b:189:ASP:CG | 33:2b:205:ASP:H | 2.29 | 0.40 |
| 34:2c:52:LEU:HD11 | 34:2c:68:VAL:HG13 | 2.03 | 0.40 |
| 37:2f:14:LEU:HD22 | 37:2f:18:GLN:HB3 | 2.03 | 0.40 |
| 41:2j:45:ARG:HD3 | 41:2j:47:PHE:CZ | 2.56 | 0.40 |
| 43:2l:33:ARG:HA | 43:2l:33:ARG:HD2 | 1.84 | 0.40 |
| 1:1A:113:G:H5' | 62:1A:4992:HOH:O | 2.19 | 0.40 |
| 1:1A:376:C:H2' | 1:1A:377:C:C6 | 2.56 | 0.40 |
| 1:1A:616:G:H2' | 1:1A:618:C:H6 | 1.87 | 0.40 |
| 1:1A:1043:C:C4 | 1:1A:1044:G:N7 | 2.90 | 0.40 |
| 1:1A:2115:G:H2' | 1:1A:2116:G:H5' | 2.03 | 0.40 |
| 1:1A:2161:C:O2' | 1:1A:2162:G:H5'' | 2.21 | 0.40 |
| 1:1A:2807:G:C2 | 1:1A:2808:U:H1' | 2.57 | 0.40 |
| 2:1B:12:C:O5' | 2:1B:12:C:H6 | 2.05 | 0.40 |
| 5:1F:24:LEU:HD23 | 5:1F:115:ALA:HA | 2.04 | 0.40 |
| 26:14:63:TYR:N | 26:14:63:TYR:CD1 | 2.86 | 0.40 |
| 32:1a:148:G:H2' | 32:1a:149:A:C8 | 2.56 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 32:1a:341:C:H2' | 32:1a:342:C:C6 | 2.55 | 0.40 |
| 32:1a:374:A:C6 | 32:1a:375:U:C4 | 3.10 | 0.40 |
| 32:1a:721:G:H4' | 32:1a:722:A:O4' | 2.20 | 0.40 |
| 41:1j:25:GLU:O | 41:1j:29:ARG:N | 2.55 | 0.40 |
| 46:1o:31:LEU:HD23 | 46:1o:31:LEU:HA | 1.84 | 0.40 |
| 47:1p:75:ARG:HE | 47:1p:75:ARG:HB2 | 1.75 | 0.40 |
| 1:2A:271(S):G:C6 | 1:2A:271(T):C:C4 | 3.10 | 0.40 |
| 1:2A:479:A:N3 | 1:2A:481:G:H5'' | 2.36 | 0.40 |
| 1:2A:1009:A:OP2 | 9:2N:37:LYS:NZ | 2.49 | 0.40 |
| 1:2A:1903:G:OP1 | 3:2D:241:PRO:HB2 | 2.21 | 0.40 |
| 5:2F:110:LEU:O | 5:2F:114:VAL:HG23 | 2.21 | 0.40 |
| 6:2G:140:ILE:HD12 | 6:2G:140:ILE:HA | 1.89 | 0.40 |
| 6:2G:152:LEU:O | 6:2G:153:ARG:HG3 | 2.22 | 0.40 |
| 6:2G:173:LEU:HD23 | 6:2G:176:LEU:HD12 | 2.03 | 0.40 |
| 7:2H:7:LEU:HD23 | 7:2H:69:ARG:NH2 | 2.37 | 0.40 |
| 9:2N:15:LEU:HB2 | 9:2N:135:PRO:HB2 | 2.03 | 0.40 |
| 10:2O:25:LEU:HD11 | 10:2O:40:VAL:HG23 | 2.02 | 0.40 |
| 15:2T:36:GLU:O | 15:2T:39:ARG:HB3 | 2.21 | 0.40 |
| 18:2W:82:LEU:HD22 | 18:2W:84:ARG:HH22 | 1.87 | 0.40 |
| 32:2a:152:A:N6 | 32:2a:170:U:C2 | 2.89 | 0.40 |
| 32:2a:719:C:N4 | 49:2r:71:LYS:HE2 | 2.37 | 0.40 |
| 32:2a:1001(A):G:C5 | 32:2a:1002:G:H1' | 2.55 | 0.40 |
| 32:2a:1520:G:H8 | 32:2a:1520:G:OP2 | 2.04 | 0.40 |
| 33:2b:185:ILE:HG22 | 33:2b:199:TYR:CB | 2.42 | 0.40 |
| 34:2c:131:ARG:NH2 | 36:2e:50:GLU:HG3 | 2.36 | 0.40 |
| 35:2d:112:VAL:H | 35:2d:116:GLN:NE2 | 2.19 | 0.40 |
| 38:2g:42:ILE:HD13 | 38:2g:116:ALA:HB3 | 2.03 | 0.40 |
| 42:2k:38:ASN:HA | 42:2k:39:PRO:HD3 | 1.87 | 0.40 |
| 43:2l:53:ARG:HB3 | 43:2l:69:TYR:HE1 | 1.86 | 0.40 |
| 43:2l:104:VAL:HG12 | 43:2l:105:TYR:CG | 2.56 | 0.40 |
| 54:2w:63:G:H2' | 54:2w:64:A:C8 | 2.56 | 0.40 |
| 1:1A:373:U:O2 | 1:1A:423:A:H2 | 2.05 | 0.40 |
| 1:1A:1312:U:OP2 | 19:1X:63:LYS:HD2 | 2.22 | 0.40 |
| 1:1A:1916:A:H2' | 1:1A:1917:PSU:O4' | 2.21 | 0.40 |
| 1:1A:2329:G:O5' | 1:1A:2329:G:H8 | 2.04 | 0.40 |
| 3:1D:26:LYS:HD3 | 3:1D:83:GLU:OE2 | 2.21 | 0.40 |
| 8:1I:47:LEU:HD23 | 8:1I:47:LEU:HA | 1.74 | 0.40 |
| 10:1O:104:ARG:CZ | 15:1T:34:VAL:HG11 | 2.52 | 0.40 |
| 14:1S:110:LEU:HD12 | 14:1S:110:LEU:HA | 1.75 | 0.40 |
| 15:1T:33:LYS:HA | 15:1T:42:ILE:HD13 | 2.03 | 0.40 |
| 32:1a:582:U:H2' | 32:1a:583:A:H8 | 1.86 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 32:1a:690:G:H2' | 32:1a:691:G:O4' | 2.22 | 0.40 |
| 32:1a:731:G:H5' | 32:1a:766:A:H4' | 2.04 | 0.40 |
| 32:1a:840:C:H4' | 32:1a:841:U:OP1 | 2.21 | 0.40 |
| 32:1a:892:A:OP2 | 62:1a:1925:HOH:O | 2.22 | 0.40 |
| 32:1a:1456:G:O3' | 51:1t:39:LYS:NZ | 2.54 | 0.40 |
| 33:1b:21:ARG:O | 33:1b:23:ARG:N | 2.46 | 0.40 |
| 33:1b:72:GLY:HA2 | 33:1b:165:VAL:CG1 | 2.52 | 0.40 |
| 33:1b:105:PHE:C | 33:1b:107:THR:N | 2.77 | 0.40 |
| 34:1c:152:ILE:HG23 | 34:1c:167:TRP:HB3 | 2.03 | 0.40 |
| 36:1e:68:GLU:CD | 36:1e:70:PRO:HG3 | 2.47 | 0.40 |
| 36:1e:90:VAL:O | 36:1e:120:THR:HA | 2.21 | 0.40 |
| 38:1g:111:ARG:HE | 38:1g:111:ARG:HB3 | 1.74 | 0.40 |
| 40:1i:5:TYR:CG | 40:1i:6:GLY:N | 2.90 | 0.40 |
| 47:1p:3:LYS:HB3 | 47:1p:3:LYS:HE2 | 1.75 | 0.40 |
| 52:1u:18:TYR:CE1 | 52:1u:24:ARG:HB3 | 2.56 | 0.40 |
| 1:2A:602:G:O2' | 1:2A:655:A:N6 | 2.55 | 0.40 |
| 1:2A:856:C:O2' | 1:2A:857:C:OP1 | 2.39 | 0.40 |
| 1:2A:1041:C:H2' | 1:2A:1042:G:O4' | 2.21 | 0.40 |
| 1:2A:1434:A:H61 | 1:2A:1558:A:N6 | 2.14 | 0.40 |
| 1:2A:1488:G:C6 | 1:2A:1489:U:C4 | 3.10 | 0.40 |
| 1:2A:2547:U:C5 | 1:2A:2566:A:C5 | 3.09 | 0.40 |
| 1:2A:2837:G:H21 | 13:2R:45:ARG:HH12 | 1.69 | 0.40 |
| 4:2E:192:ASN:HB3 | 15:2T:3:ARG:HD3 | 2.04 | 0.40 |
| 12:2Q:65:PHE:HB2 | 12:2Q:105:GLU:HB2 | 2.02 | 0.40 |
| 19:2X:32:PRO:HA | 19:2X:77:LYS:HD3 | 2.04 | 0.40 |
| 25:23:30:ARG:HB2 | 25:23:33:GLN:HB2 | 2.03 | 0.40 |
| 32:2a:137:C:H2' | 32:2a:138:G:H8 | 1.85 | 0.40 |
| 32:2a:189(L):G:H2' | 32:2a:190:U:H6 | 1.86 | 0.40 |
| 32:2a:271:C:H2' | 32:2a:272:C:H6 | 1.86 | 0.40 |
| 32:2a:603:U:H6 | 32:2a:603:U:O5' | 2.03 | 0.40 |
| 32:2a:864:A:H2' | 32:2a:865:A:C8 | 2.57 | 0.40 |
| 32:2a:1002:G:C2 | 32:2a:1039:C:N4 | 2.89 | 0.40 |
| 32:2a:1157:A:C2 | 32:2a:1180:A:H2' | 2.56 | 0.40 |
| 40:2i:31:GLN:NE2 | 40:2i:36:TYR:HD1 | 2.20 | 0.40 |
| 41:2j:50:ILE:O | 45:2n:41:ARG:NH1 | 2.54 | 0.40 |
| 51:2t:30:LYS:HE3 | 51:2t:30:LYS:HB2 | 1.85 | 0.40 |
| 54:2w:75:C:C3' | 54:2w:76:F3N:P | 3.09 | 0.40 |
| 56:2y:42:C:H2' | 56:2y:43:C:H6 | 1.86 | 0.40 |
| 1:1A:969:U:H2' | 1:1A:970:C:C6 | 2.56 | 0.40 |
| 1:1A:1142(A):A:C5 | 1:1A:1144:G:C8 | 3.10 | 0.40 |
| 1:1A:2026:C:H2' | 1:1A:2027:G:O4' | 2.21 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1A:2136:C:N4 | 1:1A:2155:G:N1 | 2.28 | 0.40 |
| 1:1A:2206:G:OP2 | 1:1A:2206:G:H4' | 2.21 | 0.40 |
| 1:1A:2629:A:HO2' | 1:1A:2630:G:P | 2.42 | 0.40 |
| 1:1A:2839:G:H5' | 13:1R:46:GLY:CA | 2.50 | 0.40 |
| 3:1D:131:LEU:HD12 | 3:1D:131:LEU:N | 2.37 | 0.40 |
| 3:1D:222:ARG:HH11 | 3:1D:222:ARG:HD2 | 1.72 | 0.40 |
| 7:1H:56:SER:HB3 | 7:1H:61:HIS:ND1 | 2.36 | 0.40 |
| 14:1S:87:PHE:HB2 | 14:1S:112:PHE:CE1 | 2.55 | 0.40 |
| 32:1a:189(D):C:C4 | 32:1a:189(E):U:C4 | 3.09 | 0.40 |
| 32:1a:422:C:H2' | 32:1a:422:C:OP2 | 2.22 | 0.40 |
| 32:1a:1176:A:H2' | 32:1a:1177:G:C8 | 2.56 | 0.40 |
| 34:1c:121:ALA:O | 34:1c:125:GLU:HG3 | 2.22 | 0.40 |
| 36:1e:82:VAL:HG21 | 36:1e:138:ALA:HA | 2.02 | 0.40 |
| 38:1g:76:ARG:HG3 | 38:1g:156:TRP:HH2 | 1.86 | 0.40 |
| 38:1g:78:ARG:HG3 | 38:1g:79:ARG:N | 2.29 | 0.40 |
| 41:1j:27:ALA:HA | 41:1j:81:THR:HG21 | 2.02 | 0.40 |
| 43:1l:79:GLU:HG2 | 43:1l:80:HIS:CD2 | 2.57 | 0.40 |
| 1:2A:720:C:H2' | 1:2A:721:C:H6 | 1.86 | 0.40 |
| 1:2A:1401:G:H2' | 1:2A:1402:C:O4' | 2.22 | 0.40 |
| 1:2A:1526:G:C6 | 1:2A:1527:G:C2 | 3.10 | 0.40 |
| 1:2A:2038:G:H2' | 1:2A:2039:C:O4' | 2.21 | 0.40 |
| 1:2A:2703:C:H2' | 1:2A:2704:C:H6 | 1.86 | 0.40 |
| 1:2A:2850:A:OP2 | 1:2A:2866:U:H5 | 2.05 | 0.40 |
| 4:2E:116:VAL:HG13 | 4:2E:122:PHE:HB2 | 2.02 | 0.40 |
| 5:2F:34:TRP:NE1 | 11:2P:8:PRO:HD3 | 2.37 | 0.40 |
| 6:2G:121:ASN:HA | 6:2G:122:PRO:HD2 | 1.99 | 0.40 |
| 7:2H:101:ARG:NH2 | 7:2H:121:ILE:O | 2.54 | 0.40 |
| 8:2I:117:GLU:H | 8:2I:117:GLU:HG3 | 1.59 | 0.40 |
| 19:2X:1:MET:H1 | 24:22:29:LYS:HE3 | 1.86 | 0.40 |
| 32:2a:344:A:H5'' | 32:2a:345:C:H5 | 1.86 | 0.40 |
| 32:2a:1152:A:OP1 | 41:2j:68:HIS:ND1 | 2.54 | 0.40 |
| 32:2a:1179:A:H4' | 40:2i:103:THR:HA | 2.03 | 0.40 |
| 35:2d:76:ARG:NH2 | 35:2d:80:GLU:OE2 | 2.51 | 0.40 |
| 36:2e:57:LYS:HE3 | 36:2e:57:LYS:HB2 | 1.96 | 0.40 |
| 38:2g:15:ASP:OD1 | 38:2g:19:GLY:N | 2.55 | 0.40 |
| 42:2k:18:ARG:O | 42:2k:32:ILE:HA | 2.21 | 0.40 |
| 51:2t:99:LEU:HD23 | 51:2t:99:LEU:HA | 1.94 | 0.40 |
| 56:2y:74:C:H2' | 56:2y:75:C:C6 | 2.56 | 0.40 |

All (1) 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) |
|----------------|------------------------|--------------------------|-------------------|
| 8:1I:87:LYS:NZ | 32:2a:358:U:O3'[3_654] | 2.18 | 0.02 |

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%) | 257 (94%) | 14 (5%) | 2 (1%) | 18 | 38 |
| 3 | 2D | 273/276 (99%) | 257 (94%) | 15 (6%) | 1 (0%) | 30 | 51 |
| 4 | 1E | 202/206 (98%) | 188 (93%) | 12 (6%) | 2 (1%) | 12 | 28 |
| 4 | 2E | 202/206 (98%) | 189 (94%) | 11 (5%) | 2 (1%) | 12 | 28 |
| 5 | 1F | 201/210 (96%) | 193 (96%) | 7 (4%) | 1 (0%) | 24 | 46 |
| 5 | 2F | 201/210 (96%) | 184 (92%) | 13 (6%) | 4 (2%) | 6 | 12 |
| 6 | 1G | 179/182 (98%) | 163 (91%) | 14 (8%) | 2 (1%) | 11 | 25 |
| 6 | 2G | 179/182 (98%) | 151 (84%) | 24 (13%) | 4 (2%) | 5 | 10 |
| 7 | 1H | 172/180 (96%) | 162 (94%) | 9 (5%) | 1 (1%) | 21 | 42 |
| 7 | 2H | 172/180 (96%) | 151 (88%) | 17 (10%) | 4 (2%) | 5 | 9 |
| 8 | 1I | 144/148 (97%) | 120 (83%) | 20 (14%) | 4 (3%) | 4 | 6 |
| 8 | 2I | 144/148 (97%) | 120 (83%) | 22 (15%) | 2 (1%) | 9 | 19 |
| 9 | 1N | 138/140 (99%) | 133 (96%) | 3 (2%) | 2 (1%) | 9 | 19 |
| 9 | 2N | 138/140 (99%) | 129 (94%) | 9 (6%) | 0 | 100 | 100 |
| 10 | 1O | 120/122 (98%) | 111 (92%) | 9 (8%) | 0 | 100 | 100 |
| 10 | 2O | 120/122 (98%) | 110 (92%) | 9 (8%) | 1 (1%) | 16 | 34 |
| 11 | 1P | 147/150 (98%) | 133 (90%) | 12 (8%) | 2 (1%) | 9 | 19 |
| 11 | 2P | 147/150 (98%) | 133 (90%) | 11 (8%) | 3 (2%) | 6 | 12 |
| 12 | 1Q | 139/141 (99%) | 127 (91%) | 12 (9%) | 0 | 100 | 100 |
| 12 | 2Q | 139/141 (99%) | 124 (89%) | 13 (9%) | 2 (1%) | 9 | 19 |
| 13 | 1R | 116/118 (98%) | 111 (96%) | 5 (4%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|------------|----------|----------|-------------|-----|
| 13 | 2R | 116/118 (98%) | 106 (91%) | 10 (9%) | 0 | 100 | 100 |
| 14 | 1S | 108/112 (96%) | 97 (90%) | 11 (10%) | 0 | 100 | 100 |
| 14 | 2S | 108/112 (96%) | 97 (90%) | 8 (7%) | 3 (3%) | 4 | 6 |
| 15 | 1T | 129/146 (88%) | 119 (92%) | 7 (5%) | 3 (2%) | 5 | 9 |
| 15 | 2T | 129/146 (88%) | 119 (92%) | 10 (8%) | 0 | 100 | 100 |
| 16 | 1U | 114/118 (97%) | 114 (100%) | 0 | 0 | 100 | 100 |
| 16 | 2U | 114/118 (97%) | 112 (98%) | 2 (2%) | 0 | 100 | 100 |
| 17 | 1V | 99/101 (98%) | 94 (95%) | 3 (3%) | 2 (2%) | 6 | 12 |
| 17 | 2V | 99/101 (98%) | 91 (92%) | 6 (6%) | 2 (2%) | 6 | 12 |
| 18 | 1W | 110/113 (97%) | 108 (98%) | 2 (2%) | 0 | 100 | 100 |
| 18 | 2W | 110/113 (97%) | 105 (96%) | 5 (4%) | 0 | 100 | 100 |
| 19 | 1X | 93/96 (97%) | 89 (96%) | 3 (3%) | 1 (1%) | 11 | 25 |
| 19 | 2X | 93/96 (97%) | 85 (91%) | 7 (8%) | 1 (1%) | 11 | 25 |
| 20 | 1Y | 105/110 (96%) | 97 (92%) | 7 (7%) | 1 (1%) | 12 | 28 |
| 20 | 2Y | 105/110 (96%) | 98 (93%) | 6 (6%) | 1 (1%) | 12 | 28 |
| 21 | 1Z | 148/206 (72%) | 131 (88%) | 14 (10%) | 3 (2%) | 6 | 12 |
| 21 | 2Z | 156/206 (76%) | 130 (83%) | 22 (14%) | 4 (3%) | 4 | 7 |
| 22 | 10 | 81/85 (95%) | 77 (95%) | 3 (4%) | 1 (1%) | 10 | 23 |
| 22 | 20 | 81/85 (95%) | 77 (95%) | 3 (4%) | 1 (1%) | 10 | 23 |
| 23 | 11 | 95/98 (97%) | 90 (95%) | 4 (4%) | 1 (1%) | 11 | 25 |
| 23 | 21 | 95/98 (97%) | 92 (97%) | 3 (3%) | 0 | 100 | 100 |
| 24 | 12 | 68/72 (94%) | 66 (97%) | 1 (2%) | 1 (2%) | 8 | 18 |
| 24 | 22 | 68/72 (94%) | 66 (97%) | 2 (3%) | 0 | 100 | 100 |
| 25 | 13 | 57/60 (95%) | 56 (98%) | 1 (2%) | 0 | 100 | 100 |
| 25 | 23 | 57/60 (95%) | 52 (91%) | 5 (9%) | 0 | 100 | 100 |
| 26 | 14 | 67/71 (94%) | 51 (76%) | 10 (15%) | 6 (9%) | 0 | 0 |
| 26 | 24 | 67/71 (94%) | 48 (72%) | 12 (18%) | 7 (10%) | 0 | 0 |
| 27 | 15 | 57/60 (95%) | 53 (93%) | 4 (7%) | 0 | 100 | 100 |
| 27 | 25 | 57/60 (95%) | 51 (90%) | 6 (10%) | 0 | 100 | 100 |
| 28 | 16 | 51/54 (94%) | 48 (94%) | 3 (6%) | 0 | 100 | 100 |
| 28 | 26 | 51/54 (94%) | 47 (92%) | 4 (8%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 29 | 17 | 46/49 (94%) | 46 (100%) | 0 | 0 | 100 | 100 |
| 29 | 27 | 46/49 (94%) | 45 (98%) | 1 (2%) | 0 | 100 | 100 |
| 30 | 18 | 62/65 (95%) | 62 (100%) | 0 | 0 | 100 | 100 |
| 30 | 28 | 62/65 (95%) | 58 (94%) | 3 (5%) | 1 (2%) | 7 | 16 |
| 31 | 19 | 35/37 (95%) | 35 (100%) | 0 | 0 | 100 | 100 |
| 31 | 29 | 35/37 (95%) | 34 (97%) | 1 (3%) | 0 | 100 | 100 |
| 33 | 1b | 229/256 (90%) | 183 (80%) | 32 (14%) | 14 (6%) | 1 | 1 |
| 33 | 2b | 229/256 (90%) | 185 (81%) | 29 (13%) | 15 (7%) | 1 | 1 |
| 34 | 1c | 204/239 (85%) | 185 (91%) | 17 (8%) | 2 (1%) | 12 | 28 |
| 34 | 2c | 204/239 (85%) | 162 (79%) | 32 (16%) | 10 (5%) | 1 | 2 |
| 35 | 1d | 206/209 (99%) | 184 (89%) | 19 (9%) | 3 (2%) | 8 | 18 |
| 35 | 2d | 206/209 (99%) | 184 (89%) | 20 (10%) | 2 (1%) | 12 | 28 |
| 36 | 1e | 146/162 (90%) | 133 (91%) | 8 (6%) | 5 (3%) | 3 | 4 |
| 36 | 2e | 146/162 (90%) | 128 (88%) | 15 (10%) | 3 (2%) | 5 | 11 |
| 37 | 1f | 98/101 (97%) | 93 (95%) | 4 (4%) | 1 (1%) | 12 | 28 |
| 37 | 2f | 98/101 (97%) | 95 (97%) | 3 (3%) | 0 | 100 | 100 |
| 38 | 1g | 153/156 (98%) | 136 (89%) | 14 (9%) | 3 (2%) | 6 | 12 |
| 38 | 2g | 153/156 (98%) | 130 (85%) | 15 (10%) | 8 (5%) | 1 | 2 |
| 39 | 1h | 135/138 (98%) | 121 (90%) | 11 (8%) | 3 (2%) | 5 | 10 |
| 39 | 2h | 135/138 (98%) | 124 (92%) | 9 (7%) | 2 (2%) | 8 | 18 |
| 40 | 1i | 125/128 (98%) | 105 (84%) | 17 (14%) | 3 (2%) | 4 | 9 |
| 40 | 2i | 125/128 (98%) | 103 (82%) | 21 (17%) | 1 (1%) | 16 | 34 |
| 41 | 1j | 95/105 (90%) | 81 (85%) | 8 (8%) | 6 (6%) | 1 | 1 |
| 41 | 2j | 94/105 (90%) | 74 (79%) | 15 (16%) | 5 (5%) | 1 | 1 |
| 42 | 1k | 112/129 (87%) | 100 (89%) | 8 (7%) | 4 (4%) | 2 | 4 |
| 42 | 2k | 112/129 (87%) | 99 (88%) | 9 (8%) | 4 (4%) | 2 | 4 |
| 43 | 1l | 119/132 (90%) | 112 (94%) | 7 (6%) | 0 | 100 | 100 |
| 43 | 2l | 119/132 (90%) | 108 (91%) | 9 (8%) | 2 (2%) | 7 | 15 |
| 44 | 1m | 123/126 (98%) | 110 (89%) | 11 (9%) | 2 (2%) | 7 | 16 |
| 44 | 2m | 120/126 (95%) | 100 (83%) | 16 (13%) | 4 (3%) | 3 | 5 |
| 45 | 1n | 58/61 (95%) | 49 (84%) | 8 (14%) | 1 (2%) | 7 | 15 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-------------------|-------------|----------|----------|-------------|-----|
| 45 | 2n | 58/61 (95%) | 50 (86%) | 6 (10%) | 2 (3%) | 3 | 4 |
| 46 | 1o | 86/89 (97%) | 78 (91%) | 7 (8%) | 1 (1%) | 10 | 23 |
| 46 | 2o | 86/89 (97%) | 82 (95%) | 3 (4%) | 1 (1%) | 10 | 23 |
| 47 | 1p | 80/88 (91%) | 71 (89%) | 8 (10%) | 1 (1%) | 9 | 21 |
| 47 | 2p | 80/88 (91%) | 71 (89%) | 8 (10%) | 1 (1%) | 9 | 21 |
| 48 | 1q | 97/105 (92%) | 90 (93%) | 7 (7%) | 0 | 100 | 100 |
| 48 | 2q | 97/105 (92%) | 89 (92%) | 7 (7%) | 1 (1%) | 12 | 28 |
| 49 | 1r | 66/88 (75%) | 57 (86%) | 8 (12%) | 1 (2%) | 8 | 18 |
| 49 | 2r | 66/88 (75%) | 63 (96%) | 3 (4%) | 0 | 100 | 100 |
| 50 | 1s | 81/93 (87%) | 70 (86%) | 6 (7%) | 5 (6%) | 1 | 1 |
| 50 | 2s | 81/93 (87%) | 67 (83%) | 11 (14%) | 3 (4%) | 2 | 3 |
| 51 | 1t | 94/106 (89%) | 84 (89%) | 6 (6%) | 4 (4%) | 2 | 2 |
| 51 | 2t | 94/106 (89%) | 82 (87%) | 8 (8%) | 4 (4%) | 2 | 2 |
| 52 | 1u | 21/27 (78%) | 19 (90%) | 2 (10%) | 0 | 100 | 100 |
| 52 | 2u | 21/27 (78%) | 19 (90%) | 2 (10%) | 0 | 100 | 100 |
| 57 | 1z | 15/17 (88%) | 13 (87%) | 2 (13%) | 0 | 100 | 100 |
| 57 | 2z | 15/17 (88%) | 10 (67%) | 5 (33%) | 0 | 100 | 100 |
| All | All | 11402/12162 (94%) | 10291 (90%) | 906 (8%) | 205 (2%) | 6 | 14 |

All (205) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5 | 1F | 130 | ALA |
| 6 | 1G | 50 | ALA |
| 15 | 1T | 55 | ASN |
| 23 | 1I | 3 | LYS |
| 33 | 1b | 8 | LYS |
| 33 | 1b | 17 | PHE |
| 35 | 1d | 173 | TRP |
| 38 | 1g | 35 | LYS |
| 42 | 1k | 89 | ALA |
| 44 | 1m | 67 | GLU |
| 50 | 1s | 24 | ALA |
| 5 | 2F | 130 | ALA |
| 11 | 2P | 90 | ARG |
| 21 | 2Z | 52 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 21 | 2Z | 146 | ILE |
| 33 | 2b | 9 | GLU |
| 33 | 2b | 17 | PHE |
| 33 | 2b | 123 | ALA |
| 38 | 2g | 7 | ALA |
| 38 | 2g | 55 | GLY |
| 38 | 2g | 80 | VAL |
| 41 | 2j | 79 | ARG |
| 42 | 2k | 49 | GLY |
| 51 | 2t | 68 | LYS |
| 51 | 2t | 95 | ALA |
| 3 | 1D | 3 | VAL |
| 8 | 1I | 34 | GLY |
| 11 | 1P | 93 | GLY |
| 15 | 1T | 37 | GLY |
| 17 | 1V | 79 | VAL |
| 19 | 1X | 93 | GLU |
| 21 | 1Z | 53 | ILE |
| 26 | 14 | 44 | THR |
| 26 | 14 | 45 | GLY |
| 26 | 14 | 47 | GLN |
| 26 | 14 | 49 | PHE |
| 26 | 14 | 59 | PHE |
| 26 | 14 | 62 | ARG |
| 33 | 1b | 31 | TYR |
| 34 | 1c | 79 | ARG |
| 35 | 1d | 172 | PRO |
| 36 | 1e | 63 | ARG |
| 36 | 1e | 85 | GLY |
| 38 | 1g | 55 | GLY |
| 39 | 1h | 54 | ASP |
| 41 | 1j | 79 | ARG |
| 49 | 1r | 54 | ARG |
| 51 | 1t | 47 | GLY |
| 51 | 1t | 100 | ILE |
| 5 | 2F | 17 | ARG |
| 6 | 2G | 28 | VAL |
| 6 | 2G | 51 | ARG |
| 11 | 2P | 39 | LYS |
| 17 | 2V | 27 | ALA |
| 17 | 2V | 79 | VAL |
| 19 | 2X | 93 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 26 | 24 | 46 | GLN |
| 26 | 24 | 47 | GLN |
| 26 | 24 | 61 | ARG |
| 33 | 2b | 10 | LEU |
| 33 | 2b | 74 | LYS |
| 33 | 2b | 121 | LEU |
| 34 | 2c | 42 | LEU |
| 34 | 2c | 43 | LEU |
| 34 | 2c | 95 | THR |
| 38 | 2g | 52 | GLU |
| 40 | 2i | 11 | LYS |
| 41 | 2j | 32 | ALA |
| 44 | 2m | 11 | ARG |
| 44 | 2m | 38 | GLY |
| 44 | 2m | 67 | GLU |
| 48 | 2q | 68 | ARG |
| 3 | 1D | 31 | LYS |
| 4 | 1E | 178 | GLU |
| 6 | 1G | 84 | LYS |
| 7 | 1H | 126 | PRO |
| 8 | 1I | 42 | SER |
| 15 | 1T | 118 | ARG |
| 17 | 1V | 43 | GLU |
| 21 | 1Z | 156 | LYS |
| 33 | 1b | 22 | LYS |
| 33 | 1b | 106 | LYS |
| 33 | 1b | 126 | GLU |
| 33 | 1b | 155 | LEU |
| 36 | 1e | 21 | ALA |
| 36 | 1e | 86 | ALA |
| 40 | 1i | 56 | LEU |
| 42 | 1k | 90 | GLY |
| 44 | 1m | 106 | ASN |
| 45 | 1n | 58 | LYS |
| 47 | 1p | 75 | ARG |
| 50 | 1s | 25 | LYS |
| 50 | 1s | 26 | GLY |
| 50 | 1s | 27 | GLU |
| 3 | 2D | 150 | LYS |
| 4 | 2E | 52 | LEU |
| 7 | 2H | 126 | PRO |
| 11 | 2P | 122 | PRO |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 14 | 2S | 84 | GLN |
| 21 | 2Z | 51 | ALA |
| 26 | 24 | 49 | PHE |
| 30 | 28 | 51 | ALA |
| 33 | 2b | 20 | GLU |
| 33 | 2b | 226 | ARG |
| 34 | 2c | 38 | ARG |
| 34 | 2c | 41 | GLY |
| 34 | 2c | 181 | ASN |
| 46 | 2o | 88 | ARG |
| 50 | 2s | 9 | VAL |
| 50 | 2s | 73 | GLU |
| 4 | 1E | 52 | LEU |
| 8 | 1I | 69 | LYS |
| 8 | 1I | 135 | GLU |
| 24 | 12 | 69 | ARG |
| 33 | 1b | 10 | LEU |
| 33 | 1b | 20 | GLU |
| 33 | 1b | 63 | MET |
| 33 | 1b | 83 | MET |
| 33 | 1b | 84 | GLU |
| 33 | 1b | 231 | GLU |
| 34 | 1c | 144 | SER |
| 36 | 1e | 69 | VAL |
| 37 | 1f | 19 | LEU |
| 40 | 1i | 127 | LYS |
| 41 | 1j | 22 | LYS |
| 5 | 2F | 18 | ARG |
| 5 | 2F | 21 | ALA |
| 6 | 2G | 43 | LEU |
| 7 | 2H | 58 | GLU |
| 8 | 2I | 40 | THR |
| 14 | 2S | 94 | TYR |
| 26 | 24 | 48 | ARG |
| 26 | 24 | 65 | ASP |
| 33 | 2b | 125 | PRO |
| 34 | 2c | 47 | LEU |
| 34 | 2c | 79 | ARG |
| 34 | 2c | 91 | LEU |
| 34 | 2c | 179 | ARG |
| 36 | 2e | 37 | ARG |
| 38 | 2g | 4 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 38 | 2g | 33 | ASP |
| 41 | 2j | 51 | ARG |
| 42 | 2k | 54 | ARG |
| 42 | 2k | 117 | ASN |
| 43 | 2l | 51 | ALA |
| 43 | 2l | 91 | LYS |
| 45 | 2n | 44 | LEU |
| 50 | 2s | 81 | ARG |
| 51 | 2t | 10 | LEU |
| 9 | 1N | 2 | LYS |
| 9 | 1N | 23 | LEU |
| 22 | 10 | 73 | GLY |
| 41 | 1j | 21 | GLN |
| 41 | 1j | 78 | ASN |
| 51 | 1t | 89 | ARG |
| 4 | 2E | 17 | ASP |
| 8 | 2I | 135 | GLU |
| 12 | 2Q | 16 | ARG |
| 20 | 2Y | 54 | LYS |
| 33 | 2b | 120 | ALA |
| 33 | 2b | 122 | PHE |
| 36 | 2e | 73 | ASN |
| 36 | 2e | 96 | PRO |
| 41 | 2j | 77 | PRO |
| 47 | 2p | 66 | PRO |
| 46 | 1o | 23 | GLY |
| 50 | 1s | 83 | HIS |
| 51 | 1t | 102 | GLY |
| 10 | 2O | 119 | PRO |
| 12 | 2Q | 15 | GLY |
| 22 | 20 | 73 | GLY |
| 26 | 24 | 45 | GLY |
| 33 | 2b | 21 | ARG |
| 33 | 2b | 131 | PRO |
| 35 | 2d | 159 | ARG |
| 39 | 2h | 22 | GLU |
| 42 | 2k | 66 | LEU |
| 45 | 2n | 14 | PRO |
| 35 | 1d | 142 | PRO |
| 42 | 1k | 35 | PRO |
| 14 | 2S | 96 | GLY |
| 33 | 2b | 231 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 39 | 2h | 73 | ASP |
| 20 | 1Y | 103 | GLY |
| 21 | 1Z | 120 | ILE |
| 21 | 2Z | 165 | VAL |
| 38 | 2g | 17 | VAL |
| 38 | 2g | 58 | PRO |
| 41 | 2j | 91 | PRO |
| 11 | 1P | 47 | ASP |
| 39 | 1h | 51 | VAL |
| 41 | 1j | 39 | PRO |
| 42 | 1k | 49 | GLY |
| 7 | 2H | 10 | PRO |
| 7 | 2H | 92 | ILE |
| 40 | 1i | 24 | GLY |
| 41 | 1j | 77 | PRO |
| 6 | 2G | 109 | VAL |
| 35 | 2d | 171 | GLY |
| 44 | 2m | 41 | PRO |
| 38 | 1g | 80 | VAL |
| 39 | 1h | 73 | ASP |
| 33 | 2b | 80 | ILE |
| 51 | 2t | 98 | PRO |
| 33 | 1b | 125 | PRO |

5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|-------------|----|
| 3 | 1D | 215/218 (99%) | 200 (93%) | 15 (7%) | 14 | 31 |
| 3 | 2D | 215/218 (99%) | 198 (92%) | 17 (8%) | 11 | 26 |
| 4 | 1E | 164/166 (99%) | 151 (92%) | 13 (8%) | 11 | 26 |
| 4 | 2E | 164/166 (99%) | 150 (92%) | 14 (8%) | 10 | 22 |
| 5 | 1F | 160/166 (96%) | 144 (90%) | 16 (10%) | 7 | 16 |
| 5 | 2F | 159/166 (96%) | 147 (92%) | 12 (8%) | 12 | 28 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 6 | 1G | 143/156 (92%) | 128 (90%) | 15 (10%) | 6 | 14 |
| 6 | 2G | 143/156 (92%) | 125 (87%) | 18 (13%) | 4 | 9 |
| 7 | 1H | 144/148 (97%) | 125 (87%) | 19 (13%) | 4 | 8 |
| 7 | 2H | 144/148 (97%) | 122 (85%) | 22 (15%) | 3 | 5 |
| 8 | 1I | 113/124 (91%) | 93 (82%) | 20 (18%) | 2 | 3 |
| 8 | 2I | 105/124 (85%) | 85 (81%) | 20 (19%) | 1 | 2 |
| 9 | 1N | 118/119 (99%) | 105 (89%) | 13 (11%) | 6 | 13 |
| 9 | 2N | 118/119 (99%) | 107 (91%) | 11 (9%) | 8 | 18 |
| 10 | 1O | 100/100 (100%) | 95 (95%) | 5 (5%) | 22 | 46 |
| 10 | 2O | 100/100 (100%) | 93 (93%) | 7 (7%) | 14 | 31 |
| 11 | 1P | 115/116 (99%) | 106 (92%) | 9 (8%) | 11 | 26 |
| 11 | 2P | 115/116 (99%) | 106 (92%) | 9 (8%) | 11 | 26 |
| 12 | 1Q | 111/111 (100%) | 105 (95%) | 6 (5%) | 20 | 42 |
| 12 | 2Q | 111/111 (100%) | 106 (96%) | 5 (4%) | 24 | 50 |
| 13 | 1R | 101/101 (100%) | 98 (97%) | 3 (3%) | 36 | 64 |
| 13 | 2R | 101/101 (100%) | 94 (93%) | 7 (7%) | 14 | 32 |
| 14 | 1S | 86/88 (98%) | 79 (92%) | 7 (8%) | 11 | 24 |
| 14 | 2S | 85/88 (97%) | 70 (82%) | 15 (18%) | 2 | 3 |
| 15 | 1T | 115/127 (91%) | 109 (95%) | 6 (5%) | 21 | 44 |
| 15 | 2T | 113/127 (89%) | 104 (92%) | 9 (8%) | 11 | 25 |
| 16 | 1U | 93/94 (99%) | 83 (89%) | 10 (11%) | 6 | 13 |
| 16 | 2U | 93/94 (99%) | 86 (92%) | 7 (8%) | 12 | 28 |
| 17 | 1V | 80/82 (98%) | 72 (90%) | 8 (10%) | 7 | 16 |
| 17 | 2V | 80/82 (98%) | 72 (90%) | 8 (10%) | 7 | 16 |
| 18 | 1W | 90/92 (98%) | 84 (93%) | 6 (7%) | 15 | 33 |
| 18 | 2W | 90/92 (98%) | 82 (91%) | 8 (9%) | 9 | 20 |
| 19 | 1X | 77/78 (99%) | 74 (96%) | 3 (4%) | 28 | 55 |
| 19 | 2X | 77/78 (99%) | 72 (94%) | 5 (6%) | 15 | 35 |
| 20 | 1Y | 85/91 (93%) | 74 (87%) | 11 (13%) | 4 | 8 |
| 20 | 2Y | 85/91 (93%) | 73 (86%) | 12 (14%) | 3 | 6 |
| 21 | 1Z | 135/179 (75%) | 120 (89%) | 15 (11%) | 6 | 12 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|-------------|-----|
| 21 | 2Z | 137/179 (76%) | 110 (80%) | 27 (20%) | 1 | 2 |
| 22 | 10 | 65/67 (97%) | 61 (94%) | 4 (6%) | 16 | 36 |
| 22 | 20 | 65/67 (97%) | 62 (95%) | 3 (5%) | 24 | 49 |
| 23 | 11 | 80/83 (96%) | 75 (94%) | 5 (6%) | 16 | 36 |
| 23 | 21 | 80/83 (96%) | 74 (92%) | 6 (8%) | 12 | 28 |
| 24 | 12 | 65/67 (97%) | 58 (89%) | 7 (11%) | 6 | 13 |
| 24 | 22 | 65/67 (97%) | 61 (94%) | 4 (6%) | 16 | 36 |
| 25 | 13 | 51/52 (98%) | 46 (90%) | 5 (10%) | 7 | 17 |
| 25 | 23 | 50/52 (96%) | 46 (92%) | 4 (8%) | 11 | 25 |
| 26 | 14 | 59/63 (94%) | 51 (86%) | 8 (14%) | 3 | 7 |
| 26 | 24 | 53/63 (84%) | 43 (81%) | 10 (19%) | 1 | 2 |
| 27 | 15 | 50/52 (96%) | 46 (92%) | 4 (8%) | 11 | 25 |
| 27 | 25 | 50/52 (96%) | 48 (96%) | 2 (4%) | 28 | 55 |
| 28 | 16 | 51/52 (98%) | 48 (94%) | 3 (6%) | 18 | 38 |
| 28 | 26 | 50/52 (96%) | 44 (88%) | 6 (12%) | 5 | 10 |
| 29 | 17 | 41/42 (98%) | 35 (85%) | 6 (15%) | 3 | 6 |
| 29 | 27 | 41/42 (98%) | 37 (90%) | 4 (10%) | 7 | 17 |
| 30 | 18 | 54/55 (98%) | 49 (91%) | 5 (9%) | 8 | 18 |
| 30 | 28 | 54/55 (98%) | 47 (87%) | 7 (13%) | 4 | 8 |
| 31 | 19 | 34/34 (100%) | 34 (100%) | 0 | 100 | 100 |
| 31 | 29 | 34/34 (100%) | 31 (91%) | 3 (9%) | 9 | 21 |
| 33 | 1b | 192/220 (87%) | 160 (83%) | 32 (17%) | 2 | 4 |
| 33 | 2b | 187/220 (85%) | 157 (84%) | 30 (16%) | 2 | 4 |
| 34 | 1c | 142/188 (76%) | 124 (87%) | 18 (13%) | 4 | 9 |
| 34 | 2c | 140/188 (74%) | 112 (80%) | 28 (20%) | 1 | 2 |
| 35 | 1d | 169/181 (93%) | 144 (85%) | 25 (15%) | 3 | 6 |
| 35 | 2d | 173/181 (96%) | 149 (86%) | 24 (14%) | 3 | 7 |
| 36 | 1e | 113/123 (92%) | 103 (91%) | 10 (9%) | 9 | 21 |
| 36 | 2e | 114/123 (93%) | 95 (83%) | 19 (17%) | 2 | 4 |
| 37 | 1f | 84/90 (93%) | 77 (92%) | 7 (8%) | 10 | 23 |
| 37 | 2f | 85/90 (94%) | 73 (86%) | 12 (14%) | 3 | 6 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|-------------|----|
| 38 | 1g | 119/127 (94%) | 99 (83%) | 20 (17%) | 2 | 4 |
| 38 | 2g | 120/127 (94%) | 106 (88%) | 14 (12%) | 5 | 11 |
| 39 | 1h | 114/119 (96%) | 108 (95%) | 6 (5%) | 20 | 43 |
| 39 | 2h | 114/119 (96%) | 101 (89%) | 13 (11%) | 5 | 11 |
| 40 | 1i | 90/99 (91%) | 79 (88%) | 11 (12%) | 5 | 10 |
| 40 | 2i | 89/99 (90%) | 78 (88%) | 11 (12%) | 4 | 9 |
| 41 | 1j | 66/92 (72%) | 55 (83%) | 11 (17%) | 2 | 4 |
| 41 | 2j | 69/92 (75%) | 55 (80%) | 14 (20%) | 1 | 2 |
| 42 | 1k | 82/99 (83%) | 70 (85%) | 12 (15%) | 3 | 6 |
| 42 | 2k | 83/99 (84%) | 77 (93%) | 6 (7%) | 13 | 30 |
| 43 | 1l | 96/108 (89%) | 94 (98%) | 2 (2%) | 47 | 73 |
| 43 | 2l | 96/108 (89%) | 90 (94%) | 6 (6%) | 16 | 36 |
| 44 | 1m | 95/101 (94%) | 81 (85%) | 14 (15%) | 3 | 6 |
| 44 | 2m | 92/101 (91%) | 81 (88%) | 11 (12%) | 5 | 10 |
| 45 | 1n | 49/50 (98%) | 44 (90%) | 5 (10%) | 7 | 15 |
| 45 | 2n | 49/50 (98%) | 41 (84%) | 8 (16%) | 2 | 4 |
| 46 | 1o | 78/80 (98%) | 73 (94%) | 5 (6%) | 16 | 35 |
| 46 | 2o | 78/80 (98%) | 73 (94%) | 5 (6%) | 16 | 35 |
| 47 | 1p | 69/74 (93%) | 59 (86%) | 10 (14%) | 3 | 6 |
| 47 | 2p | 68/74 (92%) | 57 (84%) | 11 (16%) | 2 | 4 |
| 48 | 1q | 94/97 (97%) | 87 (93%) | 7 (7%) | 13 | 29 |
| 48 | 2q | 94/97 (97%) | 86 (92%) | 8 (8%) | 10 | 22 |
| 49 | 1r | 59/77 (77%) | 51 (86%) | 8 (14%) | 3 | 7 |
| 49 | 2r | 59/77 (77%) | 52 (88%) | 7 (12%) | 5 | 10 |
| 50 | 1s | 69/80 (86%) | 60 (87%) | 9 (13%) | 4 | 8 |
| 50 | 2s | 67/80 (84%) | 54 (81%) | 13 (19%) | 1 | 2 |
| 51 | 1t | 70/82 (85%) | 61 (87%) | 9 (13%) | 4 | 8 |
| 51 | 2t | 70/82 (85%) | 67 (96%) | 3 (4%) | 26 | 51 |
| 52 | 1u | 18/22 (82%) | 16 (89%) | 2 (11%) | 6 | 12 |
| 52 | 2u | 18/22 (82%) | 17 (94%) | 1 (6%) | 19 | 40 |
| 57 | 1z | 13/13 (100%) | 9 (69%) | 4 (31%) | 0 | 0 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|-----|-------|------------------|------------|------------|-------------|
| 57 | 2z | 13/13 (100%) | 8 (62%) | 5 (38%) | 0 0 |
| All | All | 9331/10090 (92%) | 8326 (89%) | 1005 (11%) | 6 13 |

All (1005) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | 1D | 3 | VAL |
| 3 | 1D | 4 | LYS |
| 3 | 1D | 82 | ILE |
| 3 | 1D | 88 | ARG |
| 3 | 1D | 99 | ASP |
| 3 | 1D | 111 | LEU |
| 3 | 1D | 136 | ILE |
| 3 | 1D | 142 | VAL |
| 3 | 1D | 154 | LYS |
| 3 | 1D | 204 | ILE |
| 3 | 1D | 212 | SER |
| 3 | 1D | 229 | VAL |
| 3 | 1D | 242 | ARG |
| 3 | 1D | 259 | THR |
| 3 | 1D | 273 | ARG |
| 4 | 1E | 2 | LYS |
| 4 | 1E | 9 | VAL |
| 4 | 1E | 12 | THR |
| 4 | 1E | 14 | ILE |
| 4 | 1E | 38 | THR |
| 4 | 1E | 59 | VAL |
| 4 | 1E | 73 | GLU |
| 4 | 1E | 77 | ILE |
| 4 | 1E | 78 | LEU |
| 4 | 1E | 92 | THR |
| 4 | 1E | 93 | VAL |
| 4 | 1E | 116 | VAL |
| 4 | 1E | 188 | VAL |
| 5 | 1F | 33 | LEU |
| 5 | 1F | 50 | SER |
| 5 | 1F | 53 | THR |
| 5 | 1F | 57 | VAL |
| 5 | 1F | 60 | SER |
| 5 | 1F | 70 | THR |
| 5 | 1F | 74 | ARG |
| 5 | 1F | 88 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5 | 1F | 106 | ARG |
| 5 | 1F | 132 | VAL |
| 5 | 1F | 140 | LEU |
| 5 | 1F | 144 | LYS |
| 5 | 1F | 162 | LEU |
| 5 | 1F | 183 | VAL |
| 5 | 1F | 192 | LEU |
| 5 | 1F | 201 | VAL |
| 6 | 1G | 5 | VAL |
| 6 | 1G | 7 | LEU |
| 6 | 1G | 9 | ARG |
| 6 | 1G | 31 | VAL |
| 6 | 1G | 43 | LEU |
| 6 | 1G | 70 | VAL |
| 6 | 1G | 79 | ASN |
| 6 | 1G | 82 | LEU |
| 6 | 1G | 109 | VAL |
| 6 | 1G | 139 | LEU |
| 6 | 1G | 140 | ILE |
| 6 | 1G | 145 | THR |
| 6 | 1G | 148 | MET |
| 6 | 1G | 159 | VAL |
| 6 | 1G | 181 | ARG |
| 7 | 1H | 2 | SER |
| 7 | 1H | 13 | LYS |
| 7 | 1H | 37 | VAL |
| 7 | 1H | 51 | ARG |
| 7 | 1H | 53 | GLU |
| 7 | 1H | 56 | SER |
| 7 | 1H | 72 | ILE |
| 7 | 1H | 88 | LEU |
| 7 | 1H | 92 | ILE |
| 7 | 1H | 98 | LEU |
| 7 | 1H | 103 | LEU |
| 7 | 1H | 104 | GLU |
| 7 | 1H | 115 | VAL |
| 7 | 1H | 122 | THR |
| 7 | 1H | 124 | GLU |
| 7 | 1H | 130 | ARG |
| 7 | 1H | 136 | ILE |
| 7 | 1H | 153 | LYS |
| 7 | 1H | 169 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8 | 1I | 15 | VAL |
| 8 | 1I | 20 | ASP |
| 8 | 1I | 38 | LEU |
| 8 | 1I | 47 | LEU |
| 8 | 1I | 52 | ARG |
| 8 | 1I | 54 | GLN |
| 8 | 1I | 75 | LEU |
| 8 | 1I | 77 | LEU |
| 8 | 1I | 81 | VAL |
| 8 | 1I | 87 | LYS |
| 8 | 1I | 92 | VAL |
| 8 | 1I | 93 | THR |
| 8 | 1I | 97 | ILE |
| 8 | 1I | 101 | LEU |
| 8 | 1I | 103 | ARG |
| 8 | 1I | 108 | THR |
| 8 | 1I | 109 | ILE |
| 8 | 1I | 110 | ASP |
| 8 | 1I | 129 | THR |
| 8 | 1I | 144 | VAL |
| 9 | 1N | 1 | MET |
| 9 | 1N | 9 | VAL |
| 9 | 1N | 37 | LYS |
| 9 | 1N | 46 | VAL |
| 9 | 1N | 48 | MET |
| 9 | 1N | 62 | VAL |
| 9 | 1N | 68 | GLU |
| 9 | 1N | 96 | GLU |
| 9 | 1N | 112 | LEU |
| 9 | 1N | 120 | LEU |
| 9 | 1N | 121 | LYS |
| 9 | 1N | 134 | ARG |
| 9 | 1N | 138 | LEU |
| 10 | 1O | 26 | LYS |
| 10 | 1O | 42 | SER |
| 10 | 1O | 47 | ILE |
| 10 | 1O | 69 | ILE |
| 10 | 1O | 113 | LYS |
| 11 | 1P | 1 | MET |
| 11 | 1P | 94 | GLU |
| 11 | 1P | 95 | VAL |
| 11 | 1P | 98 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11 | 1P | 99 | LEU |
| 11 | 1P | 125 | VAL |
| 11 | 1P | 126 | VAL |
| 11 | 1P | 133 | SER |
| 11 | 1P | 148 | LEU |
| 12 | 1Q | 21 | THR |
| 12 | 1Q | 22 | LYS |
| 12 | 1Q | 79 | LEU |
| 12 | 1Q | 94 | VAL |
| 12 | 1Q | 109 | VAL |
| 12 | 1Q | 115 | MET |
| 13 | 1R | 36 | THR |
| 13 | 1R | 67 | LEU |
| 13 | 1R | 114 | VAL |
| 14 | 1S | 8 | GLU |
| 14 | 1S | 25 | ARG |
| 14 | 1S | 35 | ILE |
| 14 | 1S | 69 | VAL |
| 14 | 1S | 73 | LEU |
| 14 | 1S | 85 | VAL |
| 14 | 1S | 110 | LEU |
| 15 | 1T | 23 | ARG |
| 15 | 1T | 36 | GLU |
| 15 | 1T | 82 | LEU |
| 15 | 1T | 85 | LYS |
| 15 | 1T | 96 | ARG |
| 15 | 1T | 128 | GLU |
| 16 | 1U | 5 | LYS |
| 16 | 1U | 8 | VAL |
| 16 | 1U | 9 | VAL |
| 16 | 1U | 27 | LEU |
| 16 | 1U | 31 | SER |
| 16 | 1U | 60 | LEU |
| 16 | 1U | 74 | LEU |
| 16 | 1U | 77 | SER |
| 16 | 1U | 95 | LEU |
| 16 | 1U | 110 | VAL |
| 17 | 1V | 14 | VAL |
| 17 | 1V | 15 | GLU |
| 17 | 1V | 28 | GLU |
| 17 | 1V | 32 | THR |
| 17 | 1V | 45 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 17 | 1V | 61 | VAL |
| 17 | 1V | 71 | LEU |
| 17 | 1V | 79 | VAL |
| 18 | 1W | 4 | LYS |
| 18 | 1W | 6 | ILE |
| 18 | 1W | 11 | ARG |
| 18 | 1W | 85 | VAL |
| 18 | 1W | 92 | ARG |
| 18 | 1W | 96 | ILE |
| 19 | 1X | 68 | ARG |
| 19 | 1X | 88 | LYS |
| 19 | 1X | 92 | LEU |
| 20 | 1Y | 1 | MET |
| 20 | 1Y | 4 | LYS |
| 20 | 1Y | 7 | VAL |
| 20 | 1Y | 21 | LYS |
| 20 | 1Y | 26 | LYS |
| 20 | 1Y | 38 | ILE |
| 20 | 1Y | 49 | VAL |
| 20 | 1Y | 64 | GLU |
| 20 | 1Y | 90 | LEU |
| 20 | 1Y | 91 | GLU |
| 20 | 1Y | 99 | CYS |
| 21 | 1Z | 1 | MET |
| 21 | 1Z | 31 | ARG |
| 21 | 1Z | 42 | VAL |
| 21 | 1Z | 52 | SER |
| 21 | 1Z | 53 | ILE |
| 21 | 1Z | 72 | ARG |
| 21 | 1Z | 94 | GLU |
| 21 | 1Z | 100 | VAL |
| 21 | 1Z | 119 | GLU |
| 21 | 1Z | 124 | ILE |
| 21 | 1Z | 136 | PHE |
| 21 | 1Z | 154 | ASP |
| 21 | 1Z | 162 | GLU |
| 21 | 1Z | 170 | THR |
| 21 | 1Z | 171 | ILE |
| 22 | 10 | 10 | THR |
| 22 | 10 | 27 | GLU |
| 22 | 10 | 49 | LYS |
| 22 | 10 | 81 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 23 | 11 | 13 | ILE |
| 23 | 11 | 35 | THR |
| 23 | 11 | 40 | ARG |
| 23 | 11 | 57 | GLU |
| 23 | 11 | 83 | GLU |
| 24 | 12 | 1 | MET |
| 24 | 12 | 4 | SER |
| 24 | 12 | 19 | VAL |
| 24 | 12 | 30 | ARG |
| 24 | 12 | 40 | SER |
| 24 | 12 | 43 | GLN |
| 24 | 12 | 53 | LEU |
| 25 | 13 | 17 | LYS |
| 25 | 13 | 23 | LEU |
| 25 | 13 | 37 | LEU |
| 25 | 13 | 48 | GLU |
| 25 | 13 | 54 | VAL |
| 26 | 14 | 1 | MET |
| 26 | 14 | 9 | LEU |
| 26 | 14 | 21 | VAL |
| 26 | 14 | 33 | VAL |
| 26 | 14 | 49 | PHE |
| 26 | 14 | 50 | VAL |
| 26 | 14 | 53 | GLU |
| 26 | 14 | 58 | ARG |
| 27 | 15 | 6 | VAL |
| 27 | 15 | 55 | ARG |
| 27 | 15 | 57 | VAL |
| 27 | 15 | 58 | LEU |
| 28 | 16 | 7 | ILE |
| 28 | 16 | 9 | LEU |
| 28 | 16 | 14 | THR |
| 29 | 17 | 1 | MET |
| 29 | 17 | 29 | LYS |
| 29 | 17 | 35 | ARG |
| 29 | 17 | 43 | THR |
| 29 | 17 | 46 | VAL |
| 29 | 17 | 48 | LYS |
| 30 | 18 | 14 | VAL |
| 30 | 18 | 29 | LYS |
| 30 | 18 | 37 | SER |
| 30 | 18 | 39 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 30 | 18 | 46 | ARG |
| 33 | 1b | 7 | VAL |
| 33 | 1b | 10 | LEU |
| 33 | 1b | 12 | GLU |
| 33 | 1b | 16 | HIS |
| 33 | 1b | 27 | LYS |
| 33 | 1b | 39 | ILE |
| 33 | 1b | 41 | ILE |
| 33 | 1b | 45 | GLN |
| 33 | 1b | 54 | THR |
| 33 | 1b | 56 | ARG |
| 33 | 1b | 67 | THR |
| 33 | 1b | 69 | LEU |
| 33 | 1b | 73 | THR |
| 33 | 1b | 80 | ILE |
| 33 | 1b | 83 | MET |
| 33 | 1b | 93 | VAL |
| 33 | 1b | 101 | MET |
| 33 | 1b | 107 | THR |
| 33 | 1b | 108 | ILE |
| 33 | 1b | 127 | ILE |
| 33 | 1b | 128 | GLU |
| 33 | 1b | 142 | LEU |
| 33 | 1b | 154 | LEU |
| 33 | 1b | 156 | LYS |
| 33 | 1b | 158 | LEU |
| 33 | 1b | 160 | ASP |
| 33 | 1b | 185 | ILE |
| 33 | 1b | 189 | ASP |
| 33 | 1b | 197 | VAL |
| 33 | 1b | 208 | ILE |
| 33 | 1b | 224 | GLN |
| 33 | 1b | 229 | VAL |
| 34 | 1c | 3 | ASN |
| 34 | 1c | 8 | ILE |
| 34 | 1c | 15 | THR |
| 34 | 1c | 29 | TYR |
| 34 | 1c | 32 | LEU |
| 34 | 1c | 40 | ARG |
| 34 | 1c | 45 | LYS |
| 34 | 1c | 49 | SER |
| 34 | 1c | 68 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 34 | 1c | 70 | VAL |
| 34 | 1c | 72 | LYS |
| 34 | 1c | 82 | GLU |
| 34 | 1c | 98 | ASN |
| 34 | 1c | 124 | ILE |
| 34 | 1c | 154 | SER |
| 34 | 1c | 165 | THR |
| 34 | 1c | 182 | ILE |
| 34 | 1c | 195 | VAL |
| 35 | 1d | 3 | ARG |
| 35 | 1d | 19 | LEU |
| 35 | 1d | 31 | CYS |
| 35 | 1d | 45 | GLN |
| 35 | 1d | 59 | ARG |
| 35 | 1d | 70 | ILE |
| 35 | 1d | 83 | SER |
| 35 | 1d | 115 | ARG |
| 35 | 1d | 119 | GLN |
| 35 | 1d | 122 | ARG |
| 35 | 1d | 127 | THR |
| 35 | 1d | 134 | ASP |
| 35 | 1d | 135 | LEU |
| 35 | 1d | 140 | VAL |
| 35 | 1d | 157 | LEU |
| 35 | 1d | 158 | ILE |
| 35 | 1d | 174 | LEU |
| 35 | 1d | 175 | SER |
| 35 | 1d | 177 | ASP |
| 35 | 1d | 178 | VAL |
| 35 | 1d | 188 | LEU |
| 35 | 1d | 190 | ASP |
| 35 | 1d | 193 | ASP |
| 35 | 1d | 194 | LEU |
| 35 | 1d | 208 | SER |
| 36 | 1e | 8 | GLU |
| 36 | 1e | 12 | LEU |
| 36 | 1e | 24 | ARG |
| 36 | 1e | 41 | VAL |
| 36 | 1e | 51 | VAL |
| 36 | 1e | 53 | LEU |
| 36 | 1e | 63 | ARG |
| 36 | 1e | 67 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 36 | 1e | 79 | GLU |
| 36 | 1e | 131 | ILE |
| 37 | 1f | 1 | MET |
| 37 | 1f | 10 | LEU |
| 37 | 1f | 19 | LEU |
| 37 | 1f | 39 | LYS |
| 37 | 1f | 45 | LEU |
| 37 | 1f | 54 | LYS |
| 37 | 1f | 77 | ARG |
| 38 | 1g | 6 | ARG |
| 38 | 1g | 9 | VAL |
| 38 | 1g | 12 | LEU |
| 38 | 1g | 22 | LEU |
| 38 | 1g | 23 | VAL |
| 38 | 1g | 31 | MET |
| 38 | 1g | 32 | ARG |
| 38 | 1g | 50 | ILE |
| 38 | 1g | 57 | GLU |
| 38 | 1g | 59 | LEU |
| 38 | 1g | 61 | VAL |
| 38 | 1g | 63 | LYS |
| 38 | 1g | 80 | VAL |
| 38 | 1g | 90 | GLU |
| 38 | 1g | 91 | VAL |
| 38 | 1g | 98 | SER |
| 38 | 1g | 99 | LEU |
| 38 | 1g | 104 | LEU |
| 38 | 1g | 110 | GLN |
| 38 | 1g | 114 | ARG |
| 39 | 1h | 25 | ASP |
| 39 | 1h | 35 | ILE |
| 39 | 1h | 51 | VAL |
| 39 | 1h | 100 | ILE |
| 39 | 1h | 107 | LEU |
| 39 | 1h | 133 | LEU |
| 40 | 1i | 3 | GLN |
| 40 | 1i | 23 | ASN |
| 40 | 1i | 77 | ILE |
| 40 | 1i | 81 | ILE |
| 40 | 1i | 86 | VAL |
| 40 | 1i | 88 | TYR |
| 40 | 1i | 96 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 40 | 1i | 103 | THR |
| 40 | 1i | 108 | VAL |
| 40 | 1i | 111 | ARG |
| 40 | 1i | 128 | ARG |
| 41 | 1j | 8 | LEU |
| 41 | 1j | 9 | ARG |
| 41 | 1j | 13 | HIS |
| 41 | 1j | 23 | ILE |
| 41 | 1j | 42 | THR |
| 41 | 1j | 43 | ARG |
| 41 | 1j | 49 | VAL |
| 41 | 1j | 51 | ARG |
| 41 | 1j | 66 | ARG |
| 41 | 1j | 81 | THR |
| 41 | 1j | 98 | ILE |
| 42 | 1k | 33 | THR |
| 42 | 1k | 48 | ILE |
| 42 | 1k | 83 | ILE |
| 42 | 1k | 84 | VAL |
| 42 | 1k | 87 | THR |
| 42 | 1k | 91 | ARG |
| 42 | 1k | 104 | GLN |
| 42 | 1k | 107 | SER |
| 42 | 1k | 109 | VAL |
| 42 | 1k | 114 | VAL |
| 42 | 1k | 120 | ARG |
| 42 | 1k | 126 | ARG |
| 43 | 1l | 11 | VAL |
| 43 | 1l | 89 | ARG |
| 44 | 1m | 3 | ARG |
| 44 | 1m | 4 | ILE |
| 44 | 1m | 15 | VAL |
| 44 | 1m | 39 | ILE |
| 44 | 1m | 43 | THR |
| 44 | 1m | 45 | VAL |
| 44 | 1m | 64 | TRP |
| 44 | 1m | 67 | GLU |
| 44 | 1m | 70 | LEU |
| 44 | 1m | 73 | GLU |
| 44 | 1m | 109 | THR |
| 44 | 1m | 117 | VAL |
| 44 | 1m | 121 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 44 | 1m | 126 | LYS |
| 45 | 1n | 18 | VAL |
| 45 | 1n | 33 | VAL |
| 45 | 1n | 35 | ARG |
| 45 | 1n | 53 | LEU |
| 45 | 1n | 60 | SER |
| 46 | 1o | 3 | ILE |
| 46 | 1o | 27 | VAL |
| 46 | 1o | 34 | LEU |
| 46 | 1o | 76 | GLU |
| 46 | 1o | 87 | ILE |
| 47 | 1p | 20 | VAL |
| 47 | 1p | 27 | LYS |
| 47 | 1p | 33 | ILE |
| 47 | 1p | 42 | ARG |
| 47 | 1p | 45 | THR |
| 47 | 1p | 61 | SER |
| 47 | 1p | 62 | VAL |
| 47 | 1p | 67 | THR |
| 47 | 1p | 72 | ARG |
| 47 | 1p | 76 | GLN |
| 48 | 1q | 5 | VAL |
| 48 | 1q | 19 | VAL |
| 48 | 1q | 48 | GLU |
| 48 | 1q | 53 | LEU |
| 48 | 1q | 62 | SER |
| 48 | 1q | 63 | ARG |
| 48 | 1q | 79 | SER |
| 49 | 1r | 26 | LEU |
| 49 | 1r | 46 | GLU |
| 49 | 1r | 54 | ARG |
| 49 | 1r | 66 | LEU |
| 49 | 1r | 75 | ILE |
| 49 | 1r | 78 | LEU |
| 49 | 1r | 82 | THR |
| 49 | 1r | 86 | VAL |
| 50 | 1s | 4 | SER |
| 50 | 1s | 5 | LEU |
| 50 | 1s | 12 | ASP |
| 50 | 1s | 17 | GLU |
| 50 | 1s | 28 | LYS |
| 50 | 1s | 40 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 50 | 1s | 41 | VAL |
| 50 | 1s | 45 | VAL |
| 50 | 1s | 67 | VAL |
| 51 | 1t | 8 | ARG |
| 51 | 1t | 10 | LEU |
| 51 | 1t | 11 | SER |
| 51 | 1t | 24 | LEU |
| 51 | 1t | 37 | SER |
| 51 | 1t | 62 | LEU |
| 51 | 1t | 70 | SER |
| 51 | 1t | 90 | GLN |
| 51 | 1t | 91 | LEU |
| 52 | 1u | 9 | ARG |
| 52 | 1u | 20 | LYS |
| 57 | 1z | 2 | LYS |
| 57 | 1z | 4 | SER |
| 57 | 1z | 13 | ARG |
| 57 | 1z | 17 | ARG |
| 3 | 2D | 10 | THR |
| 3 | 2D | 12 | SER |
| 3 | 2D | 24 | ILE |
| 3 | 2D | 38 | LYS |
| 3 | 2D | 98 | VAL |
| 3 | 2D | 113 | VAL |
| 3 | 2D | 117 | VAL |
| 3 | 2D | 126 | GLN |
| 3 | 2D | 142 | VAL |
| 3 | 2D | 162 | SER |
| 3 | 2D | 173 | VAL |
| 3 | 2D | 183 | ARG |
| 3 | 2D | 229 | VAL |
| 3 | 2D | 242 | ARG |
| 3 | 2D | 259 | THR |
| 3 | 2D | 270 | ILE |
| 3 | 2D | 275 | LYS |
| 4 | 2E | 7 | VAL |
| 4 | 2E | 8 | LYS |
| 4 | 2E | 12 | THR |
| 4 | 2E | 21 | VAL |
| 4 | 2E | 27 | LEU |
| 4 | 2E | 38 | THR |
| 4 | 2E | 41 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | 2E | 73 | GLU |
| 4 | 2E | 95 | ILE |
| 4 | 2E | 116 | VAL |
| 4 | 2E | 117 | MET |
| 4 | 2E | 134 | ILE |
| 4 | 2E | 145 | LYS |
| 4 | 2E | 188 | VAL |
| 5 | 2F | 12 | LEU |
| 5 | 2F | 17 | ARG |
| 5 | 2F | 28 | ILE |
| 5 | 2F | 53 | THR |
| 5 | 2F | 57 | VAL |
| 5 | 2F | 70 | THR |
| 5 | 2F | 74 | ARG |
| 5 | 2F | 126 | VAL |
| 5 | 2F | 157 | VAL |
| 5 | 2F | 162 | LEU |
| 5 | 2F | 179 | GLU |
| 5 | 2F | 192 | LEU |
| 6 | 2G | 5 | VAL |
| 6 | 2G | 28 | VAL |
| 6 | 2G | 43 | LEU |
| 6 | 2G | 45 | GLU |
| 6 | 2G | 49 | ASP |
| 6 | 2G | 53 | LEU |
| 6 | 2G | 86 | MET |
| 6 | 2G | 91 | ARG |
| 6 | 2G | 107 | LEU |
| 6 | 2G | 109 | VAL |
| 6 | 2G | 111 | LEU |
| 6 | 2G | 113 | ARG |
| 6 | 2G | 124 | SER |
| 6 | 2G | 126 | ASP |
| 6 | 2G | 130 | ASN |
| 6 | 2G | 140 | ILE |
| 6 | 2G | 146 | TYR |
| 6 | 2G | 165 | THR |
| 7 | 2H | 7 | LEU |
| 7 | 2H | 9 | ILE |
| 7 | 2H | 15 | VAL |
| 7 | 2H | 17 | VAL |
| 7 | 2H | 24 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7 | 2H | 26 | VAL |
| 7 | 2H | 27 | LYS |
| 7 | 2H | 37 | VAL |
| 7 | 2H | 38 | SER |
| 7 | 2H | 40 | GLU |
| 7 | 2H | 63 | SER |
| 7 | 2H | 70 | THR |
| 7 | 2H | 76 | VAL |
| 7 | 2H | 95 | ARG |
| 7 | 2H | 98 | LEU |
| 7 | 2H | 103 | LEU |
| 7 | 2H | 113 | VAL |
| 7 | 2H | 114 | VAL |
| 7 | 2H | 125 | VAL |
| 7 | 2H | 129 | THR |
| 7 | 2H | 136 | ILE |
| 7 | 2H | 149 | ARG |
| 8 | 2I | 6 | LEU |
| 8 | 2I | 15 | VAL |
| 8 | 2I | 18 | VAL |
| 8 | 2I | 20 | ASP |
| 8 | 2I | 38 | LEU |
| 8 | 2I | 41 | GLU |
| 8 | 2I | 43 | ASN |
| 8 | 2I | 44 | LEU |
| 8 | 2I | 58 | LEU |
| 8 | 2I | 68 | LEU |
| 8 | 2I | 72 | LEU |
| 8 | 2I | 77 | LEU |
| 8 | 2I | 82 | ARG |
| 8 | 2I | 85 | GLU |
| 8 | 2I | 87 | LYS |
| 8 | 2I | 92 | VAL |
| 8 | 2I | 108 | THR |
| 8 | 2I | 117 | GLU |
| 8 | 2I | 121 | LYS |
| 8 | 2I | 127 | VAL |
| 9 | 2N | 1 | MET |
| 9 | 2N | 9 | VAL |
| 9 | 2N | 10 | GLU |
| 9 | 2N | 25 | ARG |
| 9 | 2N | 38 | HIS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9 | 2N | 55 | VAL |
| 9 | 2N | 58 | ASP |
| 9 | 2N | 60 | ILE |
| 9 | 2N | 62 | VAL |
| 9 | 2N | 65 | LYS |
| 9 | 2N | 73 | THR |
| 10 | 2O | 13 | ASN |
| 10 | 2O | 28 | SER |
| 10 | 2O | 66 | LYS |
| 10 | 2O | 69 | ILE |
| 10 | 2O | 78 | ARG |
| 10 | 2O | 102 | VAL |
| 10 | 2O | 113 | LYS |
| 11 | 2P | 56 | SER |
| 11 | 2P | 65 | ARG |
| 11 | 2P | 71 | VAL |
| 11 | 2P | 75 | ILE |
| 11 | 2P | 90 | ARG |
| 11 | 2P | 95 | VAL |
| 11 | 2P | 126 | VAL |
| 11 | 2P | 133 | SER |
| 11 | 2P | 148 | LEU |
| 12 | 2Q | 7 | MET |
| 12 | 2Q | 10 | ARG |
| 12 | 2Q | 17 | LEU |
| 12 | 2Q | 22 | LYS |
| 12 | 2Q | 127 | ILE |
| 13 | 2R | 6 | SER |
| 13 | 2R | 15 | SER |
| 13 | 2R | 20 | LEU |
| 13 | 2R | 36 | THR |
| 13 | 2R | 102 | GLU |
| 13 | 2R | 111 | LEU |
| 13 | 2R | 114 | VAL |
| 14 | 2S | 15 | ARG |
| 14 | 2S | 17 | ARG |
| 14 | 2S | 21 | THR |
| 14 | 2S | 30 | ARG |
| 14 | 2S | 36 | TYR |
| 14 | 2S | 44 | LYS |
| 14 | 2S | 50 | SER |
| 14 | 2S | 58 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 14 | 2S | 63 | THR |
| 14 | 2S | 64 | GLU |
| 14 | 2S | 65 | VAL |
| 14 | 2S | 83 | LYS |
| 14 | 2S | 93 | LYS |
| 14 | 2S | 103 | GLU |
| 14 | 2S | 110 | LEU |
| 15 | 2T | 1 | MET |
| 15 | 2T | 10 | VAL |
| 15 | 2T | 28 | VAL |
| 15 | 2T | 40 | THR |
| 15 | 2T | 63 | VAL |
| 15 | 2T | 67 | SER |
| 15 | 2T | 87 | ASP |
| 15 | 2T | 107 | ASP |
| 15 | 2T | 115 | ARG |
| 16 | 2U | 5 | LYS |
| 16 | 2U | 8 | VAL |
| 16 | 2U | 62 | ILE |
| 16 | 2U | 70 | ARG |
| 16 | 2U | 74 | LEU |
| 16 | 2U | 95 | LEU |
| 16 | 2U | 111 | GLU |
| 17 | 2V | 15 | GLU |
| 17 | 2V | 33 | VAL |
| 17 | 2V | 38 | LEU |
| 17 | 2V | 53 | GLU |
| 17 | 2V | 57 | VAL |
| 17 | 2V | 61 | VAL |
| 17 | 2V | 72 | VAL |
| 17 | 2V | 79 | VAL |
| 18 | 2W | 11 | ARG |
| 18 | 2W | 15 | ARG |
| 18 | 2W | 17 | VAL |
| 18 | 2W | 60 | ASN |
| 18 | 2W | 90 | ARG |
| 18 | 2W | 92 | ARG |
| 18 | 2W | 96 | ILE |
| 18 | 2W | 106 | ILE |
| 19 | 2X | 30 | VAL |
| 19 | 2X | 72 | LYS |
| 19 | 2X | 81 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 19 | 2X | 88 | LYS |
| 19 | 2X | 92 | LEU |
| 20 | 2Y | 3 | VAL |
| 20 | 2Y | 7 | VAL |
| 20 | 2Y | 9 | LYS |
| 20 | 2Y | 21 | LYS |
| 20 | 2Y | 39 | VAL |
| 20 | 2Y | 50 | ARG |
| 20 | 2Y | 64 | GLU |
| 20 | 2Y | 85 | VAL |
| 20 | 2Y | 90 | LEU |
| 20 | 2Y | 96 | ILE |
| 20 | 2Y | 99 | CYS |
| 20 | 2Y | 106 | LEU |
| 21 | 2Z | 6 | LYS |
| 21 | 2Z | 16 | SER |
| 21 | 2Z | 19 | ARG |
| 21 | 2Z | 28 | MET |
| 21 | 2Z | 32 | HIS |
| 21 | 2Z | 33 | LEU |
| 21 | 2Z | 36 | LYS |
| 21 | 2Z | 41 | LEU |
| 21 | 2Z | 42 | VAL |
| 21 | 2Z | 53 | ILE |
| 21 | 2Z | 58 | VAL |
| 21 | 2Z | 63 | ASP |
| 21 | 2Z | 76 | LEU |
| 21 | 2Z | 90 | VAL |
| 21 | 2Z | 91 | LEU |
| 21 | 2Z | 100 | VAL |
| 21 | 2Z | 102 | LEU |
| 21 | 2Z | 126 | VAL |
| 21 | 2Z | 128 | VAL |
| 21 | 2Z | 129 | SER |
| 21 | 2Z | 131 | ARG |
| 21 | 2Z | 137 | ILE |
| 21 | 2Z | 139 | VAL |
| 21 | 2Z | 144 | LEU |
| 21 | 2Z | 154 | ASP |
| 21 | 2Z | 171 | ILE |
| 21 | 2Z | 174 | VAL |
| 22 | 20 | 9 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 22 | 20 | 11 | ARG |
| 22 | 20 | 79 | VAL |
| 23 | 21 | 26 | ARG |
| 23 | 21 | 35 | THR |
| 23 | 21 | 40 | ARG |
| 23 | 21 | 83 | GLU |
| 23 | 21 | 85 | LEU |
| 23 | 21 | 92 | LYS |
| 24 | 22 | 19 | VAL |
| 24 | 22 | 38 | GLN |
| 24 | 22 | 53 | LEU |
| 24 | 22 | 70 | GLN |
| 25 | 23 | 31 | LEU |
| 25 | 23 | 37 | LEU |
| 25 | 23 | 57 | GLU |
| 25 | 23 | 59 | VAL |
| 26 | 24 | 13 | ARG |
| 26 | 24 | 26 | SER |
| 26 | 24 | 27 | THR |
| 26 | 24 | 31 | ILE |
| 26 | 24 | 33 | VAL |
| 26 | 24 | 34 | GLU |
| 26 | 24 | 37 | SER |
| 26 | 24 | 49 | PHE |
| 26 | 24 | 59 | PHE |
| 26 | 24 | 60 | GLN |
| 27 | 25 | 6 | VAL |
| 27 | 25 | 55 | ARG |
| 28 | 26 | 7 | ILE |
| 28 | 26 | 9 | LEU |
| 28 | 26 | 13 | CYS |
| 28 | 26 | 14 | THR |
| 28 | 26 | 32 | ASN |
| 28 | 26 | 48 | VAL |
| 29 | 27 | 41 | ARG |
| 29 | 27 | 43 | THR |
| 29 | 27 | 46 | VAL |
| 29 | 27 | 48 | LYS |
| 30 | 28 | 11 | LYS |
| 30 | 28 | 14 | VAL |
| 30 | 28 | 15 | LYS |
| 30 | 28 | 29 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 30 | 28 | 41 | ILE |
| 30 | 28 | 49 | VAL |
| 30 | 28 | 50 | LEU |
| 31 | 29 | 18 | ARG |
| 31 | 29 | 19 | ARG |
| 31 | 29 | 28 | GLU |
| 33 | 2b | 8 | LYS |
| 33 | 2b | 11 | LEU |
| 33 | 2b | 15 | VAL |
| 33 | 2b | 16 | HIS |
| 33 | 2b | 30 | ARG |
| 33 | 2b | 39 | ILE |
| 33 | 2b | 45 | GLN |
| 33 | 2b | 48 | MET |
| 33 | 2b | 49 | GLU |
| 33 | 2b | 58 | ILE |
| 33 | 2b | 67 | THR |
| 33 | 2b | 76 | GLN |
| 33 | 2b | 80 | ILE |
| 33 | 2b | 93 | VAL |
| 33 | 2b | 111 | ARG |
| 33 | 2b | 112 | VAL |
| 33 | 2b | 115 | LEU |
| 33 | 2b | 117 | GLU |
| 33 | 2b | 150 | SER |
| 33 | 2b | 168 | THR |
| 33 | 2b | 178 | ARG |
| 33 | 2b | 185 | ILE |
| 33 | 2b | 189 | ASP |
| 33 | 2b | 190 | THR |
| 33 | 2b | 198 | ASP |
| 33 | 2b | 208 | ILE |
| 33 | 2b | 215 | LEU |
| 33 | 2b | 221 | LEU |
| 33 | 2b | 223 | ILE |
| 33 | 2b | 230 | VAL |
| 34 | 2c | 4 | LYS |
| 34 | 2c | 15 | THR |
| 34 | 2c | 16 | ARG |
| 34 | 2c | 18 | TRP |
| 34 | 2c | 19 | GLU |
| 34 | 2c | 28 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 34 | 2c | 34 | LEU |
| 34 | 2c | 43 | LEU |
| 34 | 2c | 45 | LYS |
| 34 | 2c | 55 | VAL |
| 34 | 2c | 57 | ILE |
| 34 | 2c | 68 | VAL |
| 34 | 2c | 77 | ILE |
| 34 | 2c | 91 | LEU |
| 34 | 2c | 101 | LEU |
| 34 | 2c | 102 | ASN |
| 34 | 2c | 118 | GLN |
| 34 | 2c | 141 | VAL |
| 34 | 2c | 152 | ILE |
| 34 | 2c | 154 | SER |
| 34 | 2c | 175 | LEU |
| 34 | 2c | 182 | ILE |
| 34 | 2c | 188 | LEU |
| 34 | 2c | 190 | ARG |
| 34 | 2c | 192 | THR |
| 34 | 2c | 198 | VAL |
| 34 | 2c | 202 | ILE |
| 34 | 2c | 206 | GLU |
| 35 | 2d | 3 | ARG |
| 35 | 2d | 8 | VAL |
| 35 | 2d | 17 | VAL |
| 35 | 2d | 19 | LEU |
| 35 | 2d | 47 | ARG |
| 35 | 2d | 49 | ARG |
| 35 | 2d | 52 | SER |
| 35 | 2d | 53 | ASP |
| 35 | 2d | 58 | LEU |
| 35 | 2d | 59 | ARG |
| 35 | 2d | 78 | LEU |
| 35 | 2d | 85 | LYS |
| 35 | 2d | 86 | LYS |
| 35 | 2d | 94 | LEU |
| 35 | 2d | 106 | TYR |
| 35 | 2d | 135 | LEU |
| 35 | 2d | 141 | ARG |
| 35 | 2d | 150 | GLU |
| 35 | 2d | 157 | LEU |
| 35 | 2d | 162 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 35 | 2d | 175 | SER |
| 35 | 2d | 178 | VAL |
| 35 | 2d | 182 | LYS |
| 35 | 2d | 188 | LEU |
| 36 | 2e | 6 | PHE |
| 36 | 2e | 9 | LYS |
| 36 | 2e | 11 | ILE |
| 36 | 2e | 12 | LEU |
| 36 | 2e | 13 | ILE |
| 36 | 2e | 18 | ARG |
| 36 | 2e | 24 | ARG |
| 36 | 2e | 40 | ARG |
| 36 | 2e | 41 | VAL |
| 36 | 2e | 51 | VAL |
| 36 | 2e | 53 | LEU |
| 36 | 2e | 55 | VAL |
| 36 | 2e | 80 | ILE |
| 36 | 2e | 120 | THR |
| 36 | 2e | 126 | ARG |
| 36 | 2e | 142 | LEU |
| 36 | 2e | 147 | ASP |
| 36 | 2e | 148 | VAL |
| 36 | 2e | 152 | ARG |
| 37 | 2f | 9 | VAL |
| 37 | 2f | 10 | LEU |
| 37 | 2f | 23 | LYS |
| 37 | 2f | 31 | GLU |
| 37 | 2f | 37 | VAL |
| 37 | 2f | 63 | TYR |
| 37 | 2f | 69 | GLU |
| 37 | 2f | 70 | ASP |
| 37 | 2f | 75 | LEU |
| 37 | 2f | 81 | ILE |
| 37 | 2f | 93 | SER |
| 37 | 2f | 95 | GLU |
| 38 | 2g | 9 | VAL |
| 38 | 2g | 10 | ARG |
| 38 | 2g | 23 | VAL |
| 38 | 2g | 37 | ASN |
| 38 | 2g | 49 | ILE |
| 38 | 2g | 75 | VAL |
| 38 | 2g | 78 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 38 | 2g | 79 | ARG |
| 38 | 2g | 85 | TYR |
| 38 | 2g | 90 | GLU |
| 38 | 2g | 91 | VAL |
| 38 | 2g | 113 | GLU |
| 38 | 2g | 146 | GLU |
| 38 | 2g | 154 | TYR |
| 39 | 2h | 17 | THR |
| 39 | 2h | 23 | SER |
| 39 | 2h | 26 | VAL |
| 39 | 2h | 29 | SER |
| 39 | 2h | 37 | ARG |
| 39 | 2h | 42 | GLU |
| 39 | 2h | 45 | ILE |
| 39 | 2h | 48 | TYR |
| 39 | 2h | 51 | VAL |
| 39 | 2h | 52 | ASP |
| 39 | 2h | 107 | LEU |
| 39 | 2h | 120 | THR |
| 39 | 2h | 133 | LEU |
| 40 | 2i | 7 | THR |
| 40 | 2i | 29 | ASN |
| 40 | 2i | 38 | GLN |
| 40 | 2i | 51 | ARG |
| 40 | 2i | 63 | ILE |
| 40 | 2i | 64 | THR |
| 40 | 2i | 65 | VAL |
| 40 | 2i | 89 | ASN |
| 40 | 2i | 102 | LEU |
| 40 | 2i | 110 | GLU |
| 40 | 2i | 128 | ARG |
| 41 | 2j | 15 | THR |
| 41 | 2j | 21 | GLN |
| 41 | 2j | 23 | ILE |
| 41 | 2j | 34 | VAL |
| 41 | 2j | 38 | ILE |
| 41 | 2j | 46 | ARG |
| 41 | 2j | 67 | THR |
| 41 | 2j | 72 | VAL |
| 41 | 2j | 81 | THR |
| 41 | 2j | 85 | LEU |
| 41 | 2j | 89 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 41 | 2j | 94 | VAL |
| 41 | 2j | 95 | GLU |
| 41 | 2j | 100 | THR |
| 42 | 2k | 14 | VAL |
| 42 | 2k | 66 | LEU |
| 42 | 2k | 84 | VAL |
| 42 | 2k | 87 | THR |
| 42 | 2k | 105 | VAL |
| 42 | 2k | 117 | ASN |
| 43 | 2l | 18 | VAL |
| 43 | 2l | 24 | VAL |
| 43 | 2l | 36 | VAL |
| 43 | 2l | 42 | THR |
| 43 | 2l | 57 | LYS |
| 43 | 2l | 82 | VAL |
| 44 | 2m | 4 | ILE |
| 44 | 2m | 15 | VAL |
| 44 | 2m | 19 | LEU |
| 44 | 2m | 47 | ASP |
| 44 | 2m | 48 | LEU |
| 44 | 2m | 90 | LEU |
| 44 | 2m | 92 | HIS |
| 44 | 2m | 98 | VAL |
| 44 | 2m | 102 | ARG |
| 44 | 2m | 103 | THR |
| 44 | 2m | 108 | ARG |
| 45 | 2n | 3 | ARG |
| 45 | 2n | 9 | LYS |
| 45 | 2n | 17 | LYS |
| 45 | 2n | 18 | VAL |
| 45 | 2n | 33 | VAL |
| 45 | 2n | 46 | GLU |
| 45 | 2n | 53 | LEU |
| 45 | 2n | 60 | SER |
| 46 | 2o | 3 | ILE |
| 46 | 2o | 14 | GLU |
| 46 | 2o | 38 | ARG |
| 46 | 2o | 76 | GLU |
| 46 | 2o | 87 | ILE |
| 47 | 2p | 1 | MET |
| 47 | 2p | 2 | VAL |
| 47 | 2p | 4 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 47 | 2p | 20 | VAL |
| 47 | 2p | 45 | THR |
| 47 | 2p | 54 | GLU |
| 47 | 2p | 60 | LEU |
| 47 | 2p | 62 | VAL |
| 47 | 2p | 69 | THR |
| 47 | 2p | 72 | ARG |
| 47 | 2p | 74 | LEU |
| 48 | 2q | 5 | VAL |
| 48 | 2q | 36 | ILE |
| 48 | 2q | 52 | LYS |
| 48 | 2q | 53 | LEU |
| 48 | 2q | 56 | VAL |
| 48 | 2q | 60 | ILE |
| 48 | 2q | 63 | ARG |
| 48 | 2q | 99 | SER |
| 49 | 2r | 21 | LYS |
| 49 | 2r | 26 | LEU |
| 49 | 2r | 37 | VAL |
| 49 | 2r | 47 | THR |
| 49 | 2r | 68 | LYS |
| 49 | 2r | 69 | THR |
| 49 | 2r | 82 | THR |
| 50 | 2s | 6 | LYS |
| 50 | 2s | 12 | ASP |
| 50 | 2s | 17 | GLU |
| 50 | 2s | 21 | GLU |
| 50 | 2s | 22 | LEU |
| 50 | 2s | 33 | THR |
| 50 | 2s | 43 | GLU |
| 50 | 2s | 44 | MET |
| 50 | 2s | 51 | VAL |
| 50 | 2s | 58 | VAL |
| 50 | 2s | 67 | VAL |
| 50 | 2s | 77 | THR |
| 50 | 2s | 81 | ARG |
| 51 | 2t | 9 | ASN |
| 51 | 2t | 37 | SER |
| 51 | 2t | 41 | ILE |
| 52 | 2u | 15 | ARG |
| 57 | 2z | 1 | SER |
| 57 | 2z | 2 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 57 | 2z | 10 | LYS |
| 57 | 2z | 13 | ARG |
| 57 | 2z | 17 | ARG |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (150) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | 1D | 87 | ASN |
| 4 | 1E | 143 | ASN |
| 4 | 1E | 180 | ASN |
| 5 | 1F | 8 | GLN |
| 5 | 1F | 69 | HIS |
| 5 | 1F | 133 | ASN |
| 5 | 1F | 204 | ASN |
| 6 | 1G | 26 | GLN |
| 6 | 1G | 123 | ASN |
| 7 | 1H | 158 | HIS |
| 8 | 1I | 11 | ASN |
| 8 | 1I | 28 | ASN |
| 8 | 1I | 133 | HIS |
| 9 | 1N | 94 | HIS |
| 12 | 1Q | 12 | GLN |
| 12 | 1Q | 57 | HIS |
| 13 | 1R | 31 | HIS |
| 13 | 1R | 71 | GLN |
| 14 | 1S | 68 | GLN |
| 16 | 1U | 81 | HIS |
| 16 | 1U | 94 | ASN |
| 19 | 1X | 31 | HIS |
| 19 | 1X | 82 | GLN |
| 20 | 1Y | 6 | HIS |
| 21 | 1Z | 34 | ASN |
| 21 | 1Z | 54 | HIS |
| 21 | 1Z | 73 | GLN |
| 21 | 1Z | 75 | ASN |
| 21 | 1Z | 151 | HIS |
| 22 | 10 | 3 | HIS |
| 25 | 13 | 32 | GLN |
| 27 | 15 | 4 | HIS |
| 28 | 16 | 26 | ASN |
| 30 | 18 | 35 | GLN |
| 31 | 19 | 20 | HIS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 31 | 19 | 34 | GLN |
| 33 | 1b | 40 | HIS |
| 33 | 1b | 78 | GLN |
| 33 | 1b | 110 | GLN |
| 33 | 1b | 212 | GLN |
| 34 | 1c | 6 | HIS |
| 34 | 1c | 37 | GLN |
| 34 | 1c | 104 | GLN |
| 34 | 1c | 118 | GLN |
| 34 | 1c | 162 | GLN |
| 34 | 1c | 181 | ASN |
| 35 | 1d | 77 | ASN |
| 35 | 1d | 116 | GLN |
| 35 | 1d | 201 | GLN |
| 36 | 1e | 78 | HIS |
| 37 | 1f | 73 | ASN |
| 38 | 1g | 13 | GLN |
| 38 | 1g | 28 | ASN |
| 39 | 1h | 82 | HIS |
| 40 | 1i | 3 | GLN |
| 40 | 1i | 23 | ASN |
| 40 | 1i | 31 | GLN |
| 40 | 1i | 34 | ASN |
| 40 | 1i | 89 | ASN |
| 41 | 1j | 56 | HIS |
| 41 | 1j | 62 | HIS |
| 43 | 1l | 80 | HIS |
| 43 | 1l | 99 | HIS |
| 44 | 1m | 77 | ASN |
| 46 | 1o | 9 | GLN |
| 46 | 1o | 46 | HIS |
| 46 | 1o | 50 | HIS |
| 49 | 1r | 63 | GLN |
| 50 | 1s | 23 | ASN |
| 50 | 1s | 47 | HIS |
| 50 | 1s | 83 | HIS |
| 51 | 1t | 73 | HIS |
| 51 | 1t | 75 | ASN |
| 51 | 1t | 90 | GLN |
| 3 | 2D | 87 | ASN |
| 4 | 2E | 143 | ASN |
| 5 | 2F | 40 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5 | 2F | 69 | HIS |
| 5 | 2F | 75 | HIS |
| 6 | 2G | 27 | ASN |
| 8 | 2I | 104 | GLN |
| 8 | 2I | 133 | HIS |
| 10 | 2O | 3 | GLN |
| 10 | 2O | 5 | GLN |
| 12 | 2Q | 12 | GLN |
| 12 | 2Q | 57 | HIS |
| 12 | 2Q | 123 | HIS |
| 13 | 2R | 50 | HIS |
| 13 | 2R | 61 | HIS |
| 14 | 2S | 38 | GLN |
| 15 | 2T | 123 | GLN |
| 16 | 2U | 94 | ASN |
| 18 | 2W | 60 | ASN |
| 19 | 2X | 31 | HIS |
| 19 | 2X | 82 | GLN |
| 21 | 2Z | 34 | ASN |
| 21 | 2Z | 54 | HIS |
| 21 | 2Z | 55 | HIS |
| 21 | 2Z | 73 | GLN |
| 21 | 2Z | 121 | HIS |
| 22 | 20 | 35 | ASN |
| 24 | 22 | 9 | GLN |
| 25 | 23 | 32 | GLN |
| 26 | 24 | 40 | HIS |
| 26 | 24 | 46 | GLN |
| 30 | 28 | 35 | GLN |
| 30 | 28 | 43 | GLN |
| 33 | 2b | 37 | ASN |
| 33 | 2b | 45 | GLN |
| 33 | 2b | 76 | GLN |
| 33 | 2b | 78 | GLN |
| 33 | 2b | 94 | ASN |
| 33 | 2b | 95 | GLN |
| 33 | 2b | 135 | GLN |
| 33 | 2b | 146 | GLN |
| 34 | 2c | 6 | HIS |
| 34 | 2c | 102 | ASN |
| 34 | 2c | 162 | GLN |
| 34 | 2c | 181 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 35 | 2d | 77 | ASN |
| 35 | 2d | 116 | GLN |
| 35 | 2d | 119 | GLN |
| 35 | 2d | 125 | HIS |
| 35 | 2d | 201 | GLN |
| 37 | 2f | 11 | ASN |
| 37 | 2f | 100 | ASN |
| 38 | 2g | 37 | ASN |
| 38 | 2g | 86 | GLN |
| 40 | 2i | 3 | GLN |
| 41 | 2j | 13 | HIS |
| 41 | 2j | 33 | GLN |
| 41 | 2j | 62 | HIS |
| 42 | 2k | 22 | HIS |
| 42 | 2k | 104 | GLN |
| 42 | 2k | 116 | HIS |
| 43 | 2l | 99 | HIS |
| 44 | 2m | 40 | ASN |
| 44 | 2m | 62 | ASN |
| 44 | 2m | 92 | HIS |
| 45 | 2n | 49 | HIS |
| 47 | 2p | 13 | HIS |
| 47 | 2p | 16 | HIS |
| 48 | 2q | 93 | GLN |
| 49 | 2r | 63 | GLN |
| 50 | 2s | 14 | HIS |
| 50 | 2s | 47 | HIS |
| 50 | 2s | 69 | HIS |
| 50 | 2s | 83 | HIS |
| 51 | 2t | 18 | GLN |
| 51 | 2t | 75 | ASN |

5.3.3 RNA ⓘ

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1 | 1A | 2864/2915 (98%) | 477 (16%) | 35 (1%) |
| 1 | 2A | 2791/2915 (95%) | 482 (17%) | 30 (1%) |
| 2 | 1B | 119/121 (98%) | 12 (10%) | 0 |
| 2 | 2B | 118/121 (97%) | 19 (16%) | 0 |
| 32 | 1a | 1497/1521 (98%) | 237 (15%) | 0 |
| 32 | 2a | 1501/1521 (98%) | 263 (17%) | 0 |

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| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 53 | 1v | 12/24 (50%) | 3 (25%) | 0 |
| 53 | 2v | 12/24 (50%) | 1 (8%) | 0 |
| 54 | 1w | 72/76 (94%) | 16 (22%) | 0 |
| 54 | 2w | 68/76 (89%) | 22 (32%) | 0 |
| 55 | 1x | 75/77 (97%) | 11 (14%) | 0 |
| 55 | 2x | 75/77 (97%) | 11 (14%) | 0 |
| 56 | 1y | 72/76 (94%) | 25 (34%) | 0 |
| 56 | 2y | 70/76 (92%) | 29 (41%) | 0 |
| All | All | 9346/9620 (97%) | 1608 (17%) | 65 (0%) |

All (1608) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 1 | 1A | 11 | G |
| 1 | 1A | 34 | C |
| 1 | 1A | 45 | C |
| 1 | 1A | 58 | G |
| 1 | 1A | 69 | C |
| 1 | 1A | 71 | A |
| 1 | 1A | 74 | A |
| 1 | 1A | 75 | G |
| 1 | 1A | 84 | A |
| 1 | 1A | 118 | A |
| 1 | 1A | 119 | A |
| 1 | 1A | 120 | U |
| 1 | 1A | 139(A) | G |
| 1 | 1A | 182 | A |
| 1 | 1A | 196 | A |
| 1 | 1A | 197 | A |
| 1 | 1A | 199 | A |
| 1 | 1A | 205 | G |
| 1 | 1A | 214 | G |
| 1 | 1A | 215 | G |
| 1 | 1A | 216 | A |
| 1 | 1A | 221 | 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 | 269 | U |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 1 | 1A | 271(E) | U |
| 1 | 1A | 271(K) | U |
| 1 | 1A | 271(L) | U |
| 1 | 1A | 271(M) | G |
| 1 | 1A | 271(N) | U |
| 1 | 1A | 271(O) | C |
| 1 | 1A | 271(S) | G |
| 1 | 1A | 272(B) | G |
| 1 | 1A | 272(I) | U |
| 1 | 1A | 275 | G |
| 1 | 1A | 279 | C |
| 1 | 1A | 287 | C |
| 1 | 1A | 307 | G |
| 1 | 1A | 311 | A |
| 1 | 1A | 329 | G |
| 1 | 1A | 330 | A |
| 1 | 1A | 346 | A |
| 1 | 1A | 352 | G |
| 1 | 1A | 353 | G |
| 1 | 1A | 363 | G |
| 1 | 1A | 363(B) | G |
| 1 | 1A | 363(D) | G |
| 1 | 1A | 366 | C |
| 1 | 1A | 380 | U |
| 1 | 1A | 386 | G |
| 1 | 1A | 396 | G |
| 1 | 1A | 405 | U |
| 1 | 1A | 411 | G |
| 1 | 1A | 428 | A |
| 1 | 1A | 444 | C |
| 1 | 1A | 448 | U |
| 1 | 1A | 455 | C |
| 1 | 1A | 456 | C |
| 1 | 1A | 467 | G |
| 1 | 1A | 481 | G |
| 1 | 1A | 504 | U |
| 1 | 1A | 505 | A |
| 1 | 1A | 509 | C |
| 1 | 1A | 530 | G |
| 1 | 1A | 531 | C |
| 1 | 1A | 532 | A |
| 1 | 1A | 533 | G |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 1 | 1A | 545 | G |
| 1 | 1A | 549 | G |
| 1 | 1A | 563 | G |
| 1 | 1A | 573 | G |
| 1 | 1A | 575 | A |
| 1 | 1A | 586 | A |
| 1 | 1A | 593 | G |
| 1 | 1A | 603 | A |
| 1 | 1A | 604 | G |
| 1 | 1A | 607 | U |
| 1 | 1A | 614(B) | G |
| 1 | 1A | 615 | G |
| 1 | 1A | 619 | G |
| 1 | 1A | 627 | A |
| 1 | 1A | 634 | C |
| 1 | 1A | 637 | A |
| 1 | 1A | 645 | C |
| 1 | 1A | 646 | A |
| 1 | 1A | 652(D) | C |
| 1 | 1A | 652(E) | G |
| 1 | 1A | 669 | G |
| 1 | 1A | 686 | G |
| 1 | 1A | 702 | G |
| 1 | 1A | 725 | G |
| 1 | 1A | 730 | C |
| 1 | 1A | 746 | A |
| 1 | 1A | 747 | U |
| 1 | 1A | 762 | U |
| 1 | 1A | 764 | A |
| 1 | 1A | 765 | G |
| 1 | 1A | 774 | A |
| 1 | 1A | 775 | G |
| 1 | 1A | 776 | G |
| 1 | 1A | 777 | A |
| 1 | 1A | 782 | A |
| 1 | 1A | 784 | A |
| 1 | 1A | 785 | G |
| 1 | 1A | 789 | A |
| 1 | 1A | 792 | G |
| 1 | 1A | 794 | G |
| 1 | 1A | 805 | G |
| 1 | 1A | 811 | U |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | 1A | 812 | C |
| 1 | 1A | 819 | A |
| 1 | 1A | 827 | U |
| 1 | 1A | 828 | U |
| 1 | 1A | 859 | G |
| 1 | 1A | 866 | A |
| 1 | 1A | 876 | C |
| 1 | 1A | 877 | U |
| 1 | 1A | 879 | G |
| 1 | 1A | 880 | G |
| 1 | 1A | 881 | G |
| 1 | 1A | 882 | G |
| 1 | 1A | 883 | G |
| 1 | 1A | 884 | C |
| 1 | 1A | 885 | C |
| 1 | 1A | 886 | C |
| 1 | 1A | 887 | A |
| 1 | 1A | 888 | C |
| 1 | 1A | 889 | C |
| 1 | 1A | 890 | A |
| 1 | 1A | 893 | C |
| 1 | 1A | 894 | C |
| 1 | 1A | 896 | A |
| 1 | 1A | 897 | C |
| 1 | 1A | 899 | A |
| 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 | 961 | C |
| 1 | 1A | 963 | U |
| 1 | 1A | 964 | C |
| 1 | 1A | 974 | G |
| 1 | 1A | 975 | C |
| 1 | 1A | 983 | A |
| 1 | 1A | 996 | A |
| 1 | 1A | 1005 | C |
| 1 | 1A | 1012 | U |
| 1 | 1A | 1013 | C |
| 1 | 1A | 1022 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | 1A | 1026 | U |
| 1 | 1A | 1027 | A |
| 1 | 1A | 1033 | U |
| 1 | 1A | 1038 | C |
| 1 | 1A | 1040 | C |
| 1 | 1A | 1041 | C |
| 1 | 1A | 1044 | G |
| 1 | 1A | 1045 | A |
| 1 | 1A | 1046 | A |
| 1 | 1A | 1047 | G |
| 1 | 1A | 1048 | A |
| 1 | 1A | 1054 | A |
| 1 | 1A | 1057 | A |
| 1 | 1A | 1058 | G |
| 1 | 1A | 1059 | G |
| 1 | 1A | 1064 | C |
| 1 | 1A | 1066 | U |
| 1 | 1A | 1069 | A |
| 1 | 1A | 1071 | G |
| 1 | 1A | 1073 | A |
| 1 | 1A | 1075 | C |
| 1 | 1A | 1077 | A |
| 1 | 1A | 1078 | U |
| 1 | 1A | 1080 | C |
| 1 | 1A | 1087 | G |
| 1 | 1A | 1088 | A |
| 1 | 1A | 1090 | U |
| 1 | 1A | 1093 | G |
| 1 | 1A | 1094 | U |
| 1 | 1A | 1096 | A |
| 1 | 1A | 1097 | U |
| 1 | 1A | 1098 | A |
| 1 | 1A | 1101 | U |
| 1 | 1A | 1109 | C |
| 1 | 1A | 1110 | G |
| 1 | 1A | 1112 | G |
| 1 | 1A | 1115 | G |
| 1 | 1A | 1116 | C |
| 1 | 1A | 1128 | A |
| 1 | 1A | 1135 | C |
| 1 | 1A | 1136 | G |
| 1 | 1A | 1169 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 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 | 1241 | A |
| 1 | 1A | 1244 | G |
| 1 | 1A | 1253 | A |
| 1 | 1A | 1256 | G |
| 1 | 1A | 1271 | G |
| 1 | 1A | 1272 | A |
| 1 | 1A | 1274 | A |
| 1 | 1A | 1300 | U |
| 1 | 1A | 1301 | A |
| 1 | 1A | 1303 | G |
| 1 | 1A | 1321 | A |
| 1 | 1A | 1344 | G |
| 1 | 1A | 1352 | U |
| 1 | 1A | 1359 | A |
| 1 | 1A | 1360 | A |
| 1 | 1A | 1365 | A |
| 1 | 1A | 1380 | G |
| 1 | 1A | 1384 | A |
| 1 | 1A | 1385 | G |
| 1 | 1A | 1386 | C |
| 1 | 1A | 1395 | A |
| 1 | 1A | 1396 | U |
| 1 | 1A | 1416 | G |
| 1 | 1A | 1417 | C |
| 1 | 1A | 1420 | U |
| 1 | 1A | 1421 | G |
| 1 | 1A | 1428 | C |
| 1 | 1A | 1445 | A |
| 1 | 1A | 1450 | G |
| 1 | 1A | 1455 | G |
| 1 | 1A | 1459 | G |
| 1 | 1A | 1460 | A |
| 1 | 1A | 1461 | G |
| 1 | 1A | 1466 | G |
| 1 | 1A | 1467 | C |

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| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 1 | 1A | 1482 | G |
| 1 | 1A | 1493 | C |
| 1 | 1A | 1494 | A |
| 1 | 1A | 1499 | C |
| 1 | 1A | 1508 | A |
| 1 | 1A | 1509 | C |
| 1 | 1A | 1509(A) | A |
| 1 | 1A | 1523 | U |
| 1 | 1A | 1525 | G |
| 1 | 1A | 1541 | G |
| 1 | 1A | 1542 | A |
| 1 | 1A | 1543 | C |
| 1 | 1A | 1554 | A |
| 1 | 1A | 1558 | A |
| 1 | 1A | 1559 | G |
| 1 | 1A | 1569 | A |
| 1 | 1A | 1578 | U |
| 1 | 1A | 1580 | A |
| 1 | 1A | 1581 | G |
| 1 | 1A | 1582 | C |
| 1 | 1A | 1584 | C |
| 1 | 1A | 1586 | A |
| 1 | 1A | 1587 | A |
| 1 | 1A | 1608 | A |
| 1 | 1A | 1609 | A |
| 1 | 1A | 1617 | C |
| 1 | 1A | 1647 | G |
| 1 | 1A | 1648 | C |
| 1 | 1A | 1664 | A |
| 1 | 1A | 1674 | G |
| 1 | 1A | 1700 | A |
| 1 | 1A | 1701 | A |
| 1 | 1A | 1703 | G |
| 1 | 1A | 1747(A) | 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 |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | 1A | 1800 | C |
| 1 | 1A | 1801 | G |
| 1 | 1A | 1816 | G |
| 1 | 1A | 1817 | G |
| 1 | 1A | 1828 | G |
| 1 | 1A | 1829 | A |
| 1 | 1A | 1846 | G |
| 1 | 1A | 1847 | A |
| 1 | 1A | 1848 | A |
| 1 | 1A | 1878 | G |
| 1 | 1A | 1889 | A |
| 1 | 1A | 1890 | A |
| 1 | 1A | 1900 | A |
| 1 | 1A | 1906 | G |
| 1 | 1A | 1927 | A |
| 1 | 1A | 1929 | G |
| 1 | 1A | 1930 | G |
| 1 | 1A | 1931 | U |
| 1 | 1A | 1937 | A |
| 1 | 1A | 1938 | A |
| 1 | 1A | 1955 | U |
| 1 | 1A | 1963 | U |
| 1 | 1A | 1967 | C |
| 1 | 1A | 1970 | A |
| 1 | 1A | 1971 | A |
| 1 | 1A | 1972 | A |
| 1 | 1A | 1992 | G |
| 1 | 1A | 1993 | U |
| 1 | 1A | 1997 | G |
| 1 | 1A | 2020 | A |
| 1 | 1A | 2023 | G |
| 1 | 1A | 2031 | A |
| 1 | 1A | 2032 | G |
| 1 | 1A | 2033 | A |
| 1 | 1A | 2039 | C |
| 1 | 1A | 2043 | C |
| 1 | 1A | 2055 | C |
| 1 | 1A | 2056 | G |
| 1 | 1A | 2060 | A |
| 1 | 1A | 2061 | G |
| 1 | 1A | 2069 | G |
| 1 | 1A | 2093 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | 1A | 2096 | U |
| 1 | 1A | 2101 | G |
| 1 | 1A | 2107 | C |
| 1 | 1A | 2113 | U |
| 1 | 1A | 2116 | G |
| 1 | 1A | 2118 | U |
| 1 | 1A | 2119 | A |
| 1 | 1A | 2120 | G |
| 1 | 1A | 2127 | G |
| 1 | 1A | 2129 | C |
| 1 | 1A | 2131 | G |
| 1 | 1A | 2132 | U |
| 1 | 1A | 2133 | G |
| 1 | 1A | 2134 | A |
| 1 | 1A | 2135 | A |
| 1 | 1A | 2136 | C |
| 1 | 1A | 2140 | C |
| 1 | 1A | 2142 | C |
| 1 | 1A | 2143 | C |
| 1 | 1A | 2144 | U |
| 1 | 1A | 2146 | C |
| 1 | 1A | 2149 | G |
| 1 | 1A | 2150 | U |
| 1 | 1A | 2151 | G |
| 1 | 1A | 2152 | G |
| 1 | 1A | 2156 | G |
| 1 | 1A | 2157 | G |
| 1 | 1A | 2158 | A |
| 1 | 1A | 2159 | G |
| 1 | 1A | 2160 | G |
| 1 | 1A | 2161 | C |
| 1 | 1A | 2163 | C |
| 1 | 1A | 2165 | G |
| 1 | 1A | 2166 | G |
| 1 | 1A | 2167 | U |
| 1 | 1A | 2171 | A |
| 1 | 1A | 2172 | U |
| 1 | 1A | 2173 | A |
| 1 | 1A | 2180 | U |
| 1 | 1A | 2183 | C |
| 1 | 1A | 2184 | G |
| 1 | 1A | 2186 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | 1A | 2189 | U |
| 1 | 1A | 2190 | G |
| 1 | 1A | 2192 | G |
| 1 | 1A | 2198 | A |
| 1 | 1A | 2206 | G |
| 1 | 1A | 2207 | G |
| 1 | 1A | 2225 | A |
| 1 | 1A | 2235 | G |
| 1 | 1A | 2238 | G |
| 1 | 1A | 2239 | G |
| 1 | 1A | 2259 | G |
| 1 | 1A | 2268 | A |
| 1 | 1A | 2269 | A |
| 1 | 1A | 2280 | G |
| 1 | 1A | 2283 | C |
| 1 | 1A | 2287 | A |
| 1 | 1A | 2288 | A |
| 1 | 1A | 2305 | A |
| 1 | 1A | 2308 | G |
| 1 | 1A | 2320 | A |
| 1 | 1A | 2324 | C |
| 1 | 1A | 2325 | G |
| 1 | 1A | 2334 | G |
| 1 | 1A | 2336 | A |
| 1 | 1A | 2340 | G |
| 1 | 1A | 2347 | C |
| 1 | 1A | 2350 | C |
| 1 | 1A | 2354 | G |
| 1 | 1A | 2361 | A |
| 1 | 1A | 2372 | G |
| 1 | 1A | 2383 | G |
| 1 | 1A | 2385 | C |
| 1 | 1A | 2400 | G |
| 1 | 1A | 2406 | U |
| 1 | 1A | 2407 | G |
| 1 | 1A | 2414 | G |
| 1 | 1A | 2422 | A |
| 1 | 1A | 2423 | U |
| 1 | 1A | 2425 | A |
| 1 | 1A | 2429 | G |
| 1 | 1A | 2430 | A |
| 1 | 1A | 2435 | A |

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| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 1 | 1A | 2439 | A |
| 1 | 1A | 2440 | C |
| 1 | 1A | 2441 | C |
| 1 | 1A | 2448 | A |
| 1 | 1A | 2474 | C |
| 1 | 1A | 2476 | A |
| 1 | 1A | 2491 | U |
| 1 | 1A | 2498 | C |
| 1 | 1A | 2502 | G |
| 1 | 1A | 2505 | G |
| 1 | 1A | 2512 | C |
| 1 | 1A | 2518 | A |
| 1 | 1A | 2520 | C |
| 1 | 1A | 2524 | G |
| 1 | 1A | 2529 | G |
| 1 | 1A | 2550 | G |
| 1 | 1A | 2554 | U |
| 1 | 1A | 2555 | U |
| 1 | 1A | 2566 | A |
| 1 | 1A | 2567 | G |
| 1 | 1A | 2573 | C |
| 1 | 1A | 2585 | U |
| 1 | 1A | 2602 | A |
| 1 | 1A | 2611 | U |
| 1 | 1A | 2612 | C |
| 1 | 1A | 2629 | A |
| 1 | 1A | 2630 | G |
| 1 | 1A | 2654 | A |
| 1 | 1A | 2672 | G |
| 1 | 1A | 2689 | U |
| 1 | 1A | 2690 | C |
| 1 | 1A | 2691 | C |
| 1 | 1A | 2703 | C |
| 1 | 1A | 2707 | G |
| 1 | 1A | 2712(A) | A |
| 1 | 1A | 2713 | A |
| 1 | 1A | 2714 | G |
| 1 | 1A | 2726 | U |
| 1 | 1A | 2733 | A |
| 1 | 1A | 2734 | A |
| 1 | 1A | 2736 | G |
| 1 | 1A | 2752 | C |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | 1A | 2758 | A |
| 1 | 1A | 2765 | A |
| 1 | 1A | 2766 | G |
| 1 | 1A | 2769 | C |
| 1 | 1A | 2778 | A |
| 1 | 1A | 2790 | A |
| 1 | 1A | 2791 | C |
| 1 | 1A | 2794 | C |
| 1 | 1A | 2802 | G |
| 1 | 1A | 2803 | C |
| 1 | 1A | 2804 | C |
| 1 | 1A | 2805 | G |
| 1 | 1A | 2813 | A |
| 1 | 1A | 2818 | G |
| 1 | 1A | 2820 | A |
| 1 | 1A | 2821 | A |
| 1 | 1A | 2833 | G |
| 1 | 1A | 2835 | A |
| 1 | 1A | 2836 | U |
| 1 | 1A | 2839 | G |
| 1 | 1A | 2872 | G |
| 1 | 1A | 2876 | G |
| 1 | 1A | 2880 | C |
| 1 | 1A | 2882 | A |
| 1 | 1A | 2883 | A |
| 1 | 1A | 2892 | A |
| 1 | 1A | 2894 | G |
| 1 | 1A | 2895 | U |
| 2 | 1B | 2 | C |
| 2 | 1B | 10 | C |
| 2 | 1B | 12 | C |
| 2 | 1B | 13 | A |
| 2 | 1B | 25 | A |
| 2 | 1B | 42 | C |
| 2 | 1B | 56 | G |
| 2 | 1B | 66 | A |
| 2 | 1B | 67 | G |
| 2 | 1B | 73 | A |
| 2 | 1B | 92 | C |
| 2 | 1B | 110 | G |
| 32 | 1a | 7 | G |
| 32 | 1a | 9 | G |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 32 | 1a | 32 | A |
| 32 | 1a | 39 | G |
| 32 | 1a | 48 | C |
| 32 | 1a | 50 | A |
| 32 | 1a | 51 | A |
| 32 | 1a | 61 | G |
| 32 | 1a | 68 | G |
| 32 | 1a | 77 | G |
| 32 | 1a | 79 | G |
| 32 | 1a | 91 | C |
| 32 | 1a | 93 | G |
| 32 | 1a | 98 | G |
| 32 | 1a | 99 | U |
| 32 | 1a | 101 | A |
| 32 | 1a | 115 | G |
| 32 | 1a | 116 | A |
| 32 | 1a | 121 | C |
| 32 | 1a | 131 | C |
| 32 | 1a | 143 | A |
| 32 | 1a | 161 | A |
| 32 | 1a | 163 | C |
| 32 | 1a | 164 | U |
| 32 | 1a | 166 | G |
| 32 | 1a | 174 | C |
| 32 | 1a | 182 | U |
| 32 | 1a | 189 | G |
| 32 | 1a | 189(F) | U |
| 32 | 1a | 189(H) | G |
| 32 | 1a | 189(J) | G |
| 32 | 1a | 189(K) | U |
| 32 | 1a | 195 | A |
| 32 | 1a | 197 | A |
| 32 | 1a | 202 | U |
| 32 | 1a | 203 | U |
| 32 | 1a | 204 | U |
| 32 | 1a | 216 | G |
| 32 | 1a | 217 | C |
| 32 | 1a | 222 | U |
| 32 | 1a | 247 | G |
| 32 | 1a | 251 | G |
| 32 | 1a | 266 | G |
| 32 | 1a | 267 | C |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 32 | 1a | 279 | A |
| 32 | 1a | 289 | G |
| 32 | 1a | 301 | G |
| 32 | 1a | 316 | G |
| 32 | 1a | 321 | A |
| 32 | 1a | 328 | C |
| 32 | 1a | 332 | G |
| 32 | 1a | 344 | A |
| 32 | 1a | 345 | C |
| 32 | 1a | 347 | G |
| 32 | 1a | 352 | C |
| 32 | 1a | 353 | A |
| 32 | 1a | 354 | G |
| 32 | 1a | 367 | U |
| 32 | 1a | 372 | C |
| 32 | 1a | 373 | A |
| 32 | 1a | 383 | A |
| 32 | 1a | 384 | G |
| 32 | 1a | 397 | A |
| 32 | 1a | 398 | C |
| 32 | 1a | 406 | G |
| 32 | 1a | 412 | A |
| 32 | 1a | 413 | G |
| 32 | 1a | 422 | C |
| 32 | 1a | 423 | G |
| 32 | 1a | 429 | U |
| 32 | 1a | 439 | A |
| 32 | 1a | 452 | A |
| 32 | 1a | 457 | C |
| 32 | 1a | 461 | A |
| 32 | 1a | 470 | C |
| 32 | 1a | 475 | G |
| 32 | 1a | 485 | G |
| 32 | 1a | 496 | A |
| 32 | 1a | 498 | U |
| 32 | 1a | 509 | A |
| 32 | 1a | 510 | A |
| 32 | 1a | 511 | C |
| 32 | 1a | 517 | G |
| 32 | 1a | 518 | C |
| 32 | 1a | 521 | G |
| 32 | 1a | 527 | G7M |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 32 | 1a | 531 | U |
| 32 | 1a | 532 | A |
| 32 | 1a | 533 | A |
| 32 | 1a | 534 | U |
| 32 | 1a | 547 | A |
| 32 | 1a | 559 | A |
| 32 | 1a | 561 | U |
| 32 | 1a | 572 | A |
| 32 | 1a | 573 | A |
| 32 | 1a | 576 | G |
| 32 | 1a | 592 | G |
| 32 | 1a | 599 | C |
| 32 | 1a | 607 | A |
| 32 | 1a | 630 | G |
| 32 | 1a | 653 | A |
| 32 | 1a | 665 | A |
| 32 | 1a | 671 | G |
| 32 | 1a | 672 | U |
| 32 | 1a | 673 | G |
| 32 | 1a | 688 | G |
| 32 | 1a | 703 | G |
| 32 | 1a | 723 | U |
| 32 | 1a | 731 | G |
| 32 | 1a | 749 | C |
| 32 | 1a | 752 | G |
| 32 | 1a | 755 | G |
| 32 | 1a | 759 | A |
| 32 | 1a | 777 | A |
| 32 | 1a | 792 | A |
| 32 | 1a | 793 | U |
| 32 | 1a | 794 | A |
| 32 | 1a | 815 | A |
| 32 | 1a | 817 | C |
| 32 | 1a | 821 | G |
| 32 | 1a | 828 | A |
| 32 | 1a | 840 | C |
| 32 | 1a | 841 | U |
| 32 | 1a | 851 | G |
| 32 | 1a | 870 | U |
| 32 | 1a | 902 | G |
| 32 | 1a | 913 | A |
| 32 | 1a | 914 | A |

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| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 32 | 1a | 916 | G |
| 32 | 1a | 926 | G |
| 32 | 1a | 927 | G |
| 32 | 1a | 934 | C |
| 32 | 1a | 942 | G |
| 32 | 1a | 960 | U |
| 32 | 1a | 961 | U |
| 32 | 1a | 963 | G |
| 32 | 1a | 968 | A |
| 32 | 1a | 969 | A |
| 32 | 1a | 974 | A |
| 32 | 1a | 975 | A |
| 32 | 1a | 976 | G |
| 32 | 1a | 977 | A |
| 32 | 1a | 984 | C |
| 32 | 1a | 991 | U |
| 32 | 1a | 992 | U |
| 32 | 1a | 993 | G |
| 32 | 1a | 1000 | U |
| 32 | 1a | 1003 | G |
| 32 | 1a | 1005 | A |
| 32 | 1a | 1006 | C |
| 32 | 1a | 1009 | G |
| 32 | 1a | 1020 | U |
| 32 | 1a | 1022 | G |
| 32 | 1a | 1023 | G |
| 32 | 1a | 1025 | U |
| 32 | 1a | 1026 | G |
| 32 | 1a | 1027 | C |
| 32 | 1a | 1028 | C |
| 32 | 1a | 1029 | C |
| 32 | 1a | 1030 | C |
| 32 | 1a | 1030(A) | G |
| 32 | 1a | 1030(B) | C |
| 32 | 1a | 1030(C) | G |
| 32 | 1a | 1031 | G |
| 32 | 1a | 1039 | C |
| 32 | 1a | 1044 | A |
| 32 | 1a | 1068 | G |
| 32 | 1a | 1081 | G |
| 32 | 1a | 1094 | G |
| 32 | 1a | 1095 | U |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 32 | 1a | 1101 | A |
| 32 | 1a | 1108 | G |
| 32 | 1a | 1114 | C |
| 32 | 1a | 1123 | A |
| 32 | 1a | 1124 | G |
| 32 | 1a | 1132 | C |
| 32 | 1a | 1134 | G |
| 32 | 1a | 1135 | U |
| 32 | 1a | 1137 | C |
| 32 | 1a | 1138 | G |
| 32 | 1a | 1139 | G |
| 32 | 1a | 1140 | C |
| 32 | 1a | 1146 | A |
| 32 | 1a | 1152 | A |
| 32 | 1a | 1159 | U |
| 32 | 1a | 1184 | G |
| 32 | 1a | 1196 | U |
| 32 | 1a | 1197 | G |
| 32 | 1a | 1201 | A |
| 32 | 1a | 1202 | G |
| 32 | 1a | 1213 | A |
| 32 | 1a | 1214 | C |
| 32 | 1a | 1225 | A |
| 32 | 1a | 1226 | C |
| 32 | 1a | 1227 | A |
| 32 | 1a | 1236 | A |
| 32 | 1a | 1238 | A |
| 32 | 1a | 1240 | U |
| 32 | 1a | 1256 | A |
| 32 | 1a | 1257 | U |
| 32 | 1a | 1270 | C |
| 32 | 1a | 1275 | A |
| 32 | 1a | 1278 | U |
| 32 | 1a | 1280 | A |
| 32 | 1a | 1286 | A |
| 32 | 1a | 1287 | A |
| 32 | 1a | 1299 | A |
| 32 | 1a | 1300 | G |
| 32 | 1a | 1302 | U |
| 32 | 1a | 1320 | C |
| 32 | 1a | 1338 | G |
| 32 | 1a | 1340 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 32 | 1a | 1346 | A |
| 32 | 1a | 1347 | G |
| 32 | 1a | 1353 | G |
| 32 | 1a | 1363 | C |
| 32 | 1a | 1370 | G |
| 32 | 1a | 1381 | U |
| 32 | 1a | 1397 | C |
| 32 | 1a | 1419 | G |
| 32 | 1a | 1441 | G |
| 32 | 1a | 1442 | G |
| 32 | 1a | 1446 | U |
| 32 | 1a | 1447 | A |
| 32 | 1a | 1457 | G |
| 32 | 1a | 1469 | G |
| 32 | 1a | 1487 | G |
| 32 | 1a | 1491 | 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 | 1529 | G |
| 32 | 1a | 1530 | G |
| 53 | 1v | 13 | A |
| 53 | 1v | 14 | A |
| 53 | 1v | 24 | A |
| 54 | 1w | 16 | U |
| 54 | 1w | 19 | G |
| 54 | 1w | 20 | U |
| 54 | 1w | 21 | A |
| 54 | 1w | 23 | A |
| 54 | 1w | 24 | G |
| 54 | 1w | 25 | C |
| 54 | 1w | 33 | U |
| 54 | 1w | 34 | G |
| 54 | 1w | 44 | G |
| 54 | 1w | 45 | U |
| 54 | 1w | 46 | G7M |
| 54 | 1w | 47 | U |
| 54 | 1w | 48 | C |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 54 | 1w | 73 | A |
| 54 | 1w | 74 | C |
| 55 | 1x | 2 | G |
| 55 | 1x | 9 | G |
| 55 | 1x | 13 | C |
| 55 | 1x | 19 | G |
| 55 | 1x | 20 | U |
| 55 | 1x | 21 | A |
| 55 | 1x | 30 | G |
| 55 | 1x | 47 | U |
| 55 | 1x | 48 | C |
| 55 | 1x | 49 | G |
| 55 | 1x | 61 | C |
| 56 | 1y | 5 | G |
| 56 | 1y | 9 | A |
| 56 | 1y | 13 | C |
| 56 | 1y | 14 | A |
| 56 | 1y | 19 | G |
| 56 | 1y | 20 | U |
| 56 | 1y | 21 | A |
| 56 | 1y | 22 | G |
| 56 | 1y | 37 | MIA |
| 56 | 1y | 40 | C |
| 56 | 1y | 43 | C |
| 56 | 1y | 44 | G |
| 56 | 1y | 45 | U |
| 56 | 1y | 46 | G7M |
| 56 | 1y | 47 | U |
| 56 | 1y | 48 | C |
| 56 | 1y | 56 | C |
| 56 | 1y | 58 | A |
| 56 | 1y | 59 | U |
| 56 | 1y | 61 | C |
| 56 | 1y | 62 | C |
| 56 | 1y | 65 | G |
| 56 | 1y | 69 | G |
| 56 | 1y | 70 | G |
| 56 | 1y | 71 | G |
| 1 | 2A | 12 | U |
| 1 | 2A | 34 | C |
| 1 | 2A | 35 | G |
| 1 | 2A | 45 | C |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 1 | 2A | 48 | G |
| 1 | 2A | 61 | G |
| 1 | 2A | 71 | A |
| 1 | 2A | 74 | A |
| 1 | 2A | 75 | G |
| 1 | 2A | 79 | G |
| 1 | 2A | 84 | A |
| 1 | 2A | 100 | G |
| 1 | 2A | 102 | G |
| 1 | 2A | 118 | A |
| 1 | 2A | 119 | A |
| 1 | 2A | 120 | U |
| 1 | 2A | 141 | A |
| 1 | 2A | 157 | U |
| 1 | 2A | 172 | C |
| 1 | 2A | 173 | G |
| 1 | 2A | 196 | A |
| 1 | 2A | 197 | A |
| 1 | 2A | 199 | A |
| 1 | 2A | 205 | G |
| 1 | 2A | 214 | G |
| 1 | 2A | 215 | G |
| 1 | 2A | 216 | A |
| 1 | 2A | 222 | A |
| 1 | 2A | 225 | A |
| 1 | 2A | 228 | A |
| 1 | 2A | 229 | A |
| 1 | 2A | 233 | A |
| 1 | 2A | 248 | G |
| 1 | 2A | 264 | C |
| 1 | 2A | 266 | G |
| 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 | G |
| 1 | 2A | 272(B) | G |
| 1 | 2A | 274 | G |
| 1 | 2A | 277 | C |
| 1 | 2A | 278 | A |
| 1 | 2A | 283 | A |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 1 | 2A | 311 | A |
| 1 | 2A | 312 | G |
| 1 | 2A | 324 | A |
| 1 | 2A | 327 | G |
| 1 | 2A | 329 | G |
| 1 | 2A | 330 | A |
| 1 | 2A | 342 | G |
| 1 | 2A | 352 | G |
| 1 | 2A | 357 | A |
| 1 | 2A | 363(B) | G |
| 1 | 2A | 370 | G |
| 1 | 2A | 386 | G |
| 1 | 2A | 396 | G |
| 1 | 2A | 399 | G |
| 1 | 2A | 405 | U |
| 1 | 2A | 406 | G |
| 1 | 2A | 411 | G |
| 1 | 2A | 421 | U |
| 1 | 2A | 435 | C |
| 1 | 2A | 443 | A |
| 1 | 2A | 444 | C |
| 1 | 2A | 445 | C |
| 1 | 2A | 455 | C |
| 1 | 2A | 456 | C |
| 1 | 2A | 457 | A |
| 1 | 2A | 481 | G |
| 1 | 2A | 494 | G |
| 1 | 2A | 505 | A |
| 1 | 2A | 508 | G |
| 1 | 2A | 509 | C |
| 1 | 2A | 529 | A |
| 1 | 2A | 530 | G |
| 1 | 2A | 531 | C |
| 1 | 2A | 532 | A |
| 1 | 2A | 533 | G |
| 1 | 2A | 551 | G |
| 1 | 2A | 556 | G |
| 1 | 2A | 563 | G |
| 1 | 2A | 568 | U |
| 1 | 2A | 573 | G |
| 1 | 2A | 575 | A |
| 1 | 2A | 586 | A |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 1 | 2A | 588 | U |
| 1 | 2A | 602 | G |
| 1 | 2A | 603 | A |
| 1 | 2A | 604 | G |
| 1 | 2A | 607 | U |
| 1 | 2A | 614(A) | U |
| 1 | 2A | 614(B) | G |
| 1 | 2A | 615 | G |
| 1 | 2A | 616 | G |
| 1 | 2A | 627 | A |
| 1 | 2A | 634 | C |
| 1 | 2A | 637 | A |
| 1 | 2A | 645 | C |
| 1 | 2A | 652(B) | A |
| 1 | 2A | 652(C) | G |
| 1 | 2A | 652(E) | G |
| 1 | 2A | 669 | G |
| 1 | 2A | 686 | G |
| 1 | 2A | 701 | G |
| 1 | 2A | 717 | G |
| 1 | 2A | 730 | C |
| 1 | 2A | 752 | A |
| 1 | 2A | 753 | C |
| 1 | 2A | 771 | G |
| 1 | 2A | 774 | A |
| 1 | 2A | 775 | G |
| 1 | 2A | 776 | G |
| 1 | 2A | 782 | A |
| 1 | 2A | 783 | A |
| 1 | 2A | 784 | A |
| 1 | 2A | 785 | G |
| 1 | 2A | 792 | G |
| 1 | 2A | 805 | G |
| 1 | 2A | 812 | C |
| 1 | 2A | 819 | A |
| 1 | 2A | 827 | U |
| 1 | 2A | 828 | U |
| 1 | 2A | 855 | G |
| 1 | 2A | 856 | C |
| 1 | 2A | 857 | C |
| 1 | 2A | 859 | G |
| 1 | 2A | 866 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | 2A | 874 | G |
| 1 | 2A | 879 | G |
| 1 | 2A | 880 | G |
| 1 | 2A | 882 | G |
| 1 | 2A | 883 | G |
| 1 | 2A | 884 | C |
| 1 | 2A | 885 | C |
| 1 | 2A | 886 | C |
| 1 | 2A | 887 | A |
| 1 | 2A | 888 | C |
| 1 | 2A | 889 | C |
| 1 | 2A | 890 | A |
| 1 | 2A | 893 | C |
| 1 | 2A | 894 | C |
| 1 | 2A | 896 | A |
| 1 | 2A | 897 | C |
| 1 | 2A | 900 | A |
| 1 | 2A | 901 | A |
| 1 | 2A | 904 | C |
| 1 | 2A | 910 | A |
| 1 | 2A | 917 | A |
| 1 | 2A | 931 | G |
| 1 | 2A | 932 | G |
| 1 | 2A | 938 | G |
| 1 | 2A | 941 | A |
| 1 | 2A | 944 | G |
| 1 | 2A | 945 | A |
| 1 | 2A | 946 | G |
| 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 | 1005 | C |
| 1 | 2A | 1012 | U |
| 1 | 2A | 1013 | C |
| 1 | 2A | 1017 | G |
| 1 | 2A | 1022 | G |
| 1 | 2A | 1025 | G |
| 1 | 2A | 1026 | U |
| 1 | 2A | 1027 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | 2A | 1033 | U |
| 1 | 2A | 1038 | C |
| 1 | 2A | 1039 | G |
| 1 | 2A | 1043 | C |
| 1 | 2A | 1116 | C |
| 1 | 2A | 1130 | U |
| 1 | 2A | 1135 | C |
| 1 | 2A | 1136 | G |
| 1 | 2A | 1139 | G |
| 1 | 2A | 1171 | G |
| 1 | 2A | 1188 | U |
| 1 | 2A | 1211 | U |
| 1 | 2A | 1219 | G |
| 1 | 2A | 1220 | A |
| 1 | 2A | 1244 | G |
| 1 | 2A | 1253 | A |
| 1 | 2A | 1256 | G |
| 1 | 2A | 1271 | G |
| 1 | 2A | 1272 | A |
| 1 | 2A | 1273 | U |
| 1 | 2A | 1284 | A |
| 1 | 2A | 1287 | A |
| 1 | 2A | 1300 | U |
| 1 | 2A | 1301 | A |
| 1 | 2A | 1303 | G |
| 1 | 2A | 1314 | C |
| 1 | 2A | 1345 | C |
| 1 | 2A | 1352 | U |
| 1 | 2A | 1359 | A |
| 1 | 2A | 1360 | A |
| 1 | 2A | 1365 | A |
| 1 | 2A | 1368 | G |
| 1 | 2A | 1370 | C |
| 1 | 2A | 1379 | A |
| 1 | 2A | 1380 | G |
| 1 | 2A | 1384 | A |
| 1 | 2A | 1385 | G |
| 1 | 2A | 1386 | C |
| 1 | 2A | 1395 | A |
| 1 | 2A | 1416 | G |
| 1 | 2A | 1417 | C |
| 1 | 2A | 1420 | U |

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| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 1 | 2A | 1427 | A |
| 1 | 2A | 1428 | C |
| 1 | 2A | 1437 | C |
| 1 | 2A | 1445 | A |
| 1 | 2A | 1449 | A |
| 1 | 2A | 1450 | G |
| 1 | 2A | 1455 | G |
| 1 | 2A | 1460 | A |
| 1 | 2A | 1461 | G |
| 1 | 2A | 1464 | C |
| 1 | 2A | 1465 | G |
| 1 | 2A | 1467 | C |
| 1 | 2A | 1471 | A |
| 1 | 2A | 1478 | G |
| 1 | 2A | 1482 | G |
| 1 | 2A | 1490 | A |
| 1 | 2A | 1493 | C |
| 1 | 2A | 1494 | A |
| 1 | 2A | 1495 | A |
| 1 | 2A | 1496 | A |
| 1 | 2A | 1497 | U |
| 1 | 2A | 1508 | A |
| 1 | 2A | 1509 | C |
| 1 | 2A | 1509(A) | A |
| 1 | 2A | 1514 | U |
| 1 | 2A | 1531 | C |
| 1 | 2A | 1542 | A |
| 1 | 2A | 1543 | C |
| 1 | 2A | 1545 | A |
| 1 | 2A | 1547 | C |
| 1 | 2A | 1554 | A |
| 1 | 2A | 1558 | A |
| 1 | 2A | 1566 | A |
| 1 | 2A | 1569 | A |
| 1 | 2A | 1578 | U |
| 1 | 2A | 1580 | A |
| 1 | 2A | 1582 | C |
| 1 | 2A | 1584 | C |
| 1 | 2A | 1608 | A |
| 1 | 2A | 1609 | A |
| 1 | 2A | 1610 | A |
| 1 | 2A | 1640 | C |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | 2A | 1648 | C |
| 1 | 2A | 1653 | G |
| 1 | 2A | 1654 | A |
| 1 | 2A | 1664 | A |
| 1 | 2A | 1667 | G |
| 1 | 2A | 1674 | G |
| 1 | 2A | 1680 | U |
| 1 | 2A | 1696 | G |
| 1 | 2A | 1700 | A |
| 1 | 2A | 1721 | G |
| 1 | 2A | 1722 | A |
| 1 | 2A | 1740 | G |
| 1 | 2A | 1746 | G |
| 1 | 2A | 1756 | G |
| 1 | 2A | 1762 | A |
| 1 | 2A | 1763 | G |
| 1 | 2A | 1764 | G |
| 1 | 2A | 1773 | A |
| 1 | 2A | 1780 | A |
| 1 | 2A | 1782 | C |
| 1 | 2A | 1791 | A |
| 1 | 2A | 1800 | C |
| 1 | 2A | 1801 | G |
| 1 | 2A | 1816 | G |
| 1 | 2A | 1828 | G |
| 1 | 2A | 1829 | A |
| 1 | 2A | 1835 | G |
| 1 | 2A | 1839 | G |
| 1 | 2A | 1847 | A |
| 1 | 2A | 1848 | A |
| 1 | 2A | 1877 | A |
| 1 | 2A | 1878 | G |
| 1 | 2A | 1900 | A |
| 1 | 2A | 1906 | G |
| 1 | 2A | 1913 | A |
| 1 | 2A | 1914 | C |
| 1 | 2A | 1929 | G |
| 1 | 2A | 1930 | G |
| 1 | 2A | 1936 | A |
| 1 | 2A | 1937 | A |
| 1 | 2A | 1955 | U |
| 1 | 2A | 1963 | U |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | 2A | 1967 | C |
| 1 | 2A | 1970 | A |
| 1 | 2A | 1971 | A |
| 1 | 2A | 1972 | A |
| 1 | 2A | 1992 | G |
| 1 | 2A | 1993 | U |
| 1 | 2A | 1997 | G |
| 1 | 2A | 2020 | A |
| 1 | 2A | 2023 | G |
| 1 | 2A | 2031 | A |
| 1 | 2A | 2032 | G |
| 1 | 2A | 2033 | A |
| 1 | 2A | 2043 | C |
| 1 | 2A | 2055 | C |
| 1 | 2A | 2056 | G |
| 1 | 2A | 2060 | A |
| 1 | 2A | 2061 | G |
| 1 | 2A | 2063 | C |
| 1 | 2A | 2069 | G |
| 1 | 2A | 2099 | U |
| 1 | 2A | 2104 | G |
| 1 | 2A | 2111 | C |
| 1 | 2A | 2112 | G |
| 1 | 2A | 2115 | G |
| 1 | 2A | 2116 | G |
| 1 | 2A | 2119 | A |
| 1 | 2A | 2120 | G |
| 1 | 2A | 2122 | U |
| 1 | 2A | 2125 | G |
| 1 | 2A | 2126 | A |
| 1 | 2A | 2127 | G |
| 1 | 2A | 2128 | C |
| 1 | 2A | 2129 | C |
| 1 | 2A | 2131 | G |
| 1 | 2A | 2132 | U |
| 1 | 2A | 2133 | G |
| 1 | 2A | 2134 | A |
| 1 | 2A | 2135 | A |
| 1 | 2A | 2137 | C |
| 1 | 2A | 2138 | C |
| 1 | 2A | 2139 | C |
| 1 | 2A | 2142 | C |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | 2A | 2145 | C |
| 1 | 2A | 2148 | G |
| 1 | 2A | 2149 | G |
| 1 | 2A | 2150 | U |
| 1 | 2A | 2151 | G |
| 1 | 2A | 2156 | G |
| 1 | 2A | 2157 | G |
| 1 | 2A | 2158 | A |
| 1 | 2A | 2161 | C |
| 1 | 2A | 2165 | G |
| 1 | 2A | 2166 | G |
| 1 | 2A | 2167 | U |
| 1 | 2A | 2168 | G |
| 1 | 2A | 2169 | A |
| 1 | 2A | 2171 | A |
| 1 | 2A | 2172 | U |
| 1 | 2A | 2174 | C |
| 1 | 2A | 2177 | C |
| 1 | 2A | 2181 | G |
| 1 | 2A | 2185 | C |
| 1 | 2A | 2186 | G |
| 1 | 2A | 2187 | G |
| 1 | 2A | 2188 | C |
| 1 | 2A | 2189 | U |
| 1 | 2A | 2192 | G |
| 1 | 2A | 2198 | A |
| 1 | 2A | 2206 | G |
| 1 | 2A | 2207 | G |
| 1 | 2A | 2208 | A |
| 1 | 2A | 2225 | A |
| 1 | 2A | 2238 | G |
| 1 | 2A | 2239 | G |
| 1 | 2A | 2262 | U |
| 1 | 2A | 2268 | A |
| 1 | 2A | 2273 | A |
| 1 | 2A | 2275 | C |
| 1 | 2A | 2277 | G |
| 1 | 2A | 2280 | G |
| 1 | 2A | 2283 | C |
| 1 | 2A | 2287 | A |
| 1 | 2A | 2305 | A |
| 1 | 2A | 2308 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 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 | 2354 | G |
| 1 | 2A | 2355 | C |
| 1 | 2A | 2366 | A |
| 1 | 2A | 2376 | A |
| 1 | 2A | 2383 | G |
| 1 | 2A | 2385 | C |
| 1 | 2A | 2389 | G |
| 1 | 2A | 2396 | G |
| 1 | 2A | 2403 | C |
| 1 | 2A | 2406 | U |
| 1 | 2A | 2410 | G |
| 1 | 2A | 2419 | U |
| 1 | 2A | 2424 | C |
| 1 | 2A | 2425 | A |
| 1 | 2A | 2429 | G |
| 1 | 2A | 2430 | A |
| 1 | 2A | 2431 | U |
| 1 | 2A | 2434 | A |
| 1 | 2A | 2435 | A |
| 1 | 2A | 2439 | A |
| 1 | 2A | 2440 | C |
| 1 | 2A | 2441 | C |
| 1 | 2A | 2445 | G |
| 1 | 2A | 2448 | A |
| 1 | 2A | 2460 | U |
| 1 | 2A | 2469 | A |
| 1 | 2A | 2476 | A |
| 1 | 2A | 2486 | G |
| 1 | 2A | 2490 | G |
| 1 | 2A | 2491 | U |
| 1 | 2A | 2494 | G |
| 1 | 2A | 2495 | G |
| 1 | 2A | 2502 | G |
| 1 | 2A | 2505 | G |

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| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 1 | 2A | 2506 | U |
| 1 | 2A | 2518 | A |
| 1 | 2A | 2520 | C |
| 1 | 2A | 2525 | G |
| 1 | 2A | 2529 | G |
| 1 | 2A | 2549 | G |
| 1 | 2A | 2554 | U |
| 1 | 2A | 2555 | U |
| 1 | 2A | 2566 | A |
| 1 | 2A | 2567 | G |
| 1 | 2A | 2573 | C |
| 1 | 2A | 2578 | G |
| 1 | 2A | 2585 | U |
| 1 | 2A | 2602 | A |
| 1 | 2A | 2605 | PSU |
| 1 | 2A | 2611 | U |
| 1 | 2A | 2612 | C |
| 1 | 2A | 2615 | U |
| 1 | 2A | 2630 | G |
| 1 | 2A | 2666 | C |
| 1 | 2A | 2689 | U |
| 1 | 2A | 2690 | C |
| 1 | 2A | 2691 | C |
| 1 | 2A | 2703 | C |
| 1 | 2A | 2712(A) | A |
| 1 | 2A | 2713 | A |
| 1 | 2A | 2714 | G |
| 1 | 2A | 2726 | U |
| 1 | 2A | 2733 | A |
| 1 | 2A | 2744 | G |
| 1 | 2A | 2748 | A |
| 1 | 2A | 2751 | G |
| 1 | 2A | 2752 | C |
| 1 | 2A | 2758 | A |
| 1 | 2A | 2760 | C |
| 1 | 2A | 2764 | A |
| 1 | 2A | 2765 | A |
| 1 | 2A | 2766 | G |
| 1 | 2A | 2778 | A |
| 1 | 2A | 2793 | G |
| 1 | 2A | 2794 | C |
| 1 | 2A | 2802 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | 2A | 2803 | C |
| 1 | 2A | 2807 | G |
| 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 | 2839 | G |
| 1 | 2A | 2872 | G |
| 1 | 2A | 2875 | C |
| 1 | 2A | 2879 | C |
| 1 | 2A | 2880 | C |
| 1 | 2A | 2892 | A |
| 1 | 2A | 2894 | G |
| 1 | 2A | 2897 | U |
| 2 | 2B | 2 | C |
| 2 | 2B | 9 | G |
| 2 | 2B | 13 | A |
| 2 | 2B | 34 | U |
| 2 | 2B | 41 | U |
| 2 | 2B | 42 | C |
| 2 | 2B | 44 | G |
| 2 | 2B | 45 | A |
| 2 | 2B | 51 | G |
| 2 | 2B | 53 | A |
| 2 | 2B | 54 | G |
| 2 | 2B | 56 | G |
| 2 | 2B | 73 | A |
| 2 | 2B | 74 | U |
| 2 | 2B | 75 | G |
| 2 | 2B | 88 | C |
| 2 | 2B | 110 | G |
| 2 | 2B | 111 | G |
| 2 | 2B | 120 | A |
| 32 | 2a | 9 | G |
| 32 | 2a | 31 | G |
| 32 | 2a | 32 | A |
| 32 | 2a | 39 | G |
| 32 | 2a | 47 | C |
| 32 | 2a | 48 | C |
| 32 | 2a | 50 | A |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 32 | 2a | 51 | A |
| 32 | 2a | 52 | G |
| 32 | 2a | 65 | U |
| 32 | 2a | 66 | G |
| 32 | 2a | 73 | G |
| 32 | 2a | 80 | G |
| 32 | 2a | 89 | C |
| 32 | 2a | 98 | G |
| 32 | 2a | 101 | A |
| 32 | 2a | 115 | G |
| 32 | 2a | 116 | A |
| 32 | 2a | 121 | C |
| 32 | 2a | 131 | C |
| 32 | 2a | 145 | G |
| 32 | 2a | 146 | G |
| 32 | 2a | 155 | C |
| 32 | 2a | 163 | C |
| 32 | 2a | 182 | U |
| 32 | 2a | 189(F) | U |
| 32 | 2a | 195 | A |
| 32 | 2a | 197 | A |
| 32 | 2a | 201 | C |
| 32 | 2a | 202 | U |
| 32 | 2a | 203 | U |
| 32 | 2a | 204 | U |
| 32 | 2a | 216 | G |
| 32 | 2a | 231 | G |
| 32 | 2a | 247 | G |
| 32 | 2a | 251 | G |
| 32 | 2a | 258 | 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 | 355 | C |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 32 | 2a | 367 | U |
| 32 | 2a | 372 | C |
| 32 | 2a | 381 | C |
| 32 | 2a | 384 | G |
| 32 | 2a | 397 | A |
| 32 | 2a | 398 | C |
| 32 | 2a | 406 | G |
| 32 | 2a | 412 | A |
| 32 | 2a | 413 | G |
| 32 | 2a | 418 | C |
| 32 | 2a | 421 | U |
| 32 | 2a | 429 | U |
| 32 | 2a | 433 | C |
| 32 | 2a | 439 | A |
| 32 | 2a | 442 | C |
| 32 | 2a | 452 | A |
| 32 | 2a | 454 | C |
| 32 | 2a | 470 | C |
| 32 | 2a | 471 | G |
| 32 | 2a | 484 | G |
| 32 | 2a | 485 | G |
| 32 | 2a | 496 | A |
| 32 | 2a | 498 | U |
| 32 | 2a | 505 | G |
| 32 | 2a | 508 | C |
| 32 | 2a | 509 | A |
| 32 | 2a | 510 | A |
| 32 | 2a | 511 | C |
| 32 | 2a | 518 | C |
| 32 | 2a | 519 | 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 | 568 | G |
| 32 | 2a | 572 | A |
| 32 | 2a | 573 | A |
| 32 | 2a | 576 | G |
| 32 | 2a | 577 | G |
| 32 | 2a | 596 | C |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 32 | 2a | 619 | U |
| 32 | 2a | 630 | G |
| 32 | 2a | 653 | A |
| 32 | 2a | 657 | G |
| 32 | 2a | 661 | G |
| 32 | 2a | 665 | A |
| 32 | 2a | 666 | G |
| 32 | 2a | 673 | G |
| 32 | 2a | 687 | A |
| 32 | 2a | 688 | G |
| 32 | 2a | 695 | A |
| 32 | 2a | 723 | U |
| 32 | 2a | 731 | G |
| 32 | 2a | 749 | C |
| 32 | 2a | 755 | G |
| 32 | 2a | 773 | G |
| 32 | 2a | 774 | G |
| 32 | 2a | 777 | A |
| 32 | 2a | 787 | A |
| 32 | 2a | 792 | A |
| 32 | 2a | 793 | U |
| 32 | 2a | 794 | A |
| 32 | 2a | 808 | C |
| 32 | 2a | 812 | C |
| 32 | 2a | 817 | C |
| 32 | 2a | 821 | G |
| 32 | 2a | 827 | U |
| 32 | 2a | 828 | A |
| 32 | 2a | 833 | U |
| 32 | 2a | 840 | C |
| 32 | 2a | 841 | U |
| 32 | 2a | 859 | A |
| 32 | 2a | 874 | G |
| 32 | 2a | 902 | G |
| 32 | 2a | 914 | A |
| 32 | 2a | 926 | G |
| 32 | 2a | 927 | G |
| 32 | 2a | 933 | G |
| 32 | 2a | 934 | C |
| 32 | 2a | 935 | A |
| 32 | 2a | 936 | C |
| 32 | 2a | 939 | G |

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| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 32 | 2a | 957 | U |
| 32 | 2a | 958 | A |
| 32 | 2a | 960 | U |
| 32 | 2a | 961 | U |
| 32 | 2a | 963 | G |
| 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 | 991 | U |
| 32 | 2a | 993 | G |
| 32 | 2a | 996 | A |
| 32 | 2a | 997 | U |
| 32 | 2a | 998 | G |
| 32 | 2a | 999 | C |
| 32 | 2a | 1002 | G |
| 32 | 2a | 1003 | G |
| 32 | 2a | 1005 | A |
| 32 | 2a | 1006 | C |
| 32 | 2a | 1009 | G |
| 32 | 2a | 1011 | G |
| 32 | 2a | 1017 | G |
| 32 | 2a | 1019 | C |
| 32 | 2a | 1020 | U |
| 32 | 2a | 1022 | G |
| 32 | 2a | 1025 | U |
| 32 | 2a | 1026 | G |
| 32 | 2a | 1027 | C |
| 32 | 2a | 1028 | C |
| 32 | 2a | 1029 | C |
| 32 | 2a | 1030 | C |
| 32 | 2a | 1030(A) | G |
| 32 | 2a | 1031 | G |
| 32 | 2a | 1035 | A |
| 32 | 2a | 1036 | G |
| 32 | 2a | 1037 | C |
| 32 | 2a | 1039 | C |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 32 | 2a | 1040 | U |
| 32 | 2a | 1041 | A |
| 32 | 2a | 1042 | G |
| 32 | 2a | 1044 | A |
| 32 | 2a | 1045 | C |
| 32 | 2a | 1053 | G |
| 32 | 2a | 1064 | G |
| 32 | 2a | 1065 | U |
| 32 | 2a | 1066 | C |
| 32 | 2a | 1068 | G |
| 32 | 2a | 1081 | G |
| 32 | 2a | 1086 | U |
| 32 | 2a | 1092 | A |
| 32 | 2a | 1093 | A |
| 32 | 2a | 1094 | G |
| 32 | 2a | 1095 | U |
| 32 | 2a | 1097 | C |
| 32 | 2a | 1101 | A |
| 32 | 2a | 1125 | U |
| 32 | 2a | 1129 | C |
| 32 | 2a | 1130 | A |
| 32 | 2a | 1136 | U |
| 32 | 2a | 1137 | C |
| 32 | 2a | 1138 | G |
| 32 | 2a | 1139 | G |
| 32 | 2a | 1140 | C |
| 32 | 2a | 1146 | A |
| 32 | 2a | 1147 | C |
| 32 | 2a | 1150 | U |
| 32 | 2a | 1152 | A |
| 32 | 2a | 1155 | G |
| 32 | 2a | 1157 | A |
| 32 | 2a | 1158 | C |
| 32 | 2a | 1159 | U |
| 32 | 2a | 1163 | C |
| 32 | 2a | 1174 | G |
| 32 | 2a | 1181 | G |
| 32 | 2a | 1182 | G |
| 32 | 2a | 1184 | G |
| 32 | 2a | 1196 | U |
| 32 | 2a | 1197 | G |
| 32 | 2a | 1200 | C |

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| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 32 | 2a | 1201 | A |
| 32 | 2a | 1202 | G |
| 32 | 2a | 1213 | A |
| 32 | 2a | 1214 | C |
| 32 | 2a | 1227 | A |
| 32 | 2a | 1238 | A |
| 32 | 2a | 1240 | U |
| 32 | 2a | 1256 | A |
| 32 | 2a | 1257 | U |
| 32 | 2a | 1258 | G |
| 32 | 2a | 1260 | C |
| 32 | 2a | 1270 | C |
| 32 | 2a | 1273 | G |
| 32 | 2a | 1278 | U |
| 32 | 2a | 1279 | A |
| 32 | 2a | 1280 | A |
| 32 | 2a | 1286 | A |
| 32 | 2a | 1287 | A |
| 32 | 2a | 1302 | U |
| 32 | 2a | 1303 | C |
| 32 | 2a | 1305 | G |
| 32 | 2a | 1319 | A |
| 32 | 2a | 1346 | A |
| 32 | 2a | 1347 | G |
| 32 | 2a | 1363 | C |
| 32 | 2a | 1378 | C |
| 32 | 2a | 1394 | A |
| 32 | 2a | 1398 | A |
| 32 | 2a | 1419 | G |
| 32 | 2a | 1442 | G |
| 32 | 2a | 1442(A) | G |
| 32 | 2a | 1447 | A |
| 32 | 2a | 1452 | C |
| 32 | 2a | 1456 | G |
| 32 | 2a | 1491 | G |
| 32 | 2a | 1492 | A |
| 32 | 2a | 1497 | G |
| 32 | 2a | 1504 | G |
| 32 | 2a | 1506 | U |
| 32 | 2a | 1507 | A |
| 32 | 2a | 1517 | G |
| 32 | 2a | 1520 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 32 | 2a | 1529 | G |
| 32 | 2a | 1530 | G |
| 32 | 2a | 1531 | A |
| 32 | 2a | 1532 | U |
| 53 | 2v | 24 | A |
| 54 | 2w | 3 | C |
| 54 | 2w | 7 | A |
| 54 | 2w | 8 | 4SU |
| 54 | 2w | 11 | C |
| 54 | 2w | 14 | A |
| 54 | 2w | 19 | G |
| 54 | 2w | 22 | G |
| 54 | 2w | 23 | A |
| 54 | 2w | 44 | G |
| 54 | 2w | 46 | G7M |
| 54 | 2w | 47 | U |
| 54 | 2w | 48 | C |
| 54 | 2w | 53 | G |
| 54 | 2w | 61 | C |
| 54 | 2w | 65 | G |
| 54 | 2w | 67 | C |
| 54 | 2w | 69 | G |
| 54 | 2w | 70 | G |
| 54 | 2w | 71 | G |
| 54 | 2w | 72 | C |
| 54 | 2w | 73 | A |
| 54 | 2w | 74 | C |
| 55 | 2x | 2 | G |
| 55 | 2x | 9 | G |
| 55 | 2x | 10 | G |
| 55 | 2x | 13 | C |
| 55 | 2x | 21 | A |
| 55 | 2x | 37 | A |
| 55 | 2x | 42 | G |
| 55 | 2x | 44 | A |
| 55 | 2x | 47 | U |
| 55 | 2x | 53 | G |
| 55 | 2x | 61 | C |
| 56 | 2y | 2 | C |
| 56 | 2y | 7 | A |
| 56 | 2y | 11 | C |
| 56 | 2y | 12 | U |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 56 | 2y | 15 | G |
| 56 | 2y | 19 | G |
| 56 | 2y | 23 | A |
| 56 | 2y | 25 | C |
| 56 | 2y | 27 | G |
| 56 | 2y | 31 | A |
| 56 | 2y | 34 | G |
| 56 | 2y | 37 | MIA |
| 56 | 2y | 38 | A |
| 56 | 2y | 40 | C |
| 56 | 2y | 45 | U |
| 56 | 2y | 48 | C |
| 56 | 2y | 49 | C |
| 56 | 2y | 52 | G |
| 56 | 2y | 53 | G |
| 56 | 2y | 54 | 5MU |
| 56 | 2y | 55 | PSU |
| 56 | 2y | 56 | C |
| 56 | 2y | 58 | A |
| 56 | 2y | 59 | U |
| 56 | 2y | 61 | C |
| 56 | 2y | 65 | G |
| 56 | 2y | 68 | C |
| 56 | 2y | 69 | G |
| 56 | 2y | 70 | G |

All (65) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 1 | 1A | 195 | A |
| 1 | 1A | 196 | A |
| 1 | 1A | 266 | G |
| 1 | 1A | 271(K) | U |
| 1 | 1A | 278 | A |
| 1 | 1A | 310 | A |
| 1 | 1A | 548 | A |
| 1 | 1A | 669 | G |
| 1 | 1A | 685 | A |
| 1 | 1A | 746 | A |
| 1 | 1A | 764 | A |
| 1 | 1A | 774 | A |
| 1 | 1A | 776 | G |

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| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 1 | 1A | 827 | U |
| 1 | 1A | 896 | A |
| 1 | 1A | 960 | A |
| 1 | 1A | 974 | G |
| 1 | 1A | 1047 | G |
| 1 | 1A | 1067 | A |
| 1 | 1A | 1174 | A |
| 1 | 1A | 1176 | G |
| 1 | 1A | 1240 | U |
| 1 | 1A | 1379 | A |
| 1 | 1A | 1420 | U |
| 1 | 1A | 1508 | A |
| 1 | 1A | 1608 | A |
| 1 | 1A | 1762 | A |
| 1 | 1A | 1992 | G |
| 1 | 1A | 2183 | C |
| 1 | 1A | 2286 | A |
| 1 | 1A | 2406 | U |
| 1 | 1A | 2430 | A |
| 1 | 1A | 2439 | A |
| 1 | 1A | 2629 | A |
| 1 | 1A | 2689 | U |
| 1 | 2A | 195 | A |
| 1 | 2A | 196 | A |
| 1 | 2A | 228 | A |
| 1 | 2A | 249 | C |
| 1 | 2A | 266 | G |
| 1 | 2A | 271(M) | G |
| 1 | 2A | 277 | C |
| 1 | 2A | 310 | A |
| 1 | 2A | 528 | A |
| 1 | 2A | 669 | G |
| 1 | 2A | 752 | A |
| 1 | 2A | 774 | A |
| 1 | 2A | 827 | U |
| 1 | 2A | 856 | C |
| 1 | 2A | 900 | A |
| 1 | 2A | 1142(A) | A |
| 1 | 2A | 1210 | A |
| 1 | 2A | 1379 | A |
| 1 | 2A | 1396 | U |
| 1 | 2A | 1442 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 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 | 2406 | U |
| 1 | 2A | 2439 | A |
| 1 | 2A | 2689 | U |

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

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

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|----------|--------------|------|-------------|-------------|------|-------------|
| | | | | | Counts | RMSZ | $\# Z > 2$ | Counts | RMSZ | $\# Z > 2$ |
| 54 | PSU | 2w | 39 | 54 | 18,21,22 | 1.41 | 2 (11%) | 21,30,33 | 1.51 | 2 (9%) |
| 55 | PSU | 2x | 55 | 55 | 18,21,22 | 1.36 | 3 (16%) | 21,30,33 | 1.99 | 5 (23%) |
| 32 | 4OC | 2a | 1402 | 32 | 20,23,24 | 0.82 | 0 | 25,32,35 | 0.93 | 1 (4%) |
| 32 | M2G | 2a | 966 | 32 | 24,27,28 | 1.27 | 4 (16%) | 33,40,43 | 1.89 | 5 (15%) |
| 56 | 4SU | 1y | 8 | 56 | 18,21,22 | 1.56 | 5 (27%) | 25,30,33 | 1.51 | 4 (16%) |
| 1 | PSU | 2A | 2605 | 1 | 18,21,22 | 1.34 | 3 (16%) | 21,30,33 | 2.28 | 4 (19%) |
| 32 | 5MC | 2a | 967 | 32 | 19,22,23 | 1.59 | 2 (10%) | 26,32,35 | 1.30 | 4 (15%) |
| 32 | 2MG | 2a | 1207 | 58,32 | 23,26,27 | 1.28 | 3 (13%) | 33,38,41 | 2.29 | 8 (24%) |
| 32 | 5MC | 2a | 1407 | 58,32 | 19,22,23 | 1.59 | 3 (15%) | 26,32,35 | 1.45 | 4 (15%) |
| 56 | PSU | 1y | 32 | 56 | 18,21,22 | 1.43 | 2 (11%) | 21,30,33 | 1.80 | 4 (19%) |
| 32 | PSU | 2a | 516 | 32 | 18,21,22 | 1.31 | 2 (11%) | 21,30,33 | 2.06 | 5 (23%) |
| 32 | 5MC | 1a | 1400 | 32 | 19,22,23 | 1.38 | 3 (15%) | 26,32,35 | 1.34 | 4 (15%) |
| 55 | PSU | 1x | 55 | 55 | 18,21,22 | 1.47 | 3 (16%) | 21,30,33 | 1.78 | 4 (19%) |
| 32 | 4OC | 1a | 1402 | 32 | 20,23,24 | 0.76 | 0 | 25,32,35 | 1.20 | 4 (16%) |
| 55 | 31H | 2x | 76 | 58,55,59 | 31,34,35 | 1.37 | 2 (6%) | 35,47,50 | 2.47 | 13 (37%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|-------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 55 | 4SU | 2x | 8 | 55 | 18,21,22 | 1.92 | 5 (27%) | 25,30,33 | 1.18 | 3 (12%) |
| 1 | 5MU | 2A | 1939 | 58,1 | 19,22,23 | 1.52 | 4 (21%) | 27,32,35 | 2.31 | 7 (25%) |
| 32 | UR3 | 1a | 1498 | 32 | 19,22,23 | 0.95 | 1 (5%) | 26,32,35 | 1.73 | 5 (19%) |
| 54 | F3N | 1w | 76 | 1 | 33,36,37 | 1.49 | 6 (18%) | 41,51,54 | 1.85 | 11 (26%) |
| 54 | 5MU | 2w | 54 | 54 | 19,22,23 | 1.22 | 3 (15%) | 27,32,35 | 2.37 | 8 (29%) |
| 32 | G7M | 2a | 527 | 58,32 | 23,26,27 | 1.50 | 5 (21%) | 34,39,42 | 1.66 | 5 (14%) |
| 1 | OMC | 2A | 1920 | 1 | 19,22,23 | 0.86 | 1 (5%) | 25,31,34 | 1.11 | 2 (8%) |
| 54 | G7M | 1w | 46 | 54 | 23,26,27 | 1.56 | 3 (13%) | 34,39,42 | 1.80 | 4 (11%) |
| 1 | PSU | 1A | 2605 | 58,1 | 18,21,22 | 1.54 | 5 (27%) | 21,30,33 | 1.96 | 5 (23%) |
| 32 | UR3 | 2a | 1498 | 32 | 19,22,23 | 1.29 | 2 (10%) | 26,32,35 | 1.84 | 5 (19%) |
| 1 | PSU | 1A | 1911 | 1 | 18,21,22 | 1.43 | 3 (16%) | 21,30,33 | 2.04 | 3 (14%) |
| 56 | 5MU | 2y | 54 | 56 | 19,22,23 | 1.56 | 3 (15%) | 27,32,35 | 2.14 | 8 (29%) |
| 54 | F3N | 2w | 76 | 1 | 33,36,37 | 1.53 | 5 (15%) | 41,51,54 | 1.78 | 9 (21%) |
| 32 | 5MC | 2a | 1404 | 32 | 19,22,23 | 1.87 | 3 (15%) | 26,32,35 | 1.21 | 4 (15%) |
| 32 | MA6 | 1a | 1518 | 32 | 23,26,27 | 0.50 | 0 | 33,38,41 | 1.97 | 9 (27%) |
| 56 | 4SU | 2y | 8 | 56,58 | 18,21,22 | 1.71 | 5 (27%) | 25,30,33 | 2.10 | 5 (20%) |
| 1 | 5MC | 2A | 1942 | 1 | 19,22,23 | 1.20 | 3 (15%) | 26,32,35 | 1.10 | 2 (7%) |
| 54 | 4SU | 2w | 8 | 54 | 18,21,22 | 1.84 | 4 (22%) | 25,30,33 | 2.43 | 5 (20%) |
| 55 | 5MU | 2x | 54 | 55 | 19,22,23 | 1.37 | 2 (10%) | 27,32,35 | 2.26 | 6 (22%) |
| 55 | 5MC | 1x | 32 | 55 | 19,22,23 | 1.78 | 3 (15%) | 26,32,35 | 1.44 | 3 (11%) |
| 1 | PSU | 2A | 1911 | 1 | 18,21,22 | 1.44 | 2 (11%) | 21,30,33 | 2.05 | 3 (14%) |
| 1 | 5MU | 2A | 1915 | 1 | 19,22,23 | 1.38 | 5 (26%) | 27,32,35 | 2.43 | 6 (22%) |
| 56 | G7M | 1y | 46 | 56 | 23,26,27 | 1.44 | 3 (13%) | 34,39,42 | 1.76 | 5 (14%) |
| 1 | 5MC | 2A | 1962 | 58,1 | 19,22,23 | 1.49 | 3 (15%) | 26,32,35 | 1.11 | 2 (7%) |
| 1 | OMU | 1A | 2552 | 58,1 | 19,22,23 | 1.30 | 3 (15%) | 25,31,34 | 2.05 | 5 (20%) |
| 1 | 5MU | 1A | 1939 | 58,1 | 19,22,23 | 1.70 | 6 (31%) | 27,32,35 | 2.33 | 6 (22%) |
| 43 | 0TD | 1l | 92 | 43 | 8,9,10 | 3.92 | 2 (25%) | 6,11,13 | 5.45 | 2 (33%) |
| 32 | 5MC | 1a | 967 | 32 | 19,22,23 | 1.77 | 2 (10%) | 26,32,35 | 1.29 | 2 (7%) |
| 32 | 5MC | 1a | 1404 | 32 | 19,22,23 | 1.16 | 3 (15%) | 26,32,35 | 1.25 | 3 (11%) |
| 56 | MIA | 1y | 37 | 56 | 21,24,32 | 1.82 | 3 (14%) | 30,35,47 | 2.02 | 9 (30%) |
| 54 | PSU | 2w | 55 | 54 | 18,21,22 | 1.47 | 2 (11%) | 21,30,33 | 2.06 | 4 (19%) |
| 55 | 31H | 1x | 76 | 58,55 | 31,34,35 | 1.36 | 4 (12%) | 35,47,50 | 2.07 | 11 (31%) |
| 32 | MA6 | 2a | 1518 | 32 | 23,26,27 | 0.42 | 0 | 33,38,41 | 2.10 | 10 (30%) |
| 1 | 5MC | 1A | 1962 | 58,1 | 19,22,23 | 1.90 | 4 (21%) | 26,32,35 | 1.39 | 5 (19%) |
| 54 | PSU | 1w | 39 | 54 | 18,21,22 | 1.42 | 3 (16%) | 21,30,33 | 2.03 | 4 (19%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|---------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 1 | OMG | 1A | 2251 | 58,55,1 | 23,26,27 | 1.38 | 3 (13%) | 32,38,41 | 1.95 | 7 (21%) |
| 56 | PSU | 2y | 32 | 56 | 18,21,22 | 1.40 | 2 (11%) | 21,30,33 | 1.92 | 3 (14%) |
| 1 | OMG | 2A | 2251 | 58,55,1 | 23,26,27 | 1.32 | 3 (13%) | 32,38,41 | 1.96 | 7 (21%) |
| 54 | 4SU | 1w | 8 | 54 | 18,21,22 | 1.89 | 4 (22%) | 25,30,33 | 1.87 | 6 (24%) |
| 54 | MIA | 2w | 37 | 54 | 24,27,32 | 2.14 | 6 (25%) | 32,39,47 | 2.44 | 10 (31%) |
| 1 | OMU | 2A | 2552 | 58,1 | 19,22,23 | 1.10 | 2 (10%) | 25,31,34 | 1.81 | 5 (20%) |
| 1 | PSU | 2A | 1917 | 1 | 18,21,22 | 1.42 | 2 (11%) | 21,30,33 | 1.81 | 4 (19%) |
| 32 | MA6 | 1a | 1519 | 32 | 23,26,27 | 0.51 | 0 | 33,38,41 | 2.14 | 9 (27%) |
| 54 | PSU | 1w | 55 | 54 | 18,21,22 | 1.39 | 2 (11%) | 21,30,33 | 1.82 | 4 (19%) |
| 56 | PSU | 1y | 39 | 56 | 18,21,22 | 1.55 | 2 (11%) | 21,30,33 | 1.74 | 3 (14%) |
| 1 | 2MA | 1A | 2503 | 58,1 | 22,25,26 | 1.38 | 4 (18%) | 32,37,40 | 2.41 | 8 (25%) |
| 32 | 5MC | 1a | 1407 | 32 | 19,22,23 | 1.43 | 2 (10%) | 26,32,35 | 1.07 | 4 (15%) |
| 1 | 5MU | 1A | 1915 | 1 | 19,22,23 | 1.39 | 4 (21%) | 27,32,35 | 2.67 | 10 (37%) |
| 56 | PSU | 1y | 55 | 56 | 18,21,22 | 1.51 | 3 (16%) | 21,30,33 | 2.02 | 4 (19%) |
| 54 | PSU | 1w | 32 | 54 | 18,21,22 | 1.35 | 3 (16%) | 21,30,33 | 1.81 | 4 (19%) |
| 1 | PSU | 1A | 1917 | 1 | 18,21,22 | 1.33 | 3 (16%) | 21,30,33 | 2.06 | 5 (23%) |
| 32 | 5MC | 2a | 1400 | 32 | 19,22,23 | 1.74 | 3 (15%) | 26,32,35 | 1.38 | 2 (7%) |
| 32 | G7M | 1a | 527 | 32 | 23,26,27 | 1.58 | 4 (17%) | 34,39,42 | 1.45 | 3 (8%) |
| 32 | M2G | 1a | 966 | 32 | 24,27,28 | 1.37 | 4 (16%) | 33,40,43 | 2.05 | 6 (18%) |
| 54 | 5MU | 1w | 54 | 54 | 19,22,23 | 1.48 | 4 (21%) | 27,32,35 | 2.14 | 5 (18%) |
| 56 | 5MU | 1y | 54 | 56 | 19,22,23 | 1.58 | 4 (21%) | 27,32,35 | 1.87 | 7 (25%) |
| 56 | G7M | 2y | 46 | 56 | 23,26,27 | 1.68 | 5 (21%) | 34,39,42 | 2.01 | 4 (11%) |
| 32 | MA6 | 2a | 1519 | 32 | 23,26,27 | 0.49 | 0 | 33,38,41 | 2.09 | 10 (30%) |
| 54 | G7M | 2w | 46 | 54 | 23,26,27 | 1.49 | 3 (13%) | 34,39,42 | 1.64 | 5 (14%) |
| 55 | 5MC | 2x | 32 | 55 | 19,22,23 | 1.57 | 3 (15%) | 26,32,35 | 1.56 | 6 (23%) |
| 56 | PSU | 2y | 39 | 56 | 18,21,22 | 1.41 | 2 (11%) | 21,30,33 | 1.58 | 3 (14%) |
| 56 | MIA | 2y | 37 | 56 | 21,24,32 | 1.67 | 3 (14%) | 30,35,47 | 2.12 | 7 (23%) |
| 54 | PSU | 2w | 32 | 54 | 18,21,22 | 1.41 | 2 (11%) | 21,30,33 | 2.06 | 5 (23%) |
| 32 | 2MG | 1a | 1207 | 58,32 | 23,26,27 | 1.27 | 2 (8%) | 33,38,41 | 2.25 | 9 (27%) |
| 54 | MIA | 1w | 37 | 54 | 28,31,32 | 2.38 | 6 (21%) | 38,44,47 | 2.76 | 14 (36%) |
| 56 | PSU | 2y | 55 | 56 | 18,21,22 | 1.43 | 2 (11%) | 21,30,33 | 2.17 | 4 (19%) |
| 1 | 2MA | 2A | 2503 | 58,1 | 22,25,26 | 1.46 | 5 (22%) | 32,37,40 | 2.25 | 9 (28%) |
| 32 | PSU | 1a | 516 | 32 | 18,21,22 | 1.46 | 3 (16%) | 21,30,33 | 1.79 | 4 (19%) |
| 55 | 5MU | 1x | 54 | 55 | 19,22,23 | 1.49 | 5 (26%) | 27,32,35 | 2.04 | 6 (22%) |
| 1 | 5MC | 1A | 1942 | 58,1 | 19,22,23 | 1.26 | 2 (10%) | 26,32,35 | 1.50 | 5 (19%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 1 | OMC | 1A | 1920 | 1 | 19,22,23 | 0.80 | 0 | 25,31,34 | 1.08 | 2 (8%) |
| 43 | 0TD | 2l | 92 | 43 | 8,9,10 | 5.12 | 2 (25%) | 6,11,13 | 2.48 | 1 (16%) |
| 55 | 4SU | 1x | 8 | 55 | 18,21,22 | 2.24 | 5 (27%) | 25,30,33 | 1.80 | 6 (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 |
|-----|------|-------|------|----------|---------|------------|---------|
| 54 | PSU | 2w | 39 | 54 | - | 0/7/25/26 | 0/2/2/2 |
| 55 | PSU | 2x | 55 | 55 | - | 0/7/25/26 | 0/2/2/2 |
| 32 | 4OC | 2a | 1402 | 32 | - | 0/9/29/30 | 0/2/2/2 |
| 32 | M2G | 2a | 966 | 32 | - | 0/11/29/30 | 0/3/3/3 |
| 56 | 4SU | 1y | 8 | 56 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | PSU | 2A | 2605 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 32 | 5MC | 2a | 967 | 32 | - | 0/7/25/26 | 0/2/2/2 |
| 32 | 2MG | 2a | 1207 | 58,32 | - | 1/9/27/28 | 0/3/3/3 |
| 32 | 5MC | 2a | 1407 | 58,32 | - | 0/7/25/26 | 0/2/2/2 |
| 56 | PSU | 1y | 32 | 56 | - | 0/7/25/26 | 0/2/2/2 |
| 32 | PSU | 2a | 516 | 32 | - | 0/7/25/26 | 0/2/2/2 |
| 32 | 5MC | 1a | 1400 | 32 | - | 0/7/25/26 | 0/2/2/2 |
| 55 | PSU | 1x | 55 | 55 | - | 0/7/25/26 | 0/2/2/2 |
| 32 | 4OC | 1a | 1402 | 32 | - | 0/9/29/30 | 0/2/2/2 |
| 55 | 31H | 2x | 76 | 58,55,59 | - | 4/22/40/41 | 0/3/3/3 |
| 55 | 4SU | 2x | 8 | 55 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | 5MU | 2A | 1939 | 58,1 | - | 0/7/25/26 | 0/2/2/2 |
| 32 | UR3 | 1a | 1498 | 32 | - | 0/7/25/26 | 0/2/2/2 |
| 54 | F3N | 1w | 76 | 1 | - | 2/19/37/38 | 0/4/4/4 |
| 54 | 5MU | 2w | 54 | 54 | - | 0/7/25/26 | 0/2/2/2 |
| 32 | G7M | 2a | 527 | 58,32 | - | 2/7/25/26 | 0/3/3/3 |
| 1 | OMC | 2A | 1920 | 1 | - | 0/9/27/28 | 0/2/2/2 |
| 54 | G7M | 1w | 46 | 54 | - | 1/7/25/26 | 0/3/3/3 |
| 1 | PSU | 1A | 2605 | 58,1 | - | 0/7/25/26 | 0/2/2/2 |
| 32 | UR3 | 2a | 1498 | 32 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | PSU | 1A | 1911 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 56 | 5MU | 2y | 54 | 56 | - | 2/7/25/26 | 0/2/2/2 |
| 54 | F3N | 2w | 76 | 1 | - | 4/19/37/38 | 0/4/4/4 |
| 32 | 5MC | 2a | 1404 | 32 | - | 0/7/25/26 | 0/2/2/2 |
| 32 | MA6 | 1a | 1518 | 32 | - | 0/11/29/30 | 0/3/3/3 |
| 56 | 4SU | 2y | 8 | 56,58 | - | 1/7/25/26 | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|---------|---------|------------|---------|
| 1 | 5MC | 2A | 1942 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 54 | 4SU | 2w | 8 | 54 | - | 0/7/25/26 | 0/2/2/2 |
| 55 | 5MU | 2x | 54 | 55 | - | 0/7/25/26 | 0/2/2/2 |
| 55 | 5MC | 1x | 32 | 55 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | PSU | 2A | 1911 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | 5MU | 2A | 1915 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 56 | G7M | 1y | 46 | 56 | - | 2/7/25/26 | 0/3/3/3 |
| 1 | 5MC | 2A | 1962 | 58,1 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | OMU | 1A | 2552 | 58,1 | - | 0/9/27/28 | 0/2/2/2 |
| 1 | 5MU | 1A | 1939 | 58,1 | - | 0/7/25/26 | 0/2/2/2 |
| 43 | 0TD | 1l | 92 | 43 | - | 4/7/12/14 | - |
| 32 | 5MC | 1a | 967 | 32 | - | 1/7/25/26 | 0/2/2/2 |
| 32 | 5MC | 1a | 1404 | 32 | - | 0/7/25/26 | 0/2/2/2 |
| 56 | MIA | 1y | 37 | 56 | - | 3/7/25/34 | 0/3/3/3 |
| 54 | PSU | 2w | 55 | 54 | - | 0/7/25/26 | 0/2/2/2 |
| 55 | 31H | 1x | 76 | 58,55 | - | 4/22/40/41 | 0/3/3/3 |
| 32 | MA6 | 2a | 1518 | 32 | - | 0/11/29/30 | 0/3/3/3 |
| 1 | 5MC | 1A | 1962 | 58,1 | - | 0/7/25/26 | 0/2/2/2 |
| 54 | PSU | 1w | 39 | 54 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | OMG | 1A | 2251 | 58,55,1 | - | 1/9/27/28 | 0/3/3/3 |
| 56 | PSU | 2y | 32 | 56 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | OMG | 2A | 2251 | 58,55,1 | - | 0/9/27/28 | 0/3/3/3 |
| 54 | 4SU | 1w | 8 | 54 | - | 0/7/25/26 | 0/2/2/2 |
| 54 | MIA | 2w | 37 | 54 | - | 2/11/29/34 | 0/3/3/3 |
| 1 | OMU | 2A | 2552 | 58,1 | - | 0/9/27/28 | 0/2/2/2 |
| 1 | PSU | 2A | 1917 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 32 | MA6 | 1a | 1519 | 32 | - | 2/11/29/30 | 0/3/3/3 |
| 54 | PSU | 1w | 55 | 54 | - | 2/7/25/26 | 0/2/2/2 |
| 56 | PSU | 1y | 39 | 56 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | 2MA | 1A | 2503 | 58,1 | - | 1/7/25/26 | 0/3/3/3 |
| 32 | 5MC | 1a | 1407 | 32 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | 5MU | 1A | 1915 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 56 | PSU | 1y | 55 | 56 | - | 1/7/25/26 | 0/2/2/2 |
| 54 | PSU | 1w | 32 | 54 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | PSU | 1A | 1917 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 32 | 5MC | 2a | 1400 | 32 | - | 0/7/25/26 | 0/2/2/2 |
| 32 | G7M | 1a | 527 | 32 | - | 3/7/25/26 | 0/3/3/3 |
| 32 | M2G | 1a | 966 | 32 | - | 0/11/29/30 | 0/3/3/3 |
| 54 | 5MU | 1w | 54 | 54 | - | 0/7/25/26 | 0/2/2/2 |
| 56 | 5MU | 1y | 54 | 56 | - | 0/7/25/26 | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|-------|---------|------------|---------|
| 56 | G7M | 2y | 46 | 56 | - | 2/7/25/26 | 0/3/3/3 |
| 32 | MA6 | 2a | 1519 | 32 | - | 3/11/29/30 | 0/3/3/3 |
| 54 | G7M | 2w | 46 | 54 | - | 3/7/25/26 | 0/3/3/3 |
| 55 | 5MC | 2x | 32 | 55 | - | 0/7/25/26 | 0/2/2/2 |
| 56 | PSU | 2y | 39 | 56 | - | 0/7/25/26 | 0/2/2/2 |
| 56 | MIA | 2y | 37 | 56 | - | 2/7/25/34 | 0/3/3/3 |
| 54 | PSU | 2w | 32 | 54 | - | 0/7/25/26 | 0/2/2/2 |
| 32 | 2MG | 1a | 1207 | 58,32 | - | 0/9/27/28 | 0/3/3/3 |
| 54 | MIA | 1w | 37 | 54 | - | 4/15/33/34 | 0/3/3/3 |
| 56 | PSU | 2y | 55 | 56 | - | 1/7/25/26 | 0/2/2/2 |
| 1 | 2MA | 2A | 2503 | 58,1 | - | 1/7/25/26 | 0/3/3/3 |
| 32 | PSU | 1a | 516 | 32 | - | 1/7/25/26 | 0/2/2/2 |
| 55 | 5MU | 1x | 54 | 55 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | 5MC | 1A | 1942 | 58,1 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | OMC | 1A | 1920 | 1 | - | 0/9/27/28 | 0/2/2/2 |
| 43 | 0TD | 2l | 92 | 43 | - | 3/7/12/14 | - |
| 55 | 4SU | 1x | 8 | 55 | - | 0/7/25/26 | 0/2/2/2 |

All (262) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|--------|-------------|----------|
| 43 | 2l | 92 | 0TD | CB-SB | -13.70 | 1.68 | 1.82 |
| 43 | 1l | 92 | 0TD | CB-SB | -10.44 | 1.71 | 1.82 |
| 54 | 1w | 37 | MIA | C2-S10 | -7.76 | 1.69 | 1.75 |
| 1 | 1A | 1962 | 5MC | C5-C4 | 6.84 | 1.49 | 1.44 |
| 54 | 1w | 37 | MIA | C13-C14 | 6.80 | 1.52 | 1.32 |
| 32 | 2a | 1404 | 5MC | C5-C4 | 6.57 | 1.49 | 1.44 |
| 54 | 2w | 37 | MIA | C2-S10 | -6.54 | 1.70 | 1.75 |
| 55 | 1x | 32 | 5MC | C5-C4 | 6.44 | 1.49 | 1.44 |
| 32 | 1a | 967 | 5MC | C5-C4 | 6.26 | 1.48 | 1.44 |
| 32 | 2a | 1400 | 5MC | C5-C4 | 6.22 | 1.48 | 1.44 |
| 56 | 1y | 37 | MIA | C5-C4 | 5.95 | 1.49 | 1.39 |
| 32 | 2a | 967 | 5MC | C5-C4 | 5.84 | 1.48 | 1.44 |
| 32 | 2a | 1407 | 5MC | C5-C4 | 5.75 | 1.48 | 1.44 |
| 55 | 2x | 76 | 31H | C5-N7 | -5.72 | 1.28 | 1.39 |
| 55 | 1x | 8 | 4SU | C4-N3 | -5.54 | 1.31 | 1.37 |
| 55 | 2x | 32 | 5MC | C5-C4 | 5.50 | 1.48 | 1.44 |
| 56 | 2y | 37 | MIA | C5-C4 | 5.38 | 1.48 | 1.39 |
| 56 | 1y | 39 | PSU | C6-C5 | 5.29 | 1.41 | 1.35 |
| 54 | 2w | 37 | MIA | C5-C4 | 5.29 | 1.48 | 1.39 |
| 55 | 1x | 8 | 4SU | C2-N3 | -5.26 | 1.28 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 54 | 2w | 8 | 4SU | C4-S4 | -5.21 | 1.59 | 1.68 |
| 32 | 1a | 527 | G7M | C5-N7 | -5.16 | 1.33 | 1.39 |
| 1 | 2A | 1962 | 5MC | C5-C4 | 5.08 | 1.48 | 1.44 |
| 54 | 2w | 76 | F3N | CB-CG | -4.96 | 1.39 | 1.51 |
| 56 | 1y | 55 | PSU | C6-C5 | 4.79 | 1.40 | 1.35 |
| 32 | 1a | 1407 | 5MC | C5-C4 | 4.76 | 1.47 | 1.44 |
| 54 | 1w | 8 | 4SU | C4-S4 | -4.64 | 1.60 | 1.68 |
| 54 | 2w | 55 | PSU | C6-C5 | 4.64 | 1.40 | 1.35 |
| 56 | 2y | 32 | PSU | C6-C5 | 4.54 | 1.40 | 1.35 |
| 56 | 1y | 32 | PSU | C6-C5 | 4.54 | 1.40 | 1.35 |
| 55 | 2x | 8 | 4SU | C4-N3 | -4.49 | 1.33 | 1.37 |
| 56 | 2y | 46 | G7M | C5-N7 | -4.48 | 1.34 | 1.39 |
| 32 | 2a | 527 | G7M | C5-N7 | -4.47 | 1.34 | 1.39 |
| 54 | 1w | 46 | G7M | C5-N7 | -4.46 | 1.34 | 1.39 |
| 54 | 2w | 46 | G7M | C5-N7 | -4.46 | 1.34 | 1.39 |
| 56 | 2y | 8 | 4SU | C4-S4 | -4.31 | 1.61 | 1.68 |
| 54 | 1w | 37 | MIA | C5-C4 | 4.29 | 1.46 | 1.39 |
| 1 | 2A | 1911 | PSU | C6-C5 | 4.26 | 1.40 | 1.35 |
| 1 | 1A | 1911 | PSU | C6-C5 | 4.26 | 1.40 | 1.35 |
| 55 | 1x | 76 | 31H | C5-N7 | -4.17 | 1.31 | 1.39 |
| 32 | 1a | 1400 | 5MC | C5-C4 | 4.17 | 1.47 | 1.44 |
| 56 | 2y | 39 | PSU | C6-C5 | 4.16 | 1.39 | 1.35 |
| 54 | 1w | 8 | 4SU | C4-N3 | -4.12 | 1.33 | 1.37 |
| 32 | 1a | 516 | PSU | C6-C5 | 4.06 | 1.39 | 1.35 |
| 54 | 1w | 76 | F3N | CB-CG | -4.03 | 1.41 | 1.51 |
| 56 | 2y | 46 | G7M | C5-C4 | 4.02 | 1.48 | 1.38 |
| 55 | 2x | 8 | 4SU | C2-N3 | -4.00 | 1.31 | 1.38 |
| 54 | 2w | 76 | F3N | C5-N7 | -3.99 | 1.31 | 1.39 |
| 54 | 2w | 32 | PSU | C6-C5 | 3.98 | 1.39 | 1.35 |
| 32 | 2a | 516 | PSU | C6-C5 | 3.97 | 1.39 | 1.35 |
| 1 | 2A | 2503 | 2MA | C5-C4 | 3.96 | 1.46 | 1.39 |
| 54 | 1w | 76 | F3N | C5-N7 | -3.82 | 1.32 | 1.39 |
| 1 | 1A | 1942 | 5MC | C5-C4 | 3.82 | 1.47 | 1.44 |
| 54 | 1w | 55 | PSU | C6-C5 | 3.81 | 1.39 | 1.35 |
| 56 | 1y | 8 | 4SU | C4-S4 | -3.76 | 1.62 | 1.68 |
| 32 | 2a | 1404 | 5MC | C6-C5 | 3.75 | 1.40 | 1.34 |
| 1 | 2A | 1939 | 5MU | C6-C5 | 3.71 | 1.40 | 1.34 |
| 56 | 1y | 46 | G7M | C5-C4 | 3.64 | 1.47 | 1.38 |
| 1 | 2A | 1942 | 5MC | C5-C4 | 3.63 | 1.46 | 1.44 |
| 56 | 2y | 55 | PSU | C6-C5 | 3.62 | 1.39 | 1.35 |
| 1 | 2A | 1917 | PSU | C6-C5 | 3.62 | 1.39 | 1.35 |
| 55 | 2x | 8 | 4SU | C4-S4 | -3.54 | 1.62 | 1.68 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 55 | 1x | 8 | 4SU | C4-S4 | -3.53 | 1.62 | 1.68 |
| 1 | 1A | 1915 | 5MU | C2-N1 | 3.51 | 1.44 | 1.38 |
| 54 | 1w | 46 | G7M | C5-C4 | 3.48 | 1.47 | 1.38 |
| 1 | 2A | 2605 | PSU | C6-C5 | 3.48 | 1.39 | 1.35 |
| 56 | 2y | 54 | 5MU | C2-N1 | 3.44 | 1.43 | 1.38 |
| 54 | 2w | 39 | PSU | C6-C5 | 3.43 | 1.39 | 1.35 |
| 32 | 1a | 1207 | 2MG | C5-C4 | 3.41 | 1.48 | 1.38 |
| 32 | 2a | 1207 | 2MG | C5-C4 | 3.40 | 1.48 | 1.38 |
| 43 | 2l | 92 | 0TD | CB-CA | 3.36 | 1.55 | 1.54 |
| 1 | 2A | 2251 | OMG | C6-N1 | -3.35 | 1.32 | 1.38 |
| 1 | 1A | 1939 | 5MU | C4-C5 | 3.35 | 1.50 | 1.44 |
| 32 | 2a | 1498 | UR3 | C2-N1 | 3.34 | 1.43 | 1.38 |
| 55 | 2x | 55 | PSU | C6-C5 | 3.33 | 1.39 | 1.35 |
| 32 | 1a | 967 | 5MC | C6-C5 | 3.31 | 1.40 | 1.34 |
| 56 | 2y | 54 | 5MU | C6-C5 | 3.31 | 1.40 | 1.34 |
| 56 | 1y | 37 | MIA | C5-C6 | 3.29 | 1.50 | 1.41 |
| 32 | 2a | 527 | G7M | C5-C4 | 3.29 | 1.46 | 1.38 |
| 54 | 2w | 8 | 4SU | C5-C4 | -3.28 | 1.38 | 1.42 |
| 1 | 1A | 1942 | 5MC | C6-N1 | -3.28 | 1.32 | 1.38 |
| 1 | 1A | 1917 | PSU | C6-C5 | 3.27 | 1.38 | 1.35 |
| 55 | 1x | 76 | 31H | C5-C4 | -3.27 | 1.33 | 1.39 |
| 1 | 1A | 2605 | PSU | C6-C5 | 3.27 | 1.38 | 1.35 |
| 32 | 1a | 966 | M2G | C6-N1 | -3.25 | 1.32 | 1.38 |
| 1 | 2A | 2251 | OMG | C5-C4 | 3.23 | 1.47 | 1.38 |
| 54 | 1w | 32 | PSU | C6-C5 | 3.22 | 1.38 | 1.35 |
| 54 | 1w | 54 | 5MU | C6-C5 | 3.21 | 1.39 | 1.34 |
| 54 | 1w | 39 | PSU | C6-C5 | 3.16 | 1.38 | 1.35 |
| 1 | 2A | 1939 | 5MU | C4-N3 | -3.16 | 1.32 | 1.38 |
| 32 | 1a | 527 | G7M | C5-C4 | 3.16 | 1.46 | 1.38 |
| 56 | 2y | 54 | 5MU | C4-C5 | 3.16 | 1.50 | 1.44 |
| 1 | 1A | 2251 | OMG | C6-N1 | -3.16 | 1.32 | 1.38 |
| 32 | 1a | 1404 | 5MC | C5-C4 | 3.15 | 1.46 | 1.44 |
| 56 | 1y | 54 | 5MU | C2-N1 | 3.14 | 1.43 | 1.38 |
| 56 | 2y | 8 | 4SU | C2-N1 | 3.14 | 1.43 | 1.38 |
| 32 | 1a | 966 | M2G | C5-C4 | 3.11 | 1.47 | 1.38 |
| 54 | 2w | 46 | G7M | C5-C4 | 3.11 | 1.46 | 1.38 |
| 56 | 1y | 46 | G7M | C5-N7 | -3.10 | 1.35 | 1.39 |
| 56 | 1y | 54 | 5MU | C6-C5 | 3.09 | 1.39 | 1.34 |
| 55 | 2x | 54 | 5MU | C6-C5 | 3.09 | 1.39 | 1.34 |
| 32 | 2a | 966 | M2G | C5-C4 | 3.09 | 1.47 | 1.38 |
| 1 | 1A | 2503 | 2MA | C5-C4 | 3.08 | 1.44 | 1.39 |
| 55 | 1x | 54 | 5MU | C4-N3 | -3.07 | 1.33 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 54 | 2w | 76 | F3N | C5-C4 | -3.07 | 1.33 | 1.39 |
| 1 | 1A | 1939 | 5MU | C2-N1 | 3.06 | 1.43 | 1.38 |
| 54 | 1w | 54 | 5MU | C2-N1 | 3.05 | 1.43 | 1.38 |
| 32 | 1a | 1407 | 5MC | C6-C5 | 3.04 | 1.39 | 1.34 |
| 54 | 2w | 37 | MIA | C5-C6 | 3.03 | 1.49 | 1.41 |
| 1 | 1A | 1939 | 5MU | C4-N3 | -3.00 | 1.33 | 1.38 |
| 55 | 1x | 54 | 5MU | C6-C5 | 3.00 | 1.39 | 1.34 |
| 54 | 1w | 39 | PSU | C4-N3 | -3.00 | 1.33 | 1.38 |
| 55 | 1x | 76 | 31H | C5-C6 | -2.98 | 1.32 | 1.41 |
| 55 | 1x | 55 | PSU | C6-C5 | 2.97 | 1.38 | 1.35 |
| 56 | 1y | 54 | 5MU | C4-C5 | 2.97 | 1.49 | 1.44 |
| 1 | 1A | 2251 | OMG | C5-C4 | 2.96 | 1.46 | 1.38 |
| 54 | 1w | 76 | F3N | C5-C4 | -2.95 | 1.33 | 1.39 |
| 55 | 1x | 32 | 5MC | C6-N1 | -2.95 | 1.33 | 1.38 |
| 56 | 2y | 37 | MIA | C5-C6 | 2.89 | 1.49 | 1.41 |
| 54 | 1w | 37 | MIA | C5-N7 | -2.87 | 1.33 | 1.39 |
| 1 | 2A | 1915 | 5MU | C6-C5 | 2.86 | 1.39 | 1.34 |
| 54 | 2w | 8 | 4SU | C4-N3 | -2.83 | 1.34 | 1.37 |
| 54 | 1w | 8 | 4SU | C5-C4 | -2.83 | 1.39 | 1.42 |
| 1 | 1A | 1917 | PSU | C4-N3 | -2.82 | 1.33 | 1.38 |
| 54 | 2w | 32 | PSU | C4-N3 | -2.81 | 1.33 | 1.38 |
| 1 | 1A | 1962 | 5MC | C6-C5 | 2.80 | 1.39 | 1.34 |
| 54 | 2w | 39 | PSU | C4-N3 | -2.79 | 1.33 | 1.38 |
| 1 | 1A | 1939 | 5MU | C6-C5 | 2.78 | 1.39 | 1.34 |
| 54 | 1w | 32 | PSU | C4-N3 | -2.78 | 1.33 | 1.38 |
| 56 | 2y | 8 | 4SU | C4-N3 | -2.74 | 1.34 | 1.37 |
| 55 | 2x | 54 | 5MU | C4-C5 | 2.73 | 1.49 | 1.44 |
| 54 | 1w | 55 | PSU | C4-N3 | -2.72 | 1.33 | 1.38 |
| 32 | 2a | 967 | 5MC | C6-N1 | -2.71 | 1.33 | 1.38 |
| 1 | 1A | 1939 | 5MU | C2-N3 | -2.70 | 1.33 | 1.38 |
| 32 | 1a | 1400 | 5MC | C6-C5 | 2.69 | 1.39 | 1.34 |
| 1 | 1A | 2503 | 2MA | C5-N7 | -2.69 | 1.34 | 1.39 |
| 1 | 2A | 1942 | 5MC | C6-N1 | -2.69 | 1.33 | 1.38 |
| 55 | 1x | 8 | 4SU | C5-C4 | -2.68 | 1.39 | 1.42 |
| 1 | 1A | 2552 | OMU | C4-N3 | -2.68 | 1.34 | 1.38 |
| 1 | 2A | 2503 | 2MA | C8-N7 | 2.67 | 1.36 | 1.31 |
| 54 | 2w | 76 | F3N | C2'-C3' | -2.67 | 1.49 | 1.53 |
| 54 | 1w | 8 | 4SU | C2-N3 | -2.67 | 1.33 | 1.38 |
| 55 | 2x | 55 | PSU | C4-N3 | -2.67 | 1.33 | 1.38 |
| 56 | 2y | 37 | MIA | C8-N7 | 2.67 | 1.36 | 1.31 |
| 56 | 1y | 37 | MIA | C8-N7 | 2.66 | 1.36 | 1.31 |
| 32 | 2a | 1400 | 5MC | C6-C5 | 2.65 | 1.38 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1 | 2A | 1962 | 5MC | C6-C5 | 2.64 | 1.38 | 1.34 |
| 32 | 1a | 1400 | 5MC | C6-N1 | -2.64 | 1.33 | 1.38 |
| 55 | 1x | 55 | PSU | C4-N3 | -2.63 | 1.33 | 1.38 |
| 1 | 2A | 1917 | PSU | C4-N3 | -2.62 | 1.33 | 1.38 |
| 32 | 1a | 966 | M2G | C2-N2 | 2.60 | 1.39 | 1.35 |
| 55 | 2x | 32 | 5MC | C6-N1 | -2.60 | 1.33 | 1.38 |
| 55 | 2x | 76 | 31H | C8-N9 | -2.59 | 1.33 | 1.37 |
| 1 | 2A | 2503 | 2MA | C5-C6 | 2.57 | 1.48 | 1.41 |
| 1 | 1A | 1915 | 5MU | C4-C5 | 2.57 | 1.49 | 1.44 |
| 32 | 2a | 1207 | 2MG | C6-N1 | -2.55 | 1.34 | 1.38 |
| 55 | 1x | 54 | 5MU | C4-C5 | 2.54 | 1.49 | 1.44 |
| 1 | 2A | 1939 | 5MU | C2-N3 | -2.53 | 1.33 | 1.38 |
| 32 | 1a | 516 | PSU | C4-N3 | -2.53 | 1.34 | 1.38 |
| 54 | 2w | 54 | 5MU | C6-N1 | -2.53 | 1.33 | 1.38 |
| 54 | 2w | 76 | F3N | C5-C6 | -2.52 | 1.34 | 1.41 |
| 55 | 2x | 8 | 4SU | C5-C4 | -2.52 | 1.39 | 1.42 |
| 1 | 1A | 2605 | PSU | O4'-C1' | -2.50 | 1.40 | 1.43 |
| 1 | 1A | 2503 | 2MA | C5-C6 | 2.49 | 1.47 | 1.41 |
| 1 | 2A | 1939 | 5MU | C2-N1 | 2.49 | 1.42 | 1.38 |
| 1 | 2A | 2503 | 2MA | C4-N9 | -2.49 | 1.32 | 1.37 |
| 1 | 2A | 1962 | 5MC | C6-N1 | -2.48 | 1.33 | 1.38 |
| 1 | 2A | 1915 | 5MU | C2-N1 | 2.48 | 1.42 | 1.38 |
| 55 | 2x | 32 | 5MC | C6-C5 | 2.48 | 1.38 | 1.34 |
| 56 | 2y | 55 | PSU | C4-N3 | -2.47 | 1.34 | 1.38 |
| 55 | 1x | 8 | 4SU | C6-C5 | 2.47 | 1.40 | 1.35 |
| 1 | 1A | 1939 | 5MU | C6-N1 | -2.47 | 1.33 | 1.38 |
| 32 | 1a | 1207 | 2MG | C6-N1 | -2.46 | 1.34 | 1.38 |
| 1 | 2A | 1911 | PSU | C4-N3 | -2.45 | 1.34 | 1.38 |
| 56 | 1y | 54 | 5MU | C4-N3 | -2.45 | 1.34 | 1.38 |
| 32 | 1a | 527 | G7M | C4-N9 | -2.44 | 1.31 | 1.38 |
| 32 | 1a | 527 | G7M | C6-N1 | -2.44 | 1.34 | 1.38 |
| 56 | 1y | 8 | 4SU | C4-N3 | -2.44 | 1.35 | 1.37 |
| 54 | 1w | 76 | F3N | C3'-N3' | 2.43 | 1.49 | 1.45 |
| 56 | 1y | 46 | G7M | C5-C6 | 2.43 | 1.50 | 1.43 |
| 1 | 1A | 2605 | PSU | C2-N1 | -2.42 | 1.33 | 1.36 |
| 55 | 1x | 55 | PSU | C2-N3 | -2.42 | 1.33 | 1.37 |
| 32 | 2a | 1407 | 5MC | C6-N1 | -2.42 | 1.33 | 1.38 |
| 32 | 2a | 1400 | 5MC | C6-N1 | -2.41 | 1.33 | 1.38 |
| 1 | 1A | 2605 | PSU | C4-N3 | -2.40 | 1.34 | 1.38 |
| 54 | 1w | 76 | F3N | C5-C6 | -2.40 | 1.34 | 1.41 |
| 1 | 2A | 2503 | 2MA | C5-N7 | -2.40 | 1.34 | 1.39 |
| 32 | 2a | 966 | M2G | C6-N1 | -2.38 | 1.34 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 54 | 1w | 76 | F3N | C1'-N9 | 2.38 | 1.52 | 1.46 |
| 56 | 1y | 8 | 4SU | C2-N1 | 2.37 | 1.42 | 1.38 |
| 32 | 1a | 1404 | 5MC | C6-C5 | 2.36 | 1.38 | 1.34 |
| 32 | 2a | 966 | M2G | C2-N2 | 2.36 | 1.39 | 1.35 |
| 54 | 1w | 37 | MIA | C5-C6 | 2.36 | 1.47 | 1.41 |
| 54 | 1w | 54 | 5MU | C4-N3 | -2.36 | 1.34 | 1.38 |
| 55 | 2x | 8 | 4SU | C6-C5 | 2.34 | 1.40 | 1.35 |
| 1 | 2A | 1920 | OMC | C6-C5 | 2.34 | 1.40 | 1.35 |
| 54 | 2w | 54 | 5MU | C4-N3 | -2.34 | 1.34 | 1.38 |
| 32 | 2a | 1404 | 5MC | C6-N1 | -2.34 | 1.34 | 1.38 |
| 54 | 2w | 55 | PSU | C4-N3 | -2.33 | 1.34 | 1.38 |
| 1 | 1A | 2251 | OMG | C5-N7 | -2.33 | 1.34 | 1.39 |
| 56 | 2y | 39 | PSU | C4-N3 | -2.32 | 1.34 | 1.38 |
| 1 | 2A | 1915 | 5MU | C4-N3 | -2.31 | 1.34 | 1.38 |
| 55 | 1x | 32 | 5MC | C6-C5 | 2.31 | 1.38 | 1.34 |
| 54 | 2w | 37 | MIA | C8-N7 | 2.29 | 1.36 | 1.31 |
| 43 | 1l | 92 | 0TD | CSB-SB | -2.28 | 1.75 | 1.79 |
| 54 | 2w | 37 | MIA | C5-N7 | -2.27 | 1.34 | 1.39 |
| 56 | 1y | 8 | 4SU | O2-C2 | 2.25 | 1.27 | 1.23 |
| 1 | 1A | 1962 | 5MC | C6-N1 | -2.25 | 1.34 | 1.38 |
| 32 | 2a | 527 | G7M | C4-N9 | -2.23 | 1.32 | 1.38 |
| 56 | 1y | 55 | PSU | C4-C5 | 2.23 | 1.50 | 1.44 |
| 1 | 1A | 2552 | OMU | C5-C4 | -2.23 | 1.38 | 1.43 |
| 54 | 2w | 46 | G7M | C4-N9 | -2.22 | 1.32 | 1.38 |
| 54 | 1w | 46 | G7M | C6-N1 | -2.22 | 1.34 | 1.38 |
| 56 | 1y | 8 | 4SU | C6-C5 | 2.21 | 1.40 | 1.35 |
| 32 | 2a | 527 | G7M | C5-C6 | 2.21 | 1.49 | 1.43 |
| 32 | 1a | 516 | PSU | C2-N3 | -2.21 | 1.33 | 1.37 |
| 1 | 2A | 2552 | OMU | C5-C4 | -2.20 | 1.38 | 1.43 |
| 54 | 1w | 39 | PSU | C2-N3 | -2.20 | 1.33 | 1.37 |
| 32 | 1a | 1404 | 5MC | C6-N1 | -2.19 | 1.34 | 1.38 |
| 1 | 1A | 1911 | PSU | C4-N3 | -2.19 | 1.34 | 1.38 |
| 54 | 1w | 37 | MIA | C4-N9 | -2.19 | 1.33 | 1.37 |
| 1 | 1A | 1915 | 5MU | C6-N1 | -2.18 | 1.34 | 1.38 |
| 56 | 2y | 46 | G7M | C6-N1 | -2.17 | 1.34 | 1.38 |
| 1 | 1A | 1917 | PSU | C2-N3 | -2.17 | 1.33 | 1.37 |
| 56 | 2y | 8 | 4SU | C6-C5 | 2.17 | 1.40 | 1.35 |
| 1 | 2A | 1915 | 5MU | C4-C5 | 2.17 | 1.48 | 1.44 |
| 1 | 1A | 1915 | 5MU | C6-C5 | 2.16 | 1.38 | 1.34 |
| 1 | 1A | 2503 | 2MA | C4-N9 | -2.16 | 1.33 | 1.37 |
| 56 | 2y | 46 | G7M | C2-N3 | 2.16 | 1.38 | 1.33 |
| 32 | 2a | 1498 | UR3 | O2-C2 | 2.14 | 1.26 | 1.22 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1 | 2A | 2552 | OMU | C6-C5 | 2.14 | 1.40 | 1.35 |
| 56 | 2y | 46 | G7M | C5-C6 | 2.14 | 1.49 | 1.43 |
| 54 | 1w | 32 | PSU | C2-N3 | -2.13 | 1.34 | 1.37 |
| 32 | 2a | 1407 | 5MC | C6-C5 | 2.13 | 1.38 | 1.34 |
| 32 | 2a | 1207 | 2MG | C5-N7 | -2.13 | 1.34 | 1.39 |
| 54 | 2w | 37 | MIA | C2-N3 | 2.13 | 1.37 | 1.34 |
| 1 | 2A | 1915 | 5MU | C6-N1 | -2.12 | 1.34 | 1.38 |
| 55 | 1x | 76 | 31H | O4'-C4' | -2.11 | 1.40 | 1.45 |
| 55 | 1x | 54 | 5MU | C6-N1 | -2.11 | 1.34 | 1.38 |
| 56 | 1y | 55 | PSU | C4-N3 | -2.11 | 1.34 | 1.38 |
| 1 | 2A | 2251 | OMG | C5-N7 | -2.11 | 1.34 | 1.39 |
| 32 | 1a | 1498 | UR3 | C2-N1 | 2.09 | 1.41 | 1.38 |
| 55 | 2x | 55 | PSU | C4-C5 | 2.09 | 1.50 | 1.44 |
| 56 | 2y | 32 | PSU | C4-C5 | 2.09 | 1.50 | 1.44 |
| 54 | 2w | 8 | 4SU | C2-N1 | 2.08 | 1.41 | 1.38 |
| 1 | 1A | 2605 | PSU | C2-N3 | -2.07 | 1.34 | 1.37 |
| 55 | 1x | 54 | 5MU | C2-N1 | 2.07 | 1.41 | 1.38 |
| 56 | 2y | 8 | 4SU | O2-C2 | 2.06 | 1.26 | 1.23 |
| 1 | 1A | 2552 | OMU | C2-N1 | 2.05 | 1.41 | 1.38 |
| 54 | 2w | 54 | 5MU | C4-C5 | 2.05 | 1.48 | 1.44 |
| 1 | 1A | 1962 | 5MC | C2-N1 | 2.05 | 1.44 | 1.40 |
| 54 | 1w | 54 | 5MU | C2-N3 | -2.04 | 1.34 | 1.38 |
| 1 | 2A | 2605 | PSU | C4-N3 | -2.04 | 1.35 | 1.38 |
| 32 | 2a | 966 | M2G | C5-N7 | -2.03 | 1.35 | 1.39 |
| 1 | 1A | 1911 | PSU | O4'-C1' | -2.03 | 1.41 | 1.43 |
| 56 | 1y | 39 | PSU | C4-N3 | -2.02 | 1.35 | 1.38 |
| 1 | 2A | 1942 | 5MC | C6-C5 | 2.02 | 1.37 | 1.34 |
| 32 | 2a | 527 | G7M | C6-N1 | -2.02 | 1.35 | 1.38 |
| 32 | 1a | 966 | M2G | C2-N3 | 2.02 | 1.37 | 1.32 |
| 32 | 2a | 516 | PSU | C4-N3 | -2.01 | 1.35 | 1.38 |
| 1 | 2A | 2605 | PSU | C2-N3 | -2.01 | 1.34 | 1.37 |
| 56 | 1y | 32 | PSU | C4-C5 | 2.00 | 1.49 | 1.44 |

All (473) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 43 | 1l | 92 | 0TD | CSB-SB-CB | -12.53 | 79.84 | 102.36 |
| 54 | 1w | 37 | MIA | C12-C13-C14 | -9.06 | 110.74 | 127.01 |
| 1 | 2A | 2503 | 2MA | C5-C4-N3 | -8.40 | 118.33 | 127.18 |
| 1 | 1A | 2503 | 2MA | C5-C4-N3 | -8.24 | 118.50 | 127.18 |
| 54 | 2w | 37 | MIA | C5-C4-N3 | -7.76 | 119.00 | 127.18 |
| 54 | 1w | 37 | MIA | C5-C4-N3 | -7.59 | 119.18 | 127.18 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 32 | 2a | 1207 | 2MG | C2-N3-C4 | 7.28 | 121.11 | 112.00 |
| 32 | 2a | 1498 | UR3 | C4-N3-C2 | -7.12 | 118.85 | 124.58 |
| 32 | 1a | 966 | M2G | C5-C4-N3 | -6.89 | 117.43 | 128.39 |
| 56 | 2y | 55 | PSU | N1-C2-N3 | 6.86 | 122.41 | 115.17 |
| 32 | 1a | 1498 | UR3 | C4-N3-C2 | -6.80 | 119.11 | 124.58 |
| 1 | 2A | 2605 | PSU | N1-C2-N3 | 6.80 | 122.34 | 115.17 |
| 32 | 1a | 1207 | 2MG | C2-N3-C4 | 6.79 | 120.50 | 112.00 |
| 55 | 2x | 76 | 31H | O4'-C1'-N9 | -6.72 | 95.18 | 108.09 |
| 54 | 2w | 8 | 4SU | C4-N3-C2 | -6.59 | 120.99 | 127.31 |
| 54 | 2w | 8 | 4SU | C5-C4-N3 | 6.55 | 120.84 | 114.75 |
| 56 | 2y | 46 | G7M | N9-C4-N3 | 6.53 | 139.02 | 125.95 |
| 56 | 2y | 37 | MIA | C5-C4-N3 | -6.47 | 117.81 | 126.72 |
| 1 | 2A | 1911 | PSU | N1-C2-N3 | 6.41 | 121.94 | 115.17 |
| 32 | 2a | 1207 | 2MG | C5-C4-N3 | -6.28 | 118.40 | 128.39 |
| 54 | 1w | 39 | PSU | N1-C2-N3 | 6.28 | 121.79 | 115.17 |
| 1 | 1A | 2503 | 2MA | N3-C4-N9 | 6.27 | 134.95 | 126.99 |
| 1 | 2A | 2251 | OMG | C5-C4-N3 | -6.27 | 118.41 | 128.39 |
| 1 | 1A | 1911 | PSU | N1-C2-N3 | 6.26 | 121.78 | 115.17 |
| 56 | 1y | 55 | PSU | N1-C2-N3 | 6.26 | 121.77 | 115.17 |
| 54 | 2w | 37 | MIA | N3-C4-N9 | 6.24 | 134.91 | 126.99 |
| 54 | 1w | 37 | MIA | N3-C4-N9 | 6.23 | 134.89 | 126.99 |
| 32 | 2a | 966 | M2G | C5-C4-N3 | -6.20 | 118.52 | 128.39 |
| 1 | 2A | 1939 | 5MU | N3-C2-N1 | 6.20 | 122.96 | 114.89 |
| 1 | 1A | 1939 | 5MU | C5-C4-N3 | 6.17 | 120.68 | 115.32 |
| 54 | 2w | 32 | PSU | N1-C2-N3 | 6.15 | 121.66 | 115.17 |
| 55 | 2x | 55 | PSU | N1-C2-N3 | 6.13 | 121.64 | 115.17 |
| 32 | 1a | 1207 | 2MG | C5-C4-N3 | -6.06 | 118.75 | 128.39 |
| 55 | 2x | 76 | 31H | N1-C2-N3 | -6.06 | 119.41 | 128.58 |
| 56 | 2y | 8 | 4SU | C4-N3-C2 | -6.05 | 121.52 | 127.31 |
| 1 | 2A | 1915 | 5MU | O4-C4-C5 | -6.03 | 118.02 | 124.92 |
| 1 | 1A | 1915 | 5MU | N3-C2-N1 | 6.02 | 122.72 | 114.89 |
| 56 | 2y | 46 | G7M | C5-C4-N3 | -6.01 | 116.80 | 128.15 |
| 54 | 2w | 55 | PSU | N1-C2-N3 | 6.00 | 121.50 | 115.17 |
| 54 | 1w | 46 | G7M | N9-C4-N3 | 5.98 | 137.91 | 125.95 |
| 32 | 2a | 516 | PSU | N1-C2-N3 | 5.94 | 121.43 | 115.17 |
| 1 | 1A | 2552 | OMU | C4-N3-C2 | -5.93 | 119.26 | 126.61 |
| 55 | 1x | 55 | PSU | N1-C2-N3 | 5.87 | 121.36 | 115.17 |
| 56 | 2y | 32 | PSU | N1-C2-N3 | 5.85 | 121.34 | 115.17 |
| 1 | 1A | 1939 | 5MU | C4-N3-C2 | -5.78 | 119.76 | 127.34 |
| 43 | 2l | 92 | 0TD | CSB-SB-CB | -5.73 | 92.06 | 102.36 |
| 54 | 2w | 76 | F3N | N1-C2-N3 | -5.73 | 119.91 | 128.58 |
| 54 | 1w | 76 | F3N | N1-C2-N3 | -5.71 | 119.94 | 128.58 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 1 | 2A | 1915 | 5MU | C4-N3-C2 | -5.71 | 119.86 | 127.34 |
| 1 | 1A | 1917 | PSU | N1-C2-N3 | 5.68 | 121.16 | 115.17 |
| 1 | 1A | 1915 | 5MU | C4-N3-C2 | -5.60 | 120.00 | 127.34 |
| 55 | 2x | 54 | 5MU | N3-C2-N1 | 5.58 | 122.15 | 114.89 |
| 56 | 1y | 46 | G7M | N9-C4-N3 | 5.52 | 137.00 | 125.95 |
| 54 | 2w | 54 | 5MU | C4-N3-C2 | -5.52 | 120.11 | 127.34 |
| 1 | 2A | 1917 | PSU | N1-C2-N3 | 5.51 | 120.98 | 115.17 |
| 1 | 1A | 2251 | OMG | C5-C4-N3 | -5.51 | 119.63 | 128.39 |
| 1 | 1A | 1915 | 5MU | O4-C4-C5 | -5.50 | 118.63 | 124.92 |
| 1 | 2A | 1939 | 5MU | C4-N3-C2 | -5.46 | 120.18 | 127.34 |
| 1 | 1A | 2605 | PSU | N1-C2-N3 | 5.45 | 120.92 | 115.17 |
| 54 | 1w | 54 | 5MU | O4-C4-C5 | -5.45 | 118.69 | 124.92 |
| 54 | 2w | 54 | 5MU | O4-C4-C5 | -5.43 | 118.70 | 124.92 |
| 54 | 1w | 55 | PSU | N1-C2-N3 | 5.38 | 120.85 | 115.17 |
| 32 | 1a | 516 | PSU | N1-C2-N3 | 5.34 | 120.80 | 115.17 |
| 54 | 1w | 46 | G7M | C5-C4-N3 | -5.31 | 118.11 | 128.15 |
| 55 | 2x | 54 | 5MU | C4-N3-C2 | -5.29 | 120.41 | 127.34 |
| 56 | 1y | 37 | MIA | C5-C4-N3 | -5.28 | 119.45 | 126.72 |
| 54 | 2w | 8 | 4SU | C5-C4-S4 | -5.27 | 118.29 | 124.31 |
| 1 | 2A | 1915 | 5MU | C5-C4-N3 | 5.26 | 119.90 | 115.32 |
| 32 | 1a | 966 | M2G | N9-C4-N3 | 5.23 | 136.41 | 125.95 |
| 1 | 2A | 1915 | 5MU | N3-C2-N1 | 5.22 | 121.68 | 114.89 |
| 32 | 2a | 1518 | MA6 | N1-C2-N3 | -5.19 | 120.72 | 128.58 |
| 54 | 2w | 54 | 5MU | C5-C4-N3 | 5.19 | 119.83 | 115.32 |
| 32 | 2a | 527 | G7M | N9-C4-N3 | 5.16 | 136.27 | 125.95 |
| 56 | 2y | 37 | MIA | N3-C4-N9 | 5.15 | 135.93 | 127.17 |
| 54 | 1w | 76 | F3N | C5-C4-N3 | -5.14 | 119.64 | 126.72 |
| 1 | 2A | 2503 | 2MA | N3-C4-N9 | 5.12 | 133.49 | 126.99 |
| 56 | 1y | 46 | G7M | C5-C4-N3 | -5.10 | 118.51 | 128.15 |
| 56 | 2y | 54 | 5MU | C5-C4-N3 | 5.08 | 119.73 | 115.32 |
| 56 | 2y | 54 | 5MU | C4-N3-C2 | -5.07 | 120.69 | 127.34 |
| 56 | 2y | 8 | 4SU | C5-C4-N3 | 5.07 | 119.46 | 114.75 |
| 32 | 1a | 1519 | MA6 | C5-C4-N3 | -5.05 | 119.76 | 126.72 |
| 56 | 2y | 46 | G7M | C2-N3-C4 | 5.04 | 120.98 | 112.30 |
| 55 | 1x | 76 | 31H | N1-C2-N3 | -5.00 | 121.02 | 128.58 |
| 32 | 2a | 1518 | MA6 | C5-C4-N3 | -4.99 | 119.84 | 126.72 |
| 54 | 2w | 76 | F3N | C5-C4-N3 | -4.99 | 119.85 | 126.72 |
| 55 | 2x | 54 | 5MU | O4-C4-C5 | -4.98 | 119.22 | 124.92 |
| 56 | 2y | 39 | PSU | N1-C2-N3 | 4.92 | 120.35 | 115.17 |
| 1 | 2A | 2552 | OMU | O2-C2-N1 | -4.90 | 116.41 | 122.80 |
| 32 | 1a | 1519 | MA6 | N1-C2-N3 | -4.89 | 121.18 | 128.58 |
| 56 | 1y | 39 | PSU | N1-C2-N3 | 4.87 | 120.31 | 115.17 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | 2A | 1939 | 5MU | C5-C4-N3 | 4.86 | 119.55 | 115.32 |
| 1 | 1A | 1939 | 5MU | C5-C6-N1 | -4.85 | 118.05 | 123.31 |
| 55 | 1x | 54 | 5MU | N3-C2-N1 | 4.82 | 121.16 | 114.89 |
| 56 | 1y | 46 | G7M | C2-N3-C4 | 4.80 | 120.56 | 112.30 |
| 1 | 2A | 2251 | OMG | N9-C4-N3 | 4.80 | 135.54 | 125.95 |
| 32 | 2a | 527 | G7M | C5-C4-N3 | -4.78 | 119.11 | 128.15 |
| 32 | 2a | 1519 | MA6 | N1-C2-N3 | -4.76 | 121.38 | 128.58 |
| 1 | 2A | 2605 | PSU | C4-N3-C2 | -4.75 | 119.83 | 126.37 |
| 1 | 1A | 2251 | OMG | C2-N3-C4 | 4.73 | 120.44 | 112.30 |
| 55 | 1x | 32 | 5MC | C5-C6-N1 | -4.72 | 118.18 | 123.31 |
| 54 | 1w | 8 | 4SU | C4-N3-C2 | -4.71 | 122.80 | 127.31 |
| 1 | 2A | 2251 | OMG | C2-N3-C4 | 4.70 | 120.39 | 112.30 |
| 54 | 2w | 32 | PSU | C4-N3-C2 | -4.70 | 119.90 | 126.37 |
| 54 | 1w | 54 | 5MU | C4-N3-C2 | -4.69 | 121.19 | 127.34 |
| 54 | 1w | 46 | G7M | C2-N3-C4 | 4.69 | 120.37 | 112.30 |
| 55 | 1x | 54 | 5MU | C4-N3-C2 | -4.68 | 121.21 | 127.34 |
| 56 | 1y | 32 | PSU | N1-C2-N3 | 4.67 | 120.10 | 115.17 |
| 1 | 1A | 1915 | 5MU | C1'-N1-C2 | 4.63 | 125.91 | 117.59 |
| 1 | 1A | 1939 | 5MU | N3-C2-N1 | 4.60 | 120.88 | 114.89 |
| 56 | 2y | 54 | 5MU | N3-C2-N1 | 4.58 | 120.85 | 114.89 |
| 56 | 1y | 37 | MIA | N3-C4-N9 | 4.55 | 134.90 | 127.17 |
| 55 | 1x | 8 | 4SU | O2-C2-N1 | 4.52 | 128.68 | 122.80 |
| 54 | 2w | 54 | 5MU | N3-C2-N1 | 4.52 | 120.77 | 114.89 |
| 1 | 1A | 2552 | OMU | N3-C2-N1 | 4.51 | 120.77 | 114.89 |
| 32 | 1a | 967 | 5MC | C5-C6-N1 | -4.49 | 118.43 | 123.31 |
| 56 | 2y | 54 | 5MU | O4-C4-C5 | -4.43 | 119.85 | 124.92 |
| 54 | 2w | 46 | G7M | N9-C4-N3 | 4.42 | 134.79 | 125.95 |
| 54 | 1w | 8 | 4SU | C5-C4-N3 | 4.40 | 118.84 | 114.75 |
| 54 | 2w | 39 | PSU | N1-C2-N3 | 4.39 | 119.80 | 115.17 |
| 54 | 1w | 54 | 5MU | C5-C6-N1 | -4.39 | 118.55 | 123.31 |
| 54 | 2w | 46 | G7M | C5-C4-N3 | -4.38 | 119.88 | 128.15 |
| 54 | 2w | 46 | G7M | C2-N3-C4 | 4.38 | 119.84 | 112.30 |
| 54 | 1w | 37 | MIA | C15-C14-C13 | -4.36 | 109.56 | 122.66 |
| 55 | 2x | 54 | 5MU | O2-C2-N1 | -4.36 | 117.12 | 122.80 |
| 32 | 1a | 527 | G7M | C5-C4-N3 | -4.36 | 119.91 | 128.15 |
| 1 | 1A | 2251 | OMG | N9-C4-N3 | 4.35 | 134.66 | 125.95 |
| 54 | 1w | 32 | PSU | N1-C2-N3 | 4.35 | 119.75 | 115.17 |
| 56 | 2y | 55 | PSU | O2-C2-N1 | -4.35 | 118.31 | 122.79 |
| 32 | 1a | 966 | M2G | C2-N3-C4 | 4.34 | 120.54 | 112.51 |
| 54 | 2w | 37 | MIA | C12-N6-C6 | -4.34 | 118.83 | 122.85 |
| 54 | 1w | 54 | 5MU | C5-C4-N3 | 4.34 | 119.09 | 115.32 |
| 1 | 2A | 1911 | PSU | O2-C2-N1 | -4.32 | 118.33 | 122.79 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 54 | 1w | 54 | 5MU | N3-C2-N1 | 4.32 | 120.52 | 114.89 |
| 32 | 2a | 1519 | MA6 | C5-C4-N3 | -4.31 | 120.78 | 126.72 |
| 56 | 1y | 37 | MIA | N3-C2-N1 | -4.30 | 122.08 | 128.58 |
| 32 | 2a | 527 | G7M | C2-N3-C4 | 4.29 | 119.69 | 112.30 |
| 1 | 1A | 1917 | PSU | C4-N3-C2 | -4.27 | 120.50 | 126.37 |
| 56 | 1y | 8 | 4SU | C4-N3-C2 | -4.26 | 123.23 | 127.31 |
| 56 | 1y | 54 | 5MU | N3-C2-N1 | 4.24 | 120.41 | 114.89 |
| 32 | 1a | 527 | G7M | C2-N3-C4 | 4.24 | 119.61 | 112.30 |
| 1 | 1A | 2552 | OMU | C5-C4-N3 | 4.24 | 120.74 | 114.80 |
| 32 | 1a | 1518 | MA6 | N1-C2-N3 | -4.23 | 122.19 | 128.58 |
| 55 | 2x | 55 | PSU | C4-N3-C2 | -4.22 | 120.56 | 126.37 |
| 55 | 2x | 32 | 5MC | C5-C4-N3 | -4.21 | 117.44 | 121.75 |
| 32 | 2a | 966 | M2G | N9-C4-N3 | 4.20 | 134.36 | 125.95 |
| 32 | 2a | 966 | M2G | C2-N3-C4 | 4.15 | 120.18 | 112.51 |
| 1 | 1A | 1911 | PSU | C4-N3-C2 | -4.11 | 120.70 | 126.37 |
| 32 | 2a | 1519 | MA6 | C4-C5-N7 | -4.08 | 105.91 | 110.58 |
| 1 | 2A | 1939 | 5MU | O4-C4-C5 | -4.07 | 120.27 | 124.92 |
| 32 | 2a | 516 | PSU | C4-N3-C2 | -4.06 | 120.78 | 126.37 |
| 56 | 2y | 32 | PSU | C4-N3-C2 | -4.05 | 120.79 | 126.37 |
| 1 | 1A | 1917 | PSU | O2-C2-N1 | -4.04 | 118.62 | 122.79 |
| 32 | 1a | 1207 | 2MG | C6-C5-N7 | 4.04 | 137.63 | 130.29 |
| 32 | 2a | 1518 | MA6 | C2-N1-C6 | 4.02 | 121.66 | 111.83 |
| 32 | 1a | 527 | G7M | N9-C4-N3 | 4.01 | 133.98 | 125.95 |
| 56 | 2y | 8 | 4SU | N3-C2-N1 | 4.01 | 120.12 | 114.89 |
| 55 | 1x | 54 | 5MU | C5-C6-N1 | -3.99 | 118.98 | 123.31 |
| 32 | 2a | 1400 | 5MC | C5-C6-N1 | -3.98 | 118.98 | 123.31 |
| 56 | 1y | 54 | 5MU | C5-C4-N3 | 3.98 | 118.78 | 115.32 |
| 1 | 1A | 2605 | PSU | C4-N3-C2 | -3.98 | 120.89 | 126.37 |
| 56 | 2y | 55 | PSU | C4-N3-C2 | -3.97 | 120.90 | 126.37 |
| 55 | 1x | 76 | 31H | C5-C4-N3 | -3.97 | 121.25 | 126.72 |
| 54 | 1w | 8 | 4SU | N3-C2-N1 | 3.97 | 120.06 | 114.89 |
| 54 | 2w | 55 | PSU | C4-N3-C2 | -3.95 | 120.93 | 126.37 |
| 32 | 1a | 1518 | MA6 | N9-C8-N7 | -3.93 | 108.36 | 113.94 |
| 32 | 2a | 1519 | MA6 | C2-N1-C6 | 3.93 | 121.42 | 111.83 |
| 1 | 2A | 2503 | 2MA | C4-C5-N7 | -3.92 | 106.10 | 110.58 |
| 1 | 2A | 2552 | OMU | C4-N3-C2 | -3.92 | 121.75 | 126.61 |
| 32 | 1a | 1518 | MA6 | C5-N7-C8 | 3.92 | 109.61 | 103.45 |
| 55 | 2x | 76 | 31H | N9-C8-N7 | -3.92 | 108.38 | 113.94 |
| 32 | 1a | 1519 | MA6 | C5-N7-C8 | 3.91 | 109.59 | 103.45 |
| 56 | 1y | 54 | 5MU | C4-N3-C2 | -3.90 | 122.22 | 127.34 |
| 55 | 1x | 54 | 5MU | C5-C4-N3 | 3.90 | 118.71 | 115.32 |
| 54 | 1w | 39 | PSU | O2-C2-N1 | -3.89 | 118.78 | 122.79 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | 2A | 2605 | PSU | O2-C2-N1 | -3.88 | 118.79 | 122.79 |
| 32 | 1a | 1519 | MA6 | C4-C5-N7 | -3.88 | 106.14 | 110.58 |
| 55 | 1x | 8 | 4SU | C4-N3-C2 | 3.85 | 131.00 | 127.31 |
| 32 | 1a | 1518 | MA6 | C5-C4-N3 | -3.84 | 121.42 | 126.72 |
| 56 | 1y | 32 | PSU | C6-C5-C4 | -3.82 | 115.59 | 118.17 |
| 1 | 1A | 2503 | 2MA | C4-C5-N7 | -3.82 | 106.21 | 110.58 |
| 56 | 1y | 8 | 4SU | C5-C4-N3 | 3.81 | 118.29 | 114.75 |
| 56 | 1y | 37 | MIA | C2-N3-C4 | 3.81 | 121.13 | 111.83 |
| 55 | 2x | 76 | 31H | C4'-O4'-C1' | -3.81 | 101.06 | 109.47 |
| 54 | 2w | 8 | 4SU | N3-C2-N1 | 3.80 | 119.84 | 114.89 |
| 54 | 2w | 54 | 5MU | O2-C2-N1 | -3.80 | 117.85 | 122.80 |
| 1 | 1A | 1911 | PSU | O2-C2-N1 | -3.79 | 118.88 | 122.79 |
| 1 | 2A | 1939 | 5MU | C5-C6-N1 | -3.78 | 119.20 | 123.31 |
| 32 | 1a | 1207 | 2MG | N9-C4-N3 | 3.78 | 133.51 | 125.95 |
| 56 | 2y | 37 | MIA | C2-N3-C4 | 3.78 | 121.06 | 111.83 |
| 56 | 1y | 55 | PSU | C4-N3-C2 | -3.77 | 121.17 | 126.37 |
| 32 | 2a | 1519 | MA6 | C5-N7-C8 | 3.77 | 109.38 | 103.45 |
| 32 | 1a | 1519 | MA6 | C2-N3-C4 | 3.77 | 121.03 | 111.83 |
| 32 | 2a | 1518 | MA6 | C2-N3-C4 | 3.76 | 121.02 | 111.83 |
| 55 | 1x | 8 | 4SU | C6-C5-C4 | -3.76 | 116.70 | 119.95 |
| 54 | 1w | 39 | PSU | C4-N3-C2 | -3.75 | 121.20 | 126.37 |
| 32 | 2a | 1518 | MA6 | C4-C5-N7 | -3.71 | 106.34 | 110.58 |
| 55 | 2x | 54 | 5MU | C5-C4-N3 | 3.71 | 118.55 | 115.32 |
| 55 | 1x | 76 | 31H | O2'-C2'-C3' | 3.71 | 120.24 | 111.16 |
| 54 | 2w | 37 | MIA | C4-C5-N7 | -3.70 | 106.35 | 110.58 |
| 1 | 1A | 2251 | OMG | C6-C5-N7 | 3.70 | 137.02 | 130.29 |
| 54 | 1w | 32 | PSU | C4-N3-C2 | -3.69 | 121.29 | 126.37 |
| 32 | 2a | 1207 | 2MG | N1-C2-N2 | 3.68 | 120.32 | 116.56 |
| 32 | 2a | 516 | PSU | O2-C2-N1 | -3.67 | 119.01 | 122.79 |
| 56 | 1y | 39 | PSU | C6-C5-C4 | -3.66 | 115.70 | 118.17 |
| 1 | 2A | 1917 | PSU | C4-N3-C2 | -3.65 | 121.34 | 126.37 |
| 32 | 2a | 1404 | 5MC | C5-C6-N1 | -3.65 | 119.35 | 123.31 |
| 32 | 2a | 1207 | 2MG | N9-C4-N3 | 3.64 | 133.23 | 125.95 |
| 43 | 1l | 92 | 0TD | OD2-CG-CB | 3.64 | 121.01 | 113.15 |
| 1 | 2A | 2552 | OMU | N3-C2-N1 | 3.62 | 119.61 | 114.89 |
| 32 | 2a | 1207 | 2MG | C6-C5-N7 | 3.61 | 136.87 | 130.29 |
| 54 | 1w | 55 | PSU | C4-N3-C2 | -3.61 | 121.40 | 126.37 |
| 55 | 1x | 32 | 5MC | C5-C4-N3 | -3.60 | 118.06 | 121.75 |
| 32 | 1a | 1519 | MA6 | C2-N1-C6 | 3.59 | 120.60 | 111.83 |
| 55 | 2x | 76 | 31H | C5-C4-N3 | -3.59 | 121.78 | 126.72 |
| 1 | 1A | 1915 | 5MU | C5-C4-N3 | 3.58 | 118.43 | 115.32 |
| 1 | 2A | 1911 | PSU | C4-N3-C2 | -3.57 | 121.46 | 126.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 32 | 2a | 1400 | 5MC | O2-C2-N3 | -3.56 | 116.72 | 122.33 |
| 55 | 2x | 76 | 31H | C2-N3-C4 | 3.56 | 120.52 | 111.83 |
| 32 | 1a | 516 | PSU | C4-N3-C2 | -3.56 | 121.47 | 126.37 |
| 55 | 1x | 76 | 31H | C5-N7-C8 | 3.53 | 109.00 | 103.45 |
| 54 | 2w | 55 | PSU | C6-C5-C4 | -3.52 | 115.80 | 118.17 |
| 55 | 1x | 54 | 5MU | O2-C2-N1 | -3.51 | 118.23 | 122.80 |
| 55 | 1x | 76 | 31H | C4'-O4'-C1' | -3.49 | 101.75 | 109.47 |
| 32 | 1a | 1518 | MA6 | C2-N1-C6 | 3.49 | 120.37 | 111.83 |
| 32 | 2a | 1207 | 2MG | N2-C2-N3 | -3.49 | 116.07 | 120.51 |
| 54 | 2w | 76 | F3N | N9-C8-N7 | -3.48 | 109.00 | 113.94 |
| 55 | 2x | 76 | 31H | CA-N-CN | -3.48 | 117.48 | 122.82 |
| 32 | 1a | 1207 | 2MG | C4-C5-N7 | -3.48 | 105.16 | 110.67 |
| 54 | 1w | 76 | F3N | C2-N3-C4 | 3.47 | 120.31 | 111.83 |
| 56 | 2y | 37 | MIA | C4-C5-N7 | -3.47 | 106.62 | 110.58 |
| 1 | 1A | 1915 | 5MU | C6-N1-C2 | -3.45 | 117.87 | 121.30 |
| 54 | 1w | 37 | MIA | C2-N3-C4 | 3.44 | 121.30 | 112.29 |
| 32 | 1a | 1519 | MA6 | N9-C8-N7 | -3.43 | 109.07 | 113.94 |
| 55 | 1x | 76 | 31H | N9-C8-N7 | -3.43 | 109.07 | 113.94 |
| 56 | 1y | 32 | PSU | O2-C2-N1 | -3.42 | 119.26 | 122.79 |
| 32 | 2a | 1407 | 5MC | C5-C6-N1 | -3.42 | 119.60 | 123.31 |
| 1 | 1A | 1942 | 5MC | C5-C4-N3 | -3.42 | 118.25 | 121.75 |
| 54 | 1w | 76 | F3N | N9-C8-N7 | -3.42 | 109.09 | 113.94 |
| 32 | 2a | 1407 | 5MC | O2-C2-N3 | -3.41 | 116.95 | 122.33 |
| 54 | 2w | 76 | F3N | C2-N3-C4 | 3.40 | 120.13 | 111.83 |
| 1 | 2A | 1915 | 5MU | C5-C6-N1 | -3.39 | 119.63 | 123.31 |
| 55 | 2x | 76 | 31H | N3-C4-N9 | 3.37 | 132.90 | 127.17 |
| 1 | 1A | 1942 | 5MC | C1'-N1-C6 | -3.37 | 115.60 | 121.15 |
| 1 | 2A | 1962 | 5MC | C5-C4-N3 | -3.37 | 118.30 | 121.75 |
| 32 | 2a | 1519 | MA6 | C2-N3-C4 | 3.36 | 120.04 | 111.83 |
| 32 | 2a | 1518 | MA6 | C5-N7-C8 | 3.35 | 108.72 | 103.45 |
| 32 | 2a | 1407 | 5MC | C5-C4-N3 | -3.34 | 118.33 | 121.75 |
| 54 | 1w | 32 | PSU | C6-C5-C4 | -3.33 | 115.93 | 118.17 |
| 32 | 1a | 1518 | MA6 | C4-C5-N7 | -3.31 | 106.80 | 110.58 |
| 56 | 2y | 37 | MIA | N3-C2-N1 | -3.30 | 123.58 | 128.58 |
| 1 | 1A | 2552 | OMU | O4-C4-C5 | -3.30 | 119.47 | 125.16 |
| 55 | 1x | 55 | PSU | C4-N3-C2 | -3.29 | 121.84 | 126.37 |
| 54 | 1w | 8 | 4SU | C5-C4-S4 | -3.27 | 120.58 | 124.31 |
| 55 | 1x | 8 | 4SU | S4-C4-N3 | -3.26 | 116.80 | 120.20 |
| 55 | 1x | 54 | 5MU | O4-C4-C5 | -3.25 | 121.19 | 124.92 |
| 1 | 1A | 1942 | 5MC | CM5-C5-C6 | -3.25 | 118.45 | 122.85 |
| 56 | 1y | 55 | PSU | O2-C2-N1 | -3.25 | 119.43 | 122.79 |
| 54 | 2w | 54 | 5MU | C5M-C5-C4 | 3.24 | 122.24 | 118.78 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 56 | 1y | 8 | 4SU | N3-C2-N1 | 3.24 | 119.11 | 114.89 |
| 56 | 1y | 54 | 5MU | O4-C4-C5 | -3.24 | 121.21 | 124.92 |
| 1 | 1A | 2503 | 2MA | C5-N7-C8 | 3.24 | 108.54 | 103.45 |
| 55 | 2x | 76 | 31H | C5-N7-C8 | 3.22 | 108.52 | 103.45 |
| 54 | 1w | 37 | MIA | C16-C14-C13 | -3.21 | 113.01 | 122.66 |
| 1 | 1A | 1915 | 5MU | C5M-C5-C4 | 3.21 | 122.21 | 118.78 |
| 32 | 2a | 1498 | UR3 | C5-C4-N3 | 3.19 | 119.25 | 115.04 |
| 1 | 1A | 1939 | 5MU | O4-C4-C5 | -3.19 | 121.27 | 124.92 |
| 32 | 2a | 966 | M2G | C6-C5-N7 | 3.17 | 136.05 | 130.29 |
| 1 | 2A | 2251 | OMG | C6-C5-N7 | 3.16 | 136.04 | 130.29 |
| 1 | 2A | 1942 | 5MC | C5-C6-N1 | -3.16 | 119.88 | 123.31 |
| 32 | 1a | 1404 | 5MC | C5-C4-N3 | -3.14 | 118.54 | 121.75 |
| 54 | 1w | 37 | MIA | C4-C5-N7 | -3.13 | 107.00 | 110.58 |
| 55 | 2x | 32 | 5MC | C5-C6-N1 | -3.13 | 119.91 | 123.31 |
| 32 | 1a | 1519 | MA6 | N3-C4-N9 | 3.12 | 132.48 | 127.17 |
| 54 | 2w | 76 | F3N | C5-N7-C8 | 3.12 | 108.35 | 103.45 |
| 32 | 2a | 1207 | 2MG | C4-C5-N7 | -3.12 | 105.73 | 110.67 |
| 56 | 1y | 39 | PSU | C4-N3-C2 | -3.11 | 122.09 | 126.37 |
| 55 | 2x | 76 | 31H | O2'-C2'-C3' | 3.09 | 118.73 | 111.16 |
| 32 | 2a | 966 | M2G | C4-C5-N7 | -3.08 | 105.78 | 110.67 |
| 32 | 1a | 1518 | MA6 | C2-N3-C4 | 3.08 | 119.35 | 111.83 |
| 1 | 1A | 2503 | 2MA | C4-N9-C8 | 3.08 | 108.97 | 105.74 |
| 54 | 1w | 37 | MIA | C6-C5-N7 | 3.07 | 135.78 | 132.43 |
| 1 | 1A | 2605 | PSU | O2-C2-N1 | -3.07 | 119.62 | 122.79 |
| 55 | 1x | 76 | 31H | CA-N-CN | -3.07 | 118.10 | 122.82 |
| 32 | 1a | 1400 | 5MC | C5-C4-N3 | -3.07 | 118.61 | 121.75 |
| 1 | 2A | 1917 | PSU | O2-C2-N1 | -3.06 | 119.63 | 122.79 |
| 32 | 2a | 1519 | MA6 | N9-C8-N7 | -3.06 | 109.59 | 113.94 |
| 32 | 2a | 1404 | 5MC | C5-C4-N3 | -3.06 | 118.62 | 121.75 |
| 1 | 1A | 1915 | 5MU | C5M-C5-C6 | -3.06 | 118.71 | 122.85 |
| 55 | 2x | 54 | 5MU | C5-C6-N1 | -3.03 | 120.02 | 123.31 |
| 54 | 1w | 76 | F3N | C5-N7-C8 | 3.03 | 108.21 | 103.45 |
| 32 | 1a | 1400 | 5MC | C5-C6-N1 | -3.03 | 120.02 | 123.31 |
| 56 | 1y | 32 | PSU | C4-N3-C2 | -3.01 | 122.22 | 126.37 |
| 1 | 1A | 1915 | 5MU | C1'-N1-C6 | -3.00 | 116.20 | 121.15 |
| 54 | 2w | 37 | MIA | C2-N3-C4 | 3.00 | 120.16 | 112.29 |
| 54 | 2w | 55 | PSU | O2-C2-N1 | -3.00 | 119.69 | 122.79 |
| 55 | 1x | 76 | 31H | C5-C4-N9 | 3.00 | 109.08 | 105.81 |
| 32 | 2a | 516 | PSU | C6-C5-C4 | -3.00 | 116.15 | 118.17 |
| 1 | 1A | 1962 | 5MC | O2-C2-N3 | -3.00 | 117.61 | 122.33 |
| 1 | 2A | 1962 | 5MC | C5-C6-N1 | -2.99 | 120.06 | 123.31 |
| 32 | 2a | 967 | 5MC | C1'-N1-C6 | -2.98 | 116.25 | 121.15 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | 2A | 1915 | 5MU | O2-C2-N1 | -2.98 | 118.92 | 122.80 |
| 55 | 2x | 32 | 5MC | CM5-C5-C6 | -2.97 | 118.83 | 122.85 |
| 32 | 2a | 967 | 5MC | C5-C6-N1 | -2.96 | 120.09 | 123.31 |
| 1 | 1A | 2503 | 2MA | N9-C8-N7 | -2.96 | 109.73 | 113.94 |
| 1 | 2A | 2552 | OMU | O4-C4-C5 | -2.93 | 120.10 | 125.16 |
| 32 | 1a | 1404 | 5MC | C5-C6-N1 | -2.92 | 120.14 | 123.31 |
| 1 | 1A | 2552 | OMU | O2-C2-N1 | -2.92 | 118.99 | 122.80 |
| 1 | 2A | 2552 | OMU | C5-C4-N3 | 2.91 | 118.88 | 114.80 |
| 56 | 1y | 37 | MIA | C4-C5-N7 | -2.89 | 107.27 | 110.58 |
| 54 | 2w | 37 | MIA | C6-C5-N7 | 2.89 | 135.58 | 132.43 |
| 56 | 2y | 8 | 4SU | C5-C4-S4 | -2.88 | 121.01 | 124.31 |
| 54 | 2w | 54 | 5MU | C5-C6-N1 | -2.86 | 120.20 | 123.31 |
| 32 | 1a | 966 | M2G | C4-C5-N7 | -2.86 | 106.13 | 110.67 |
| 1 | 1A | 1920 | OMC | O2-C2-N3 | -2.86 | 117.82 | 122.33 |
| 54 | 1w | 76 | F3N | C5-C4-N9 | 2.86 | 108.93 | 105.81 |
| 56 | 2y | 32 | PSU | O2-C2-N1 | -2.86 | 119.84 | 122.79 |
| 32 | 1a | 1498 | UR3 | C5-C4-N3 | 2.86 | 118.80 | 115.04 |
| 54 | 1w | 37 | MIA | C4-N9-C8 | 2.85 | 108.73 | 105.74 |
| 32 | 1a | 1518 | MA6 | N3-C4-N9 | 2.81 | 131.95 | 127.17 |
| 54 | 2w | 37 | MIA | C5-N7-C8 | 2.81 | 107.87 | 103.45 |
| 56 | 1y | 54 | 5MU | C5M-C5-C4 | 2.81 | 121.78 | 118.78 |
| 55 | 2x | 8 | 4SU | C6-C5-C4 | -2.81 | 117.52 | 119.95 |
| 32 | 1a | 966 | M2G | C6-C5-N7 | 2.81 | 135.40 | 130.29 |
| 55 | 2x | 76 | 31H | O4'-C1'-C2' | -2.81 | 100.61 | 106.62 |
| 54 | 2w | 46 | G7M | O6-C6-C5 | -2.80 | 121.76 | 128.01 |
| 1 | 2A | 1939 | 5MU | O2-C2-N3 | -2.79 | 116.34 | 121.49 |
| 32 | 1a | 1407 | 5MC | O2-C2-N3 | -2.78 | 117.95 | 122.33 |
| 32 | 2a | 1518 | MA6 | N3-C4-N9 | 2.78 | 131.89 | 127.17 |
| 32 | 1a | 1402 | 4OC | C6-C5-C4 | 2.78 | 120.34 | 117.00 |
| 32 | 1a | 1207 | 2MG | N2-C2-N3 | -2.77 | 116.98 | 120.51 |
| 54 | 2w | 39 | PSU | C4-N3-C2 | -2.76 | 122.57 | 126.37 |
| 54 | 2w | 37 | MIA | C2-N1-C6 | 2.76 | 122.77 | 117.54 |
| 54 | 2w | 32 | PSU | C5-C6-N1 | -2.75 | 118.32 | 122.14 |
| 32 | 1a | 1518 | MA6 | C4-N9-C8 | 2.75 | 108.62 | 105.74 |
| 32 | 2a | 967 | 5MC | CM5-C5-C6 | -2.75 | 119.13 | 122.85 |
| 56 | 1y | 37 | MIA | C2-N1-C6 | 2.74 | 123.23 | 118.73 |
| 56 | 2y | 39 | PSU | C4-N3-C2 | -2.72 | 122.62 | 126.37 |
| 55 | 1x | 76 | 31H | OCN-CN-N | -2.72 | 118.28 | 125.32 |
| 55 | 1x | 76 | 31H | C2-N3-C4 | 2.72 | 118.47 | 111.83 |
| 56 | 2y | 37 | MIA | C5-N7-C8 | 2.71 | 107.71 | 103.45 |
| 56 | 2y | 54 | 5MU | C5-C6-N1 | -2.71 | 120.37 | 123.31 |
| 55 | 1x | 8 | 4SU | O2-C2-N3 | -2.70 | 116.51 | 121.49 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 56 | 1y | 55 | PSU | C6-C5-C4 | -2.70 | 116.35 | 118.17 |
| 55 | 2x | 32 | 5MC | C1'-N1-C6 | -2.69 | 116.71 | 121.15 |
| 54 | 1w | 37 | MIA | N3-C2-N1 | -2.69 | 122.09 | 127.00 |
| 1 | 1A | 1915 | 5MU | O2-C2-N1 | -2.69 | 119.30 | 122.80 |
| 1 | 2A | 1942 | 5MC | C5-C4-N3 | -2.68 | 119.00 | 121.75 |
| 1 | 2A | 2503 | 2MA | C6-C5-N7 | 2.68 | 137.26 | 132.09 |
| 54 | 1w | 37 | MIA | C2-N1-C6 | 2.67 | 122.61 | 117.54 |
| 1 | 1A | 1962 | 5MC | C5-C6-N1 | -2.67 | 120.42 | 123.31 |
| 1 | 1A | 2251 | OMG | C4-C5-N7 | -2.66 | 106.45 | 110.67 |
| 54 | 2w | 37 | MIA | C4-N9-C8 | 2.66 | 108.53 | 105.74 |
| 1 | 1A | 1962 | 5MC | CM5-C5-C6 | -2.66 | 119.25 | 122.85 |
| 32 | 2a | 1518 | MA6 | C4-C5-C6 | 2.66 | 118.66 | 115.91 |
| 32 | 2a | 1498 | UR3 | C1'-N1-C2 | 2.65 | 121.38 | 117.04 |
| 1 | 1A | 2503 | 2MA | C6-C5-N7 | 2.64 | 137.18 | 132.09 |
| 55 | 1x | 8 | 4SU | C5-C4-S4 | 2.63 | 127.30 | 124.31 |
| 54 | 2w | 76 | F3N | C5-C4-N9 | 2.62 | 108.67 | 105.81 |
| 32 | 1a | 1498 | UR3 | C3U-N3-C4 | 2.62 | 121.50 | 117.87 |
| 1 | 1A | 1962 | 5MC | C5-C4-N3 | -2.60 | 119.09 | 121.75 |
| 32 | 2a | 1518 | MA6 | N9-C8-N7 | -2.59 | 110.26 | 113.94 |
| 56 | 1y | 37 | MIA | C4-N9-C8 | 2.58 | 108.44 | 105.74 |
| 1 | 1A | 2605 | PSU | C6-C5-C4 | -2.57 | 116.44 | 118.17 |
| 32 | 1a | 1402 | 4OC | C5-C6-N1 | -2.56 | 117.67 | 121.84 |
| 55 | 2x | 8 | 4SU | O2-C2-N1 | 2.56 | 126.12 | 122.80 |
| 32 | 1a | 1407 | 5MC | C5-C6-N1 | -2.54 | 120.55 | 123.31 |
| 54 | 2w | 76 | F3N | N3-C4-N9 | 2.54 | 131.48 | 127.17 |
| 32 | 1a | 1400 | 5MC | C1'-N1-C6 | -2.53 | 116.99 | 121.15 |
| 32 | 1a | 1400 | 5MC | O2-C2-N3 | -2.53 | 118.34 | 122.33 |
| 54 | 1w | 76 | F3N | N3-C4-N9 | 2.51 | 131.43 | 127.17 |
| 54 | 1w | 37 | MIA | C5-N7-C8 | 2.50 | 107.37 | 103.45 |
| 54 | 1w | 37 | MIA | C11-S10-C2 | 2.49 | 104.12 | 102.25 |
| 32 | 1a | 516 | PSU | C5-C6-N1 | -2.49 | 118.69 | 122.14 |
| 54 | 1w | 76 | F3N | O2'-C2'-C3' | -2.48 | 105.10 | 111.16 |
| 55 | 1x | 55 | PSU | O2-C2-N3 | -2.47 | 117.47 | 121.86 |
| 1 | 1A | 2503 | 2MA | N6-C6-N1 | 2.46 | 120.35 | 117.03 |
| 1 | 1A | 1939 | 5MU | O2-C2-N3 | -2.46 | 116.95 | 121.49 |
| 1 | 1A | 1942 | 5MC | C1'-N1-C2 | 2.46 | 123.86 | 118.44 |
| 54 | 1w | 46 | G7M | O6-C6-C5 | -2.45 | 122.53 | 128.01 |
| 56 | 1y | 54 | 5MU | C1'-N1-C2 | 2.45 | 122.00 | 117.59 |
| 56 | 1y | 46 | G7M | O6-C6-C5 | -2.44 | 122.56 | 128.01 |
| 55 | 2x | 55 | PSU | O2-C2-N1 | -2.44 | 120.27 | 122.79 |
| 32 | 2a | 967 | 5MC | C5-C4-N3 | -2.44 | 119.26 | 121.75 |
| 1 | 1A | 1920 | OMC | CM2-O2'-C2' | -2.43 | 108.23 | 114.47 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 54 | 1w | 55 | PSU | O2-C2-N1 | -2.43 | 120.28 | 122.79 |
| 1 | 2A | 2251 | OMG | C4-C5-N7 | -2.42 | 106.83 | 110.67 |
| 1 | 2A | 1920 | OMC | CM2-O2'-C2' | -2.40 | 108.32 | 114.47 |
| 32 | 1a | 1402 | 4OC | CM4-N4-C4 | -2.37 | 117.82 | 122.45 |
| 1 | 1A | 1942 | 5MC | C5-C6-N1 | -2.37 | 120.74 | 123.31 |
| 55 | 2x | 76 | 31H | C5-C6-N6 | -2.37 | 117.42 | 123.29 |
| 32 | 1a | 1519 | MA6 | C4-C5-C6 | 2.37 | 118.36 | 115.91 |
| 32 | 1a | 1207 | 2MG | N1-C2-N2 | 2.36 | 118.97 | 116.56 |
| 1 | 2A | 2503 | 2MA | CM2-C2-N1 | 2.36 | 120.66 | 117.13 |
| 1 | 1A | 1917 | PSU | C5-C6-N1 | -2.35 | 118.88 | 122.14 |
| 55 | 1x | 76 | 31H | C4-C5-N7 | -2.35 | 107.90 | 110.58 |
| 55 | 2x | 76 | 31H | OCN-CN-N | -2.35 | 119.26 | 125.32 |
| 32 | 2a | 527 | G7M | C5-C6-N1 | 2.34 | 116.68 | 111.84 |
| 54 | 1w | 76 | F3N | O4'-C4'-C3' | 2.33 | 107.52 | 104.13 |
| 54 | 1w | 32 | PSU | O4-C4-C5 | -2.33 | 118.22 | 124.01 |
| 54 | 2w | 32 | PSU | O2-C2-N3 | -2.33 | 117.72 | 121.86 |
| 56 | 1y | 54 | 5MU | C5-C6-N1 | -2.33 | 120.79 | 123.31 |
| 32 | 2a | 1519 | MA6 | C5-C4-N9 | 2.33 | 108.34 | 105.81 |
| 32 | 2a | 1498 | UR3 | C3U-N3-C2 | 2.30 | 121.33 | 117.33 |
| 32 | 1a | 1207 | 2MG | C8-N7-C5 | 2.29 | 108.34 | 104.26 |
| 54 | 1w | 8 | 4SU | C6-N1-C2 | -2.29 | 118.21 | 121.00 |
| 54 | 2w | 76 | F3N | C4-C5-N7 | -2.28 | 107.97 | 110.58 |
| 55 | 2x | 55 | PSU | C5-C6-N1 | -2.27 | 118.99 | 122.14 |
| 55 | 1x | 55 | PSU | C5-C6-N1 | -2.26 | 119.00 | 122.14 |
| 32 | 1a | 1207 | 2MG | C2-N1-C6 | -2.25 | 121.83 | 124.55 |
| 32 | 2a | 1518 | MA6 | C5-C4-N9 | 2.25 | 108.26 | 105.81 |
| 54 | 1w | 76 | F3N | C4-C5-N7 | -2.25 | 108.02 | 110.58 |
| 32 | 2a | 527 | G7M | O6-C6-C5 | -2.24 | 123.02 | 128.01 |
| 1 | 1A | 2251 | OMG | C8-N7-C5 | 2.22 | 108.22 | 104.26 |
| 55 | 2x | 32 | 5MC | C1'-N1-C2 | 2.22 | 123.34 | 118.44 |
| 55 | 2x | 8 | 4SU | C4-N3-C2 | 2.21 | 129.44 | 127.31 |
| 32 | 2a | 1402 | 4OC | C6-C5-C4 | 2.21 | 119.66 | 117.00 |
| 56 | 2y | 8 | 4SU | O3'-C3'-C4' | 2.21 | 117.42 | 111.08 |
| 1 | 2A | 2605 | PSU | O4-C4-C5 | -2.19 | 118.56 | 124.01 |
| 56 | 2y | 54 | 5MU | C1'-N1-C2 | 2.19 | 121.52 | 117.59 |
| 32 | 2a | 1519 | MA6 | N3-C4-N9 | 2.18 | 130.88 | 127.17 |
| 56 | 1y | 8 | 4SU | C5-C4-S4 | -2.18 | 121.81 | 124.31 |
| 32 | 1a | 516 | PSU | O2-C2-N3 | -2.18 | 118.00 | 121.86 |
| 1 | 1A | 2605 | PSU | O4-C4-C5 | -2.17 | 118.61 | 124.01 |
| 32 | 1a | 1402 | 4OC | O2-C2-N3 | -2.17 | 118.91 | 122.33 |
| 1 | 2A | 2503 | 2MA | C2-N1-C6 | 2.17 | 121.43 | 118.10 |
| 32 | 1a | 967 | 5MC | C5-C4-N3 | -2.16 | 119.54 | 121.75 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | 2A | 2503 | 2MA | C5-C4-N9 | 2.16 | 108.16 | 105.81 |
| 32 | 2a | 1404 | 5MC | O2-C2-N3 | -2.14 | 118.95 | 122.33 |
| 1 | 1A | 1962 | 5MC | C1'-N1-C6 | -2.14 | 117.62 | 121.15 |
| 32 | 2a | 1407 | 5MC | CM5-C5-C6 | -2.14 | 119.96 | 122.85 |
| 55 | 2x | 32 | 5MC | O2-C2-N3 | -2.14 | 118.96 | 122.33 |
| 54 | 2w | 46 | G7M | N2-C2-N1 | 2.13 | 121.27 | 116.76 |
| 54 | 1w | 76 | F3N | C6-C5-C4 | 2.13 | 120.09 | 117.18 |
| 54 | 2w | 37 | MIA | N3-C2-N1 | -2.13 | 123.11 | 127.00 |
| 56 | 2y | 46 | G7M | O6-C6-C5 | -2.13 | 123.26 | 128.01 |
| 56 | 1y | 37 | MIA | C5-N7-C8 | 2.13 | 106.79 | 103.45 |
| 1 | 1A | 1917 | PSU | O4'-C1'-C2' | 2.13 | 108.09 | 105.15 |
| 54 | 1w | 55 | PSU | C6-C5-C4 | -2.13 | 116.74 | 118.17 |
| 55 | 2x | 55 | PSU | O2-C2-N3 | -2.13 | 118.08 | 121.86 |
| 56 | 2y | 54 | 5MU | C5M-C5-C4 | 2.12 | 121.05 | 118.78 |
| 56 | 1y | 46 | G7M | C5-C6-N1 | 2.11 | 116.21 | 111.84 |
| 32 | 2a | 1404 | 5MC | N1-C2-N3 | 2.11 | 122.46 | 118.80 |
| 54 | 2w | 32 | PSU | O2-C2-N1 | -2.11 | 120.61 | 122.79 |
| 1 | 2A | 2251 | OMG | O6-C6-C5 | -2.11 | 120.97 | 126.53 |
| 32 | 2a | 1519 | MA6 | C4-C5-C6 | 2.10 | 118.09 | 115.91 |
| 54 | 2w | 76 | F3N | C6-C5-C4 | 2.10 | 120.05 | 117.18 |
| 32 | 1a | 1498 | UR3 | O2-C2-N3 | -2.10 | 118.43 | 121.33 |
| 1 | 2A | 2503 | 2MA | C5-N7-C8 | 2.10 | 106.75 | 103.45 |
| 1 | 2A | 2503 | 2MA | C2-N3-C4 | 2.10 | 122.20 | 115.02 |
| 54 | 2w | 54 | 5MU | C5M-C5-C6 | -2.09 | 120.02 | 122.85 |
| 32 | 1a | 1498 | UR3 | C6-N1-C2 | -2.09 | 120.09 | 121.80 |
| 54 | 1w | 37 | MIA | N9-C8-N7 | -2.09 | 110.97 | 113.94 |
| 32 | 1a | 966 | M2G | C8-N7-C5 | 2.08 | 107.97 | 104.26 |
| 32 | 1a | 1407 | 5MC | C5-C4-N3 | -2.08 | 119.62 | 121.75 |
| 32 | 2a | 1498 | UR3 | C6-N1-C2 | -2.07 | 120.11 | 121.80 |
| 56 | 2y | 54 | 5MU | C1'-N1-C6 | -2.07 | 117.75 | 121.15 |
| 56 | 2y | 39 | PSU | O2-C2-N3 | -2.06 | 118.20 | 121.86 |
| 54 | 1w | 8 | 4SU | C1'-N1-C2 | 2.06 | 121.29 | 117.59 |
| 56 | 2y | 37 | MIA | C4-N9-C8 | 2.06 | 107.90 | 105.74 |
| 56 | 1y | 37 | MIA | C6-C5-N7 | 2.06 | 136.05 | 132.09 |
| 1 | 2A | 1917 | PSU | C5-C6-N1 | -2.05 | 119.30 | 122.14 |
| 54 | 2w | 8 | 4SU | C6-N1-C2 | -2.05 | 118.51 | 121.00 |
| 32 | 1a | 1407 | 5MC | N1-C2-N3 | 2.04 | 122.34 | 118.80 |
| 32 | 2a | 1207 | 2MG | C2-N1-C6 | -2.04 | 122.08 | 124.55 |
| 1 | 2A | 1920 | OMC | C2'-C1'-N1 | -2.04 | 110.37 | 114.24 |
| 32 | 1a | 1404 | 5MC | N4-C4-N3 | 2.03 | 122.19 | 118.51 |
| 32 | 2a | 516 | PSU | O4'-C1'-C2' | 2.03 | 107.95 | 105.15 |
| 56 | 2y | 55 | PSU | O4'-C1'-C2' | 2.03 | 107.95 | 105.15 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 1 | 2A | 1939 | 5MU | C6-N1-C2 | -2.03 | 119.28 | 121.30 |
| 1 | 2A | 2251 | OMG | C5-C6-N1 | 2.02 | 118.39 | 113.25 |
| 54 | 1w | 39 | PSU | C5-C6-N1 | -2.02 | 119.34 | 122.14 |
| 55 | 1x | 32 | 5MC | O2-C2-N3 | -2.02 | 119.15 | 122.33 |
| 1 | 1A | 2251 | OMG | C8-N9-C4 | 2.01 | 109.79 | 106.03 |

There are no chirality outliers.

All (63) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 1 | 1A | 2251 | OMG | C1'-C2'-O2'-CM2 |
| 32 | 1a | 1519 | MA6 | O4'-C4'-C5'-O5' |
| 43 | 1l | 92 | 0TD | CA-CB-SB-CSB |
| 43 | 1l | 92 | 0TD | CG-CB-SB-CSB |
| 54 | 1w | 37 | MIA | C5-C6-N6-C12 |
| 54 | 1w | 37 | MIA | C12-C13-C14-C15 |
| 54 | 1w | 37 | MIA | C12-C13-C14-C16 |
| 56 | 1y | 46 | G7M | C4'-C5'-O5'-P |
| 32 | 2a | 1207 | 2MG | N3-C2-N2-CM2 |
| 43 | 2l | 92 | 0TD | CA-CB-SB-CSB |
| 43 | 2l | 92 | 0TD | CG-CB-SB-CSB |
| 54 | 2w | 37 | MIA | C5-C6-N6-C12 |
| 54 | 2w | 37 | MIA | N1-C6-N6-C12 |
| 54 | 2w | 46 | G7M | O4'-C4'-C5'-O5' |
| 55 | 2x | 76 | 31H | O4'-C4'-C5'-O5' |
| 56 | 2y | 54 | 5MU | O4'-C4'-C5'-O5' |
| 55 | 2x | 76 | 31H | C3'-C4'-C5'-O5' |
| 56 | 1y | 37 | MIA | C3'-C4'-C5'-O5' |
| 32 | 2a | 1519 | MA6 | O4'-C4'-C5'-O5' |
| 54 | 2w | 46 | G7M | C3'-C4'-C5'-O5' |
| 54 | 2w | 76 | F3N | O4'-C4'-C5'-O5' |
| 56 | 2y | 37 | MIA | C3'-C4'-C5'-O5' |
| 56 | 2y | 54 | 5MU | C3'-C4'-C5'-O5' |
| 55 | 1x | 76 | 31H | CB-CG-SD-CE |
| 55 | 1x | 76 | 31H | C3'-C4'-C5'-O5' |
| 55 | 1x | 76 | 31H | O4'-C4'-C5'-O5' |
| 56 | 1y | 37 | MIA | O4'-C4'-C5'-O5' |
| 32 | 1a | 527 | G7M | C3'-C4'-C5'-O5' |
| 32 | 1a | 1519 | MA6 | C3'-C4'-C5'-O5' |
| 55 | 2x | 76 | 31H | CB-CG-SD-CE |
| 32 | 2a | 527 | G7M | C3'-C4'-C5'-O5' |
| 54 | 2w | 46 | G7M | C4'-C5'-O5'-P |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 56 | 2y | 46 | G7M | O4'-C1'-N9-C4 |
| 56 | 2y | 37 | MIA | O4'-C4'-C5'-O5' |
| 54 | 1w | 37 | MIA | N1-C6-N6-C12 |
| 54 | 2w | 76 | F3N | N-CA-CB-CG |
| 32 | 2a | 1519 | MA6 | C3'-C4'-C5'-O5' |
| 54 | 2w | 76 | F3N | C3'-C4'-C5'-O5' |
| 32 | 1a | 967 | 5MC | O4'-C4'-C5'-O5' |
| 54 | 1w | 76 | F3N | C3'-C4'-C5'-O5' |
| 43 | 1l | 92 | 0TD | SB-CB-CG-OD1 |
| 43 | 2l | 92 | 0TD | SB-CB-CG-OD1 |
| 32 | 1a | 527 | G7M | O4'-C4'-C5'-O5' |
| 55 | 1x | 76 | 31H | C4'-C5'-O5'-P |
| 55 | 2x | 76 | 31H | C4'-C5'-O5'-P |
| 54 | 1w | 55 | PSU | O4'-C1'-C5-C4 |
| 56 | 1y | 55 | PSU | O4'-C1'-C5-C4 |
| 56 | 2y | 55 | PSU | O4'-C1'-C5-C4 |
| 54 | 1w | 46 | G7M | C4'-C5'-O5'-P |
| 32 | 1a | 527 | G7M | C4'-C5'-O5'-P |
| 32 | 2a | 1519 | MA6 | C4'-C5'-O5'-P |
| 56 | 2y | 46 | G7M | O4'-C1'-N9-C8 |
| 43 | 1l | 92 | 0TD | SB-CB-CG-OD2 |
| 54 | 2w | 76 | F3N | C-CA-CB-CG |
| 54 | 1w | 55 | PSU | O4'-C1'-C5-C6 |
| 54 | 1w | 76 | F3N | O4'-C4'-C5'-O5' |
| 56 | 1y | 46 | G7M | C3'-C4'-C5'-O5' |
| 1 | 2A | 2503 | 2MA | O4'-C4'-C5'-O5' |
| 1 | 1A | 2503 | 2MA | C4'-C5'-O5'-P |
| 32 | 1a | 516 | PSU | O4'-C4'-C5'-O5' |
| 32 | 2a | 527 | G7M | O4'-C4'-C5'-O5' |
| 56 | 1y | 37 | MIA | C4'-C5'-O5'-P |
| 56 | 2y | 8 | 4SU | C2'-C1'-N1-C2 |

There are no ring outliers.

38 monomers are involved in 54 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 54 | 2w | 39 | PSU | 2 | 0 |
| 56 | 1y | 8 | 4SU | 1 | 0 |
| 32 | 2a | 967 | 5MC | 2 | 0 |
| 32 | 2a | 1207 | 2MG | 1 | 0 |
| 32 | 1a | 1402 | 4OC | 1 | 0 |
| 55 | 2x | 76 | 31H | 1 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 55 | 2x | 8 | 4SU | 1 | 0 |
| 1 | 2A | 1939 | 5MU | 1 | 0 |
| 54 | 1w | 76 | F3N | 4 | 0 |
| 54 | 1w | 46 | G7M | 1 | 0 |
| 54 | 2w | 76 | F3N | 3 | 0 |
| 32 | 1a | 1518 | MA6 | 2 | 0 |
| 56 | 2y | 8 | 4SU | 2 | 0 |
| 54 | 2w | 8 | 4SU | 1 | 0 |
| 55 | 2x | 54 | 5MU | 3 | 0 |
| 1 | 1A | 2552 | OMU | 1 | 0 |
| 1 | 1A | 1939 | 5MU | 1 | 0 |
| 43 | 1l | 92 | 0TD | 1 | 0 |
| 32 | 1a | 967 | 5MC | 1 | 0 |
| 56 | 1y | 37 | MIA | 2 | 0 |
| 55 | 1x | 76 | 31H | 1 | 0 |
| 32 | 2a | 1518 | MA6 | 3 | 0 |
| 1 | 1A | 2251 | OMG | 1 | 0 |
| 54 | 1w | 8 | 4SU | 1 | 0 |
| 1 | 2A | 2552 | OMU | 1 | 0 |
| 32 | 1a | 1519 | MA6 | 1 | 0 |
| 56 | 1y | 39 | PSU | 1 | 0 |
| 1 | 1A | 1917 | PSU | 1 | 0 |
| 32 | 2a | 1400 | 5MC | 2 | 0 |
| 32 | 1a | 527 | G7M | 1 | 0 |
| 32 | 1a | 966 | M2G | 3 | 0 |
| 56 | 2y | 46 | G7M | 3 | 0 |
| 32 | 2a | 1519 | MA6 | 2 | 0 |
| 54 | 2w | 46 | G7M | 2 | 0 |
| 56 | 2y | 39 | PSU | 2 | 0 |
| 1 | 1A | 1920 | OMC | 1 | 0 |
| 43 | 2l | 92 | 0TD | 1 | 0 |
| 55 | 1x | 8 | 4SU | 1 | 0 |

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2820 ligands modelled in this entry, 2818 are monoatomic - leaving 2 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 | $\# Z > 2$ |
| 61 | SF4 | 1d | 302 | 35 | 0,12,12 | - | - | - | | |
| 61 | SF4 | 2d | 302 | 35 | 0,12,12 | - | - | - | | |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|----------|---------|
| 61 | SF4 | 1d | 302 | 35 | - | - | 0/6/5/5 |
| 61 | SF4 | 2d | 302 | 35 | - | - | 0/6/5/5 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 61 | 1d | 302 | SF4 | 2 | 0 |

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 54 | 2w | 1 |

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| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 54 | 1w | 1 |
| 17 | 1V | 1 |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1 | 2w | 75:C | O3' | 76:F3N | P | 2.56 |
| 1 | 1w | 75:C | O3' | 76:F3N | P | 2.32 |
| 1 | 1V | 34:GLU | C | 35:LEU | N | 1.14 |

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | | | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|----------|-----|-----|-----------------------|-------|
| 1 | 1A | 2860/2915 (98%) | -0.59 | 187 (6%) | 25 | 19 | 11, 27, 82, 92 | 0 |
| 1 | 2A | 2789/2915 (95%) | -0.11 | 162 (5%) | 29 | 23 | 23, 44, 80, 96 | 0 |
| 2 | 1B | 120/121 (99%) | -0.43 | 0 | 100 | 100 | 21, 39, 54, 74 | 0 |
| 2 | 2B | 120/121 (99%) | 0.26 | 1 (0%) | 82 | 80 | 43, 57, 66, 80 | 0 |
| 3 | 1D | 275/276 (99%) | -0.37 | 2 (0%) | 84 | 82 | 13, 28, 42, 71 | 0 |
| 3 | 2D | 275/276 (99%) | -0.09 | 5 (1%) | 67 | 63 | 21, 38, 50, 68 | 0 |
| 4 | 1E | 204/206 (99%) | -0.36 | 0 | 100 | 100 | 12, 30, 49, 65 | 0 |
| 4 | 2E | 204/206 (99%) | 0.19 | 2 (0%) | 79 | 76 | 26, 48, 60, 69 | 0 |
| 5 | 1F | 203/210 (96%) | -0.32 | 0 | 100 | 100 | 12, 31, 54, 69 | 0 |
| 5 | 2F | 203/210 (96%) | 0.33 | 5 (2%) | 58 | 52 | 24, 52, 65, 71 | 0 |
| 6 | 1G | 181/182 (99%) | 0.27 | 8 (4%) | 39 | 33 | 28, 44, 59, 72 | 0 |
| 6 | 2G | 181/182 (99%) | 0.68 | 9 (4%) | 34 | 28 | 48, 58, 68, 76 | 0 |
| 7 | 1H | 174/180 (96%) | 0.15 | 5 (2%) | 53 | 48 | 29, 43, 55, 64 | 0 |
| 7 | 2H | 174/180 (96%) | 1.48 | 43 (24%) | 2 | 1 | 59, 71, 78, 88 | 0 |
| 8 | 1I | 146/148 (98%) | 0.58 | 2 (1%) | 73 | 69 | 34, 59, 67, 70 | 0 |
| 8 | 2I | 146/148 (98%) | 0.76 | 8 (5%) | 30 | 25 | 42, 59, 69, 73 | 0 |
| 9 | 1N | 140/140 (100%) | -0.31 | 0 | 100 | 100 | 18, 28, 46, 61 | 0 |
| 9 | 2N | 140/140 (100%) | 0.51 | 6 (4%) | 40 | 34 | 36, 50, 67, 73 | 0 |
| 10 | 1O | 122/122 (100%) | -0.28 | 0 | 100 | 100 | 19, 31, 48, 53 | 0 |
| 10 | 2O | 122/122 (100%) | 0.25 | 2 (1%) | 70 | 66 | 35, 48, 58, 62 | 0 |
| 11 | 1P | 149/150 (99%) | -0.14 | 0 | 100 | 100 | 14, 37, 55, 62 | 0 |
| 11 | 2P | 149/150 (99%) | 0.38 | 3 (2%) | 65 | 60 | 28, 52, 66, 73 | 0 |
| 12 | 1Q | 141/141 (100%) | -0.17 | 1 (0%) | 84 | 82 | 17, 30, 48, 62 | 0 |
| 12 | 2Q | 141/141 (100%) | 0.44 | 4 (2%) | 55 | 49 | 34, 50, 62, 67 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|----------------|--------|---------------|-----------------------|-------|
| 13 | 1R | 118/118 (100%) | -0.53 | 0 100 100 | 17, 25, 38, 44 | 0 |
| 13 | 2R | 118/118 (100%) | 0.04 | 0 100 100 | 31, 42, 54, 61 | 0 |
| 14 | 1S | 110/112 (98%) | -0.04 | 0 100 100 | 26, 39, 51, 53 | 0 |
| 14 | 2S | 110/112 (98%) | 0.51 | 1 (0%) 81 78 | 45, 54, 62, 68 | 0 |
| 15 | 1T | 131/146 (89%) | -0.14 | 2 (1%) 72 68 | 23, 35, 56, 69 | 0 |
| 15 | 2T | 131/146 (89%) | 0.47 | 3 (2%) 61 55 | 40, 50, 62, 68 | 0 |
| 16 | 1U | 116/118 (98%) | -0.60 | 0 100 100 | 15, 21, 34, 47 | 0 |
| 16 | 2U | 116/118 (98%) | 0.33 | 3 (2%) 57 51 | 30, 47, 59, 64 | 0 |
| 17 | 1V | 101/101 (100%) | -0.41 | 0 100 100 | 14, 27, 47, 56 | 0 |
| 17 | 2V | 101/101 (100%) | 0.53 | 0 100 100 | 29, 56, 62, 66 | 0 |
| 18 | 1W | 112/113 (99%) | -0.52 | 1 (0%) 81 78 | 13, 22, 39, 66 | 0 |
| 18 | 2W | 112/113 (99%) | -0.02 | 1 (0%) 81 78 | 30, 38, 56, 75 | 0 |
| 19 | 1X | 95/96 (98%) | -0.28 | 1 (1%) 78 74 | 16, 29, 50, 65 | 0 |
| 19 | 2X | 95/96 (98%) | 0.21 | 2 (2%) 63 58 | 34, 44, 61, 71 | 0 |
| 20 | 1Y | 107/110 (97%) | 0.01 | 1 (0%) 81 78 | 24, 39, 55, 65 | 0 |
| 20 | 2Y | 107/110 (97%) | 0.83 | 12 (11%) 10 8 | 45, 57, 69, 75 | 0 |
| 21 | 1Z | 154/206 (74%) | 0.65 | 5 (3%) 50 44 | 26, 52, 70, 76 | 0 |
| 21 | 2Z | 160/206 (77%) | 1.26 | 33 (20%) 2 2 | 53, 66, 76, 79 | 0 |
| 22 | 10 | 83/85 (97%) | -0.24 | 1 (1%) 76 73 | 15, 26, 40, 51 | 0 |
| 22 | 20 | 83/85 (97%) | 0.42 | 2 (2%) 59 54 | 35, 45, 54, 62 | 0 |
| 23 | 11 | 97/98 (98%) | 0.08 | 2 (2%) 63 58 | 19, 37, 58, 65 | 0 |
| 23 | 21 | 97/98 (98%) | 0.37 | 5 (5%) 33 27 | 29, 45, 61, 67 | 0 |
| 24 | 12 | 70/72 (97%) | -0.04 | 1 (1%) 73 69 | 23, 37, 47, 63 | 0 |
| 24 | 22 | 70/72 (97%) | 0.66 | 2 (2%) 53 48 | 42, 54, 64, 70 | 0 |
| 25 | 13 | 59/60 (98%) | -0.19 | 0 100 100 | 15, 26, 49, 62 | 0 |
| 25 | 23 | 59/60 (98%) | 0.44 | 2 (3%) 48 42 | 40, 50, 61, 68 | 0 |
| 26 | 14 | 69/71 (97%) | 0.73 | 7 (10%) 12 9 | 38, 59, 74, 78 | 0 |
| 26 | 24 | 69/71 (97%) | 1.17 | 10 (14%) 6 4 | 56, 68, 76, 79 | 0 |
| 27 | 15 | 59/60 (98%) | -0.49 | 0 100 100 | 12, 22, 39, 46 | 0 |
| 27 | 25 | 59/60 (98%) | 0.08 | 0 100 100 | 28, 39, 54, 70 | 0 |
| 28 | 16 | 53/54 (98%) | -0.20 | 0 100 100 | 24, 32, 47, 53 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 28 | 26 | 53/54 (98%) | 0.38 | 1 (1%) 66 61 | 37, 46, 54, 60 | 0 |
| 29 | 17 | 48/49 (97%) | -0.50 | 2 (4%) 40 35 | 14, 19, 43, 50 | 0 |
| 29 | 27 | 48/49 (97%) | 0.00 | 4 (8%) 17 13 | 24, 31, 51, 59 | 0 |
| 30 | 18 | 64/65 (98%) | -0.54 | 0 100 100 | 20, 25, 32, 46 | 0 |
| 30 | 28 | 64/65 (98%) | 0.07 | 1 (1%) 70 66 | 33, 40, 46, 54 | 0 |
| 31 | 19 | 37/37 (100%) | -0.31 | 0 100 100 | 19, 29, 45, 51 | 0 |
| 31 | 29 | 37/37 (100%) | 0.81 | 2 (5%) 31 26 | 44, 54, 66, 68 | 0 |
| 32 | 1a | 1488/1521 (97%) | 0.19 | 67 (4%) 38 32 | 25, 52, 79, 94 | 0 |
| 32 | 2a | 1491/1521 (98%) | 0.39 | 74 (4%) 34 28 | 34, 58, 79, 96 | 0 |
| 33 | 1b | 231/256 (90%) | 1.03 | 33 (14%) 6 5 | 50, 64, 74, 78 | 0 |
| 33 | 2b | 231/256 (90%) | 1.15 | 27 (11%) 9 7 | 51, 68, 75, 79 | 0 |
| 34 | 1c | 206/239 (86%) | 0.68 | 8 (3%) 43 38 | 43, 56, 69, 75 | 0 |
| 34 | 2c | 206/239 (86%) | 1.14 | 23 (11%) 10 8 | 56, 64, 73, 77 | 0 |
| 35 | 1d | 208/209 (99%) | 1.10 | 30 (14%) 6 5 | 44, 56, 66, 75 | 0 |
| 35 | 2d | 208/209 (99%) | 0.69 | 11 (5%) 32 26 | 45, 54, 63, 71 | 0 |
| 36 | 1e | 148/162 (91%) | 0.42 | 1 (0%) 84 82 | 35, 51, 61, 68 | 0 |
| 36 | 2e | 148/162 (91%) | 0.62 | 8 (5%) 31 26 | 45, 57, 65, 75 | 0 |
| 37 | 1f | 100/101 (99%) | 0.58 | 0 100 100 | 43, 55, 63, 68 | 0 |
| 37 | 2f | 100/101 (99%) | 0.49 | 1 (1%) 79 76 | 41, 52, 60, 70 | 0 |
| 38 | 1g | 155/156 (99%) | 0.68 | 10 (6%) 25 19 | 47, 57, 72, 77 | 0 |
| 38 | 2g | 155/156 (99%) | 0.92 | 17 (10%) 10 8 | 54, 63, 72, 76 | 0 |
| 39 | 1h | 137/138 (99%) | 0.43 | 3 (2%) 62 57 | 42, 53, 59, 65 | 0 |
| 39 | 2h | 137/138 (99%) | 0.48 | 2 (1%) 72 68 | 49, 58, 64, 69 | 0 |
| 40 | 1i | 127/128 (99%) | 0.96 | 12 (9%) 14 11 | 41, 61, 70, 74 | 0 |
| 40 | 2i | 127/128 (99%) | 1.38 | 28 (22%) 2 2 | 52, 68, 73, 75 | 0 |
| 41 | 1j | 97/105 (92%) | 1.23 | 18 (18%) 3 3 | 43, 63, 71, 76 | 0 |
| 41 | 2j | 96/105 (91%) | 1.62 | 29 (30%) 1 1 | 55, 68, 76, 78 | 0 |
| 42 | 1k | 114/129 (88%) | 0.46 | 4 (3%) 47 41 | 33, 52, 63, 67 | 0 |
| 42 | 2k | 114/129 (88%) | 0.87 | 11 (9%) 13 10 | 38, 56, 67, 74 | 0 |
| 43 | 1l | 121/132 (91%) | 0.10 | 3 (2%) 58 52 | 33, 40, 53, 64 | 0 |
| 43 | 2l | 121/132 (91%) | 0.54 | 4 (3%) 49 43 | 42, 50, 61, 67 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-------------------|--------|-----------------|-----------------------|-------|
| 44 | 1m | 125/126 (99%) | 0.58 | 9 (7%) 21 17 | 38, 52, 61, 66 | 0 |
| 44 | 2m | 122/126 (96%) | 0.89 | 10 (8%) 17 14 | 47, 61, 67, 69 | 0 |
| 45 | 1n | 60/61 (98%) | 0.73 | 2 (3%) 49 43 | 45, 52, 58, 64 | 0 |
| 45 | 2n | 60/61 (98%) | 1.39 | 11 (18%) 3 3 | 59, 63, 69, 75 | 0 |
| 46 | 1o | 88/89 (98%) | 0.30 | 2 (2%) 61 55 | 36, 51, 63, 66 | 0 |
| 46 | 2o | 88/89 (98%) | 0.51 | 2 (2%) 61 55 | 45, 54, 67, 69 | 0 |
| 47 | 1p | 82/88 (93%) | 0.95 | 7 (8%) 16 13 | 41, 56, 64, 70 | 0 |
| 47 | 2p | 82/88 (93%) | 0.68 | 3 (3%) 45 39 | 47, 56, 64, 66 | 0 |
| 48 | 1q | 99/105 (94%) | 0.56 | 2 (2%) 65 60 | 41, 54, 63, 64 | 0 |
| 48 | 2q | 99/105 (94%) | 0.62 | 2 (2%) 65 60 | 48, 57, 66, 68 | 0 |
| 49 | 1r | 68/88 (77%) | 0.59 | 1 (1%) 72 68 | 44, 52, 64, 67 | 0 |
| 49 | 2r | 68/88 (77%) | 0.31 | 1 (1%) 72 68 | 46, 52, 61, 67 | 0 |
| 50 | 1s | 83/93 (89%) | 0.67 | 4 (4%) 35 30 | 46, 54, 64, 68 | 0 |
| 50 | 2s | 83/93 (89%) | 1.16 | 7 (8%) 17 13 | 53, 64, 73, 76 | 0 |
| 51 | 1t | 96/106 (90%) | 0.71 | 3 (3%) 51 45 | 46, 57, 68, 71 | 0 |
| 51 | 2t | 96/106 (90%) | 0.67 | 6 (6%) 26 20 | 47, 56, 67, 72 | 0 |
| 52 | 1u | 23/27 (85%) | 0.92 | 2 (8%) 16 12 | 46, 52, 57, 58 | 0 |
| 52 | 2u | 23/27 (85%) | 1.14 | 1 (4%) 40 34 | 54, 62, 65, 72 | 0 |
| 53 | 1v | 13/24 (54%) | 0.58 | 4 (30%) 1 1 | 32, 39, 82, 89 | 0 |
| 53 | 2v | 13/24 (54%) | 0.90 | 4 (30%) 1 1 | 47, 53, 81, 93 | 0 |
| 54 | 1w | 67/76 (88%) | 0.51 | 5 (7%) 20 16 | 18, 63, 78, 85 | 0 |
| 54 | 2w | 64/76 (84%) | 0.91 | 6 (9%) 14 11 | 36, 71, 80, 87 | 0 |
| 55 | 1x | 72/77 (93%) | -0.03 | 2 (2%) 55 49 | 16, 48, 66, 79 | 0 |
| 55 | 2x | 72/77 (93%) | 0.26 | 1 (1%) 73 69 | 31, 56, 70, 87 | 0 |
| 56 | 1y | 67/76 (88%) | 2.43 | 51 (76%) 0 0 | 50, 85, 89, 90 | 0 |
| 56 | 2y | 66/76 (86%) | 2.53 | 50 (75%) 0 0 | 56, 86, 91, 93 | 0 |
| 57 | 1z | 17/17 (100%) | 0.16 | 0 100 100 | 40, 45, 51, 52 | 0 |
| 57 | 2z | 17/17 (100%) | 0.76 | 1 (5%) 28 23 | 56, 59, 65, 68 | 0 |
| All | All | 20910/21782 (95%) | 0.20 | 1185 (5%) 29 24 | 11, 49, 74, 96 | 0 |

All (1185) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|---------|------|------|
| 1 | 2A | 2174 | C | 8.9 |
| 45 | 1n | 2 | ALA | 8.6 |
| 1 | 1A | 2174 | C | 8.1 |
| 1 | 1A | 2129 | C | 7.9 |
| 1 | 1A | 2130 | U | 7.7 |
| 1 | 2A | 2802 | G | 7.7 |
| 1 | 1A | 1096 | A | 7.2 |
| 1 | 1A | 2175 | C | 7.1 |
| 45 | 2n | 2 | ALA | 6.8 |
| 1 | 1A | 897 | C | 6.6 |
| 1 | 2A | 2128 | C | 6.6 |
| 1 | 1A | 2173 | A | 6.5 |
| 1 | 2A | 2173 | A | 6.4 |
| 1 | 1A | 1059 | G | 6.1 |
| 1 | 1A | 2135 | A | 6.0 |
| 1 | 1A | 2160 | G | 6.0 |
| 1 | 2A | 2175 | C | 5.9 |
| 1 | 2A | 2803 | C | 5.9 |
| 1 | 2A | 2125 | G | 5.8 |
| 32 | 1a | 1003 | G | 5.8 |
| 7 | 1H | 2 | SER | 5.8 |
| 1 | 1A | 2161 | C | 5.8 |
| 1 | 2A | 2160 | G | 5.7 |
| 32 | 2a | 1032 | G | 5.6 |
| 21 | 1Z | 141 | VAL | 5.6 |
| 55 | 2x | 47 | U | 5.5 |
| 1 | 1A | 2133 | G | 5.5 |
| 32 | 2a | 1001(A) | G | 5.5 |
| 1 | 2A | 2896 | C | 5.4 |
| 33 | 1b | 127 | ILE | 5.4 |
| 1 | 1A | 2162 | G | 5.4 |
| 1 | 1A | 2159 | G | 5.3 |
| 32 | 2a | 1002 | G | 5.3 |
| 29 | 27 | 48 | LYS | 5.3 |
| 1 | 2A | 2138 | C | 5.3 |
| 1 | 1A | 2121 | G | 5.3 |
| 1 | 2A | 2123 | G | 5.3 |
| 1 | 2A | 1536 | C | 5.2 |
| 1 | 1A | 2116 | G | 5.2 |
| 1 | 1A | 2134 | A | 5.2 |
| 33 | 2b | 237 | ALA | 5.2 |
| 1 | 1A | 2128 | C | 5.2 |
| 7 | 2H | 2 | SER | 5.2 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|---------|------|------|
| 1 | 1A | 2170 | A | 5.1 |
| 1 | 1A | 2803 | C | 5.1 |
| 32 | 2a | 1039 | C | 5.1 |
| 1 | 1A | 896 | A | 5.1 |
| 1 | 2A | 883 | G | 5.1 |
| 1 | 2A | 2129 | C | 5.1 |
| 1 | 1A | 2801(A) | A | 5.0 |
| 1 | 1A | 2115 | G | 5.0 |
| 1 | 2A | 2117 | A | 5.0 |
| 1 | 2A | 2126 | A | 5.0 |
| 1 | 1A | 2802 | G | 4.9 |
| 1 | 2A | 2127 | G | 4.9 |
| 1 | 2A | 2113 | U | 4.9 |
| 33 | 1b | 237 | ALA | 4.9 |
| 1 | 1A | 1095 | A | 4.9 |
| 1 | 2A | 2116 | G | 4.9 |
| 1 | 1A | 1094 | U | 4.9 |
| 1 | 1A | 2108 | C | 4.8 |
| 1 | 1A | 2136 | C | 4.8 |
| 56 | 1y | 35 | A | 4.8 |
| 38 | 1g | 80 | VAL | 4.8 |
| 1 | 2A | 2139 | C | 4.7 |
| 54 | 1w | 20 | U | 4.7 |
| 1 | 2A | 2894 | G | 4.7 |
| 1 | 2A | 882 | G | 4.7 |
| 40 | 1i | 8 | GLY | 4.6 |
| 32 | 2a | 1027 | C | 4.6 |
| 1 | 1A | 2110 | G | 4.6 |
| 1 | 1A | 2131 | G | 4.6 |
| 1 | 1A | 2172 | U | 4.5 |
| 26 | 14 | 56 | VAL | 4.5 |
| 1 | 1A | 2127 | G | 4.5 |
| 32 | 2a | 1033 | G | 4.5 |
| 1 | 1A | 2117 | A | 4.5 |
| 1 | 2A | 2114 | A | 4.5 |
| 38 | 2g | 82 | GLY | 4.5 |
| 1 | 1A | 2169 | A | 4.5 |
| 3 | 1D | 276 | LYS | 4.4 |
| 1 | 2A | 2161 | C | 4.4 |
| 41 | 2j | 32 | ALA | 4.4 |
| 20 | 2Y | 1 | MET | 4.4 |
| 1 | 2A | 2130 | U | 4.4 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|---------|------|------|
| 32 | 1a | 1002 | G | 4.4 |
| 1 | 2A | 2137 | C | 4.4 |
| 21 | 2Z | 174 | VAL | 4.4 |
| 1 | 1A | 884 | C | 4.4 |
| 1 | 1A | 1057 | A | 4.3 |
| 32 | 1a | 1035 | A | 4.3 |
| 33 | 2b | 236 | TYR | 4.3 |
| 1 | 1A | 1097 | U | 4.3 |
| 1 | 2A | 2122 | U | 4.3 |
| 49 | 1r | 20 | ALA | 4.3 |
| 44 | 1m | 2 | ALA | 4.3 |
| 1 | 1A | 898 | C | 4.3 |
| 32 | 1a | 344 | A | 4.3 |
| 35 | 2d | 5 | ILE | 4.3 |
| 1 | 1A | 2151 | G | 4.3 |
| 1 | 2A | 2112 | G | 4.3 |
| 1 | 2A | 896 | A | 4.3 |
| 47 | 2p | 82 | GLN | 4.2 |
| 1 | 1A | 1081 | U | 4.2 |
| 1 | 1A | 2171 | A | 4.2 |
| 32 | 2a | 1035 | A | 4.2 |
| 1 | 1A | 885 | C | 4.2 |
| 1 | 1A | 2892 | A | 4.2 |
| 1 | 1A | 2120 | G | 4.2 |
| 1 | 2A | 2115 | G | 4.2 |
| 23 | 2l | 2 | SER | 4.2 |
| 56 | 1y | 15 | G | 4.2 |
| 21 | 1Z | 146 | ILE | 4.2 |
| 1 | 1A | 1060 | U | 4.2 |
| 1 | 1A | 1098 | A | 4.2 |
| 44 | 2m | 102 | ARG | 4.2 |
| 1 | 1A | 2112 | G | 4.2 |
| 1 | 2A | 10 | G | 4.2 |
| 1 | 2A | 2801(A) | A | 4.1 |
| 1 | 2A | 2124 | G | 4.1 |
| 46 | 2o | 89 | GLY | 4.1 |
| 1 | 1A | 1082 | U | 4.1 |
| 7 | 1H | 174 | GLY | 4.1 |
| 1 | 1A | 1058 | G | 4.0 |
| 56 | 1y | 34 | G | 4.0 |
| 21 | 2Z | 146 | ILE | 4.0 |
| 41 | 2j | 74 | ILE | 4.0 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | 2A | 2135 | A | 4.0 |
| 1 | 2A | 2169 | A | 4.0 |
| 1 | 2A | 2111 | C | 4.0 |
| 1 | 2A | 2136 | C | 4.0 |
| 1 | 2A | 11 | G | 4.0 |
| 1 | 2A | 2121 | G | 4.0 |
| 40 | 2i | 9 | ARG | 4.0 |
| 1 | 2A | 2119 | A | 4.0 |
| 56 | 2y | 36 | A | 4.0 |
| 56 | 1y | 75 | C | 4.0 |
| 15 | 2T | 131 | ALA | 4.0 |
| 1 | 1A | 1069 | A | 4.0 |
| 1 | 1A | 2107 | C | 4.0 |
| 35 | 1d | 70 | ILE | 4.0 |
| 35 | 2d | 6 | GLY | 4.0 |
| 1 | 1A | 2109 | U | 4.0 |
| 1 | 2A | 2150 | U | 4.0 |
| 38 | 1g | 79 | ARG | 3.9 |
| 1 | 1A | 2168 | G | 3.9 |
| 1 | 2A | 2149 | G | 3.9 |
| 32 | 2a | 1036 | G | 3.9 |
| 56 | 2y | 6 | G | 3.9 |
| 1 | 1A | 2138 | C | 3.9 |
| 50 | 1s | 84 | GLY | 3.9 |
| 1 | 1A | 879 | G | 3.9 |
| 1 | 2A | 2154 | G | 3.9 |
| 32 | 2a | 1034 | G | 3.9 |
| 1 | 2A | 2134 | A | 3.9 |
| 1 | 1A | 1064 | C | 3.9 |
| 8 | 1I | 146 | ALA | 3.9 |
| 1 | 1A | 2132 | U | 3.9 |
| 50 | 2s | 84 | GLY | 3.9 |
| 1 | 1A | 2149 | G | 3.8 |
| 32 | 2a | 1024 | G | 3.8 |
| 53 | 2v | 12 | A | 3.8 |
| 7 | 2H | 120 | GLY | 3.8 |
| 44 | 2m | 100 | GLY | 3.8 |
| 54 | 2w | 72 | C | 3.8 |
| 1 | 1A | 2893 | G | 3.8 |
| 32 | 1a | 1024 | G | 3.8 |
| 32 | 1a | 1031 | G | 3.8 |
| 1 | 2A | 2170 | A | 3.8 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|---------|------|------|
| 32 | 2a | 1004 | A | 3.8 |
| 43 | 2l | 18 | VAL | 3.8 |
| 1 | 1A | 1070 | A | 3.8 |
| 1 | 1A | 2114 | A | 3.8 |
| 32 | 1a | 1023 | G | 3.8 |
| 32 | 1a | 1034 | G | 3.8 |
| 32 | 2a | 1003 | G | 3.8 |
| 54 | 2w | 73 | A | 3.8 |
| 56 | 2y | 14 | A | 3.8 |
| 32 | 2a | 1150 | U | 3.8 |
| 21 | 1Z | 1 | MET | 3.8 |
| 22 | 20 | 84 | LEU | 3.8 |
| 33 | 2b | 121 | LEU | 3.8 |
| 33 | 2b | 134 | GLU | 3.7 |
| 35 | 1d | 194 | LEU | 3.7 |
| 1 | 1A | 2894 | G | 3.7 |
| 1 | 2A | 2167 | U | 3.7 |
| 1 | 1A | 2145 | C | 3.7 |
| 56 | 2y | 7 | A | 3.7 |
| 1 | 1A | 1068 | G | 3.7 |
| 1 | 1A | 2123 | G | 3.7 |
| 1 | 1A | 2125 | G | 3.7 |
| 1 | 2A | 881 | G | 3.7 |
| 32 | 1a | 1030(A) | G | 3.7 |
| 32 | 2a | 1030(A) | G | 3.7 |
| 32 | 2a | 1030 | C | 3.7 |
| 32 | 1a | 1025 | U | 3.7 |
| 1 | 1A | 882 | G | 3.7 |
| 1 | 2A | 2153 | G | 3.7 |
| 32 | 2a | 1117 | G | 3.7 |
| 32 | 1a | 1028 | C | 3.7 |
| 21 | 2Z | 136 | PHE | 3.7 |
| 33 | 1b | 125 | PRO | 3.7 |
| 56 | 2y | 15 | G | 3.6 |
| 56 | 2y | 44 | G | 3.6 |
| 1 | 2A | 888 | C | 3.6 |
| 32 | 2a | 1030(B) | C | 3.6 |
| 43 | 2l | 63 | GLY | 3.6 |
| 1 | 2A | 2176 | A | 3.6 |
| 53 | 1v | 13 | A | 3.6 |
| 42 | 2k | 25 | TYR | 3.6 |
| 1 | 1A | 880 | G | 3.6 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|---------|------|------|
| 1 | 2A | 2133 | G | 3.6 |
| 1 | 2A | 2151 | G | 3.6 |
| 1 | 2A | 2162 | G | 3.6 |
| 32 | 1a | 1026 | G | 3.6 |
| 32 | 2a | 1038 | C | 3.6 |
| 35 | 1d | 118 | ARG | 3.6 |
| 1 | 1A | 2189 | U | 3.6 |
| 1 | 1A | 2111 | C | 3.6 |
| 56 | 1y | 27 | G | 3.6 |
| 34 | 1c | 177 | THR | 3.6 |
| 1 | 1A | 1084 | A | 3.6 |
| 32 | 2a | 1005 | A | 3.6 |
| 32 | 1a | 1027 | C | 3.5 |
| 32 | 1a | 1001(A) | G | 3.5 |
| 18 | 1W | 112 | GLY | 3.5 |
| 41 | 1j | 36 | GLY | 3.5 |
| 56 | 1y | 45 | U | 3.5 |
| 1 | 2A | 2629 | A | 3.5 |
| 1 | 1A | 2178 | C | 3.5 |
| 1 | 2A | 897 | C | 3.5 |
| 32 | 1a | 163 | C | 3.5 |
| 1 | 2A | 2110 | G | 3.5 |
| 32 | 1a | 346 | G | 3.5 |
| 32 | 2a | 1031 | G | 3.5 |
| 1 | 2A | 2895 | U | 3.5 |
| 19 | 2X | 94 | GLY | 3.5 |
| 7 | 2H | 29 | PRO | 3.5 |
| 1 | 1A | 1072 | C | 3.5 |
| 7 | 2H | 6 | ARG | 3.5 |
| 32 | 2a | 1149 | C | 3.5 |
| 1 | 2A | 892 | G | 3.5 |
| 1 | 1A | 1066 | U | 3.5 |
| 41 | 1j | 87 | THR | 3.5 |
| 34 | 2c | 2 | GLY | 3.5 |
| 41 | 2j | 91 | PRO | 3.5 |
| 42 | 2k | 14 | VAL | 3.5 |
| 56 | 2y | 75 | C | 3.4 |
| 40 | 2i | 11 | LYS | 3.4 |
| 1 | 1A | 2180 | U | 3.4 |
| 1 | 2A | 2120 | G | 3.4 |
| 1 | 2A | 2155 | G | 3.4 |
| 1 | 2A | 2893 | G | 3.4 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|---------|------|------|
| 1 | 2A | 899 | A | 3.4 |
| 35 | 2d | 8 | VAL | 3.4 |
| 28 | 26 | 20 | ASN | 3.4 |
| 51 | 2t | 103 | GLY | 3.4 |
| 1 | 2A | 2172 | U | 3.4 |
| 1 | 1A | 2181 | G | 3.4 |
| 1 | 2A | 2100 | G | 3.4 |
| 1 | 1A | 2119 | A | 3.4 |
| 1 | 2A | 652(B) | A | 3.4 |
| 53 | 2v | 13 | A | 3.4 |
| 6 | 1G | 50 | ALA | 3.4 |
| 38 | 2g | 81 | GLY | 3.4 |
| 56 | 1y | 67 | C | 3.4 |
| 6 | 2G | 52 | ILE | 3.4 |
| 55 | 1x | 47 | U | 3.4 |
| 23 | 1l | 2 | SER | 3.4 |
| 38 | 2g | 85 | TYR | 3.4 |
| 1 | 1A | 1063 | G | 3.4 |
| 1 | 1A | 2166 | G | 3.4 |
| 1 | 2A | 2190 | G | 3.4 |
| 1 | 1A | 2896 | C | 3.3 |
| 1 | 2A | 885 | C | 3.3 |
| 32 | 2a | 1029 | C | 3.3 |
| 35 | 2d | 4 | TYR | 3.3 |
| 32 | 1a | 1030(D) | A | 3.3 |
| 1 | 1A | 1093 | G | 3.3 |
| 56 | 1y | 44 | G | 3.3 |
| 34 | 2c | 207 | VAL | 3.3 |
| 1 | 2A | 2107 | C | 3.3 |
| 1 | 2A | 2179 | C | 3.3 |
| 38 | 2g | 32 | ARG | 3.3 |
| 3 | 2D | 99 | ASP | 3.3 |
| 33 | 2b | 17 | PHE | 3.3 |
| 1 | 1A | 1177 | A | 3.3 |
| 1 | 2A | 2152 | G | 3.3 |
| 6 | 1G | 146 | TYR | 3.3 |
| 29 | 27 | 47 | ARG | 3.3 |
| 32 | 1a | 1257 | U | 3.3 |
| 43 | 1l | 63 | GLY | 3.3 |
| 56 | 2y | 12 | U | 3.3 |
| 1 | 1A | 2804 | C | 3.3 |
| 1 | 1A | 1073 | A | 3.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 56 | 1y | 36 | A | 3.3 |
| 1 | 1A | 2124 | G | 3.3 |
| 32 | 2a | 1026 | G | 3.3 |
| 33 | 2b | 11 | LEU | 3.3 |
| 56 | 2y | 19 | G | 3.3 |
| 7 | 2H | 134 | SER | 3.3 |
| 21 | 2Z | 106 | GLY | 3.3 |
| 29 | 17 | 48 | LYS | 3.3 |
| 7 | 2H | 52 | VAL | 3.3 |
| 38 | 2g | 80 | VAL | 3.3 |
| 1 | 1A | 888 | C | 3.2 |
| 1 | 2A | 898 | C | 3.2 |
| 35 | 1d | 122 | ARG | 3.2 |
| 40 | 2i | 102 | LEU | 3.2 |
| 51 | 2t | 99 | LEU | 3.2 |
| 41 | 1j | 32 | ALA | 3.2 |
| 56 | 1y | 57 | G | 3.2 |
| 56 | 2y | 45 | U | 3.2 |
| 1 | 2A | 884 | C | 3.2 |
| 32 | 2a | 1006 | C | 3.2 |
| 47 | 1p | 13 | HIS | 3.2 |
| 42 | 1k | 25 | TYR | 3.2 |
| 54 | 1w | 73 | A | 3.2 |
| 40 | 1i | 18 | PHE | 3.2 |
| 26 | 14 | 51 | ASP | 3.2 |
| 1 | 1A | 2152 | G | 3.2 |
| 1 | 2A | 1533 | G | 3.2 |
| 32 | 2a | 485 | G | 3.2 |
| 32 | 2a | 1040 | U | 3.2 |
| 56 | 2y | 22 | G | 3.2 |
| 1 | 1A | 2163 | C | 3.1 |
| 38 | 2g | 84 | ASN | 3.1 |
| 6 | 1G | 182 | LYS | 3.1 |
| 20 | 2Y | 54 | LYS | 3.1 |
| 1 | 1A | 1088 | A | 3.1 |
| 20 | 2Y | 90 | LEU | 3.1 |
| 53 | 1v | 12 | A | 3.1 |
| 41 | 2j | 87 | THR | 3.1 |
| 35 | 2d | 69 | GLY | 3.1 |
| 1 | 1A | 9 | U | 3.1 |
| 1 | 1A | 2122 | U | 3.1 |
| 1 | 2A | 362 | U | 3.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|---------|------|------|
| 32 | 2a | 1257 | U | 3.1 |
| 32 | 2a | 1532 | U | 3.1 |
| 1 | 2A | 886 | C | 3.1 |
| 26 | 14 | 57 | GLU | 3.1 |
| 32 | 1a | 221 | C | 3.1 |
| 56 | 1y | 68 | C | 3.1 |
| 1 | 2A | 2892 | A | 3.1 |
| 15 | 2T | 130 | ALA | 3.1 |
| 7 | 2H | 19 | VAL | 3.1 |
| 7 | 2H | 26 | VAL | 3.1 |
| 33 | 1b | 122 | PHE | 3.1 |
| 33 | 2b | 165 | VAL | 3.1 |
| 1 | 1A | 2150 | U | 3.1 |
| 1 | 2A | 2109 | U | 3.1 |
| 56 | 1y | 12 | U | 3.1 |
| 26 | 24 | 51 | ASP | 3.1 |
| 51 | 1t | 10 | LEU | 3.1 |
| 1 | 1A | 883 | G | 3.1 |
| 1 | 1A | 2141 | G | 3.1 |
| 1 | 1A | 2165 | G | 3.1 |
| 32 | 1a | 1030(C) | G | 3.1 |
| 32 | 1a | 1036 | G | 3.1 |
| 56 | 2y | 57 | G | 3.1 |
| 41 | 1j | 77 | PRO | 3.1 |
| 1 | 2A | 2164 | C | 3.1 |
| 1 | 2A | 2804 | C | 3.1 |
| 38 | 1g | 82 | GLY | 3.1 |
| 41 | 2j | 86 | MET | 3.1 |
| 1 | 2A | 2189 | U | 3.1 |
| 1 | 2A | 2897 | U | 3.1 |
| 42 | 2k | 117 | ASN | 3.1 |
| 21 | 2Z | 87 | ASP | 3.1 |
| 44 | 2m | 124 | PRO | 3.1 |
| 41 | 1j | 33 | GLN | 3.1 |
| 32 | 1a | 1139 | G | 3.1 |
| 56 | 1y | 24 | G | 3.1 |
| 41 | 1j | 4 | ILE | 3.1 |
| 33 | 2b | 96 | ARG | 3.1 |
| 56 | 2y | 67 | C | 3.1 |
| 1 | 2A | 2809 | A | 3.0 |
| 35 | 2d | 156 | GLU | 3.0 |
| 56 | 1y | 20 | U | 3.0 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 41 | 1j | 38 | ILE | 3.0 |
| 15 | 1T | 131 | ALA | 3.0 |
| 39 | 1h | 93 | VAL | 3.0 |
| 1 | 1A | 2207 | G | 3.0 |
| 32 | 1a | 630 | G | 3.0 |
| 19 | 2X | 95 | LEU | 3.0 |
| 1 | 1A | 886 | C | 3.0 |
| 1 | 1A | 2137 | C | 3.0 |
| 32 | 2a | 1018 | C | 3.0 |
| 7 | 2H | 118 | PRO | 3.0 |
| 42 | 2k | 13 | GLN | 3.0 |
| 1 | 1A | 1078 | U | 3.0 |
| 1 | 2A | 9 | U | 3.0 |
| 38 | 1g | 4 | ARG | 3.0 |
| 21 | 2Z | 172 | ALA | 3.0 |
| 21 | 2Z | 166 | SER | 3.0 |
| 41 | 2j | 59 | SER | 3.0 |
| 40 | 1i | 2 | GLU | 3.0 |
| 1 | 2A | 2168 | G | 3.0 |
| 32 | 1a | 1033 | G | 3.0 |
| 32 | 2a | 1023 | G | 3.0 |
| 56 | 2y | 70 | G | 3.0 |
| 1 | 1A | 2164 | C | 3.0 |
| 1 | 2A | 2140 | C | 3.0 |
| 32 | 1a | 1029 | C | 3.0 |
| 32 | 2a | 1286 | A | 3.0 |
| 44 | 2m | 123 | ALA | 3.0 |
| 1 | 2A | 12 | U | 3.0 |
| 1 | 2A | 895 | U | 3.0 |
| 7 | 2H | 7 | LEU | 3.0 |
| 34 | 2c | 105 | GLU | 3.0 |
| 41 | 2j | 37 | PRO | 3.0 |
| 3 | 2D | 276 | LYS | 3.0 |
| 50 | 2s | 13 | ASP | 3.0 |
| 21 | 2Z | 103 | ARG | 3.0 |
| 25 | 23 | 29 | ARG | 3.0 |
| 35 | 2d | 115 | ARG | 3.0 |
| 1 | 1A | 2156 | G | 3.0 |
| 56 | 1y | 49 | C | 3.0 |
| 56 | 1y | 74 | C | 3.0 |
| 21 | 1Z | 105 | VAL | 3.0 |
| 41 | 2j | 78 | ASN | 2.9 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|---------|------|------|
| 20 | 2Y | 55 | TYR | 2.9 |
| 16 | 2U | 88 | ILE | 2.9 |
| 40 | 2i | 19 | LEU | 2.9 |
| 1 | 1A | 1076 | C | 2.9 |
| 1 | 2A | 2108 | C | 2.9 |
| 1 | 2A | 878 | A | 2.9 |
| 1 | 2A | 2148 | G | 2.9 |
| 1 | 2A | 2165 | G | 2.9 |
| 32 | 1a | 162 | A | 2.9 |
| 32 | 1a | 1032 | G | 2.9 |
| 9 | 2N | 44 | PRO | 2.9 |
| 56 | 1y | 59 | U | 2.9 |
| 26 | 24 | 63 | TYR | 2.9 |
| 38 | 1g | 85 | TYR | 2.9 |
| 44 | 2m | 87 | TYR | 2.9 |
| 18 | 2W | 112 | GLY | 2.9 |
| 43 | 1l | 18 | VAL | 2.9 |
| 21 | 2Z | 150 | LEU | 2.9 |
| 38 | 2g | 156 | TRP | 2.9 |
| 47 | 1p | 82 | GLN | 2.9 |
| 1 | 2A | 2171 | A | 2.9 |
| 1 | 2A | 2794 | C | 2.9 |
| 32 | 1a | 160 | A | 2.9 |
| 51 | 2t | 8 | ARG | 2.9 |
| 56 | 1y | 11 | C | 2.9 |
| 1 | 1A | 171 | G | 2.9 |
| 1 | 1A | 2106 | G | 2.9 |
| 1 | 1A | 2155 | G | 2.9 |
| 1 | 2A | 171 | G | 2.9 |
| 1 | 2A | 2159 | G | 2.9 |
| 32 | 2a | 220 | G | 2.9 |
| 32 | 2a | 630 | G | 2.9 |
| 32 | 2a | 1030(C) | G | 2.9 |
| 56 | 1y | 1 | G | 2.9 |
| 56 | 2y | 5 | G | 2.9 |
| 56 | 2y | 18 | G | 2.9 |
| 56 | 2y | 24 | G | 2.9 |
| 34 | 2c | 47 | LEU | 2.9 |
| 35 | 1d | 135 | LEU | 2.9 |
| 8 | 2I | 82 | ARG | 2.9 |
| 35 | 1d | 73 | ARG | 2.9 |
| 1 | 2A | 894 | C | 2.9 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|--------|------|------|
| 32 | 2a | 1531 | A | 2.9 |
| 41 | 2j | 36 | GLY | 2.9 |
| 56 | 1y | 61 | C | 2.9 |
| 56 | 2y | 23 | A | 2.9 |
| 56 | 2y | 59 | U | 2.9 |
| 56 | 2y | 68 | C | 2.9 |
| 40 | 2i | 7 | THR | 2.9 |
| 15 | 1T | 130 | ALA | 2.9 |
| 32 | 1a | 220 | G | 2.9 |
| 56 | 1y | 22 | G | 2.9 |
| 33 | 1b | 130 | ARG | 2.8 |
| 9 | 2N | 45 | ASN | 2.8 |
| 38 | 1g | 81 | GLY | 2.8 |
| 43 | 2l | 126 | LYS | 2.8 |
| 8 | 2I | 146 | ALA | 2.8 |
| 9 | 2N | 9 | VAL | 2.8 |
| 32 | 1a | 1041 | A | 2.8 |
| 7 | 2H | 39 | PRO | 2.8 |
| 1 | 1A | 1087 | G | 2.8 |
| 1 | 2A | 2147 | G | 2.8 |
| 35 | 1d | 137 | SER | 2.8 |
| 35 | 1d | 171 | GLY | 2.8 |
| 33 | 1b | 11 | LEU | 2.8 |
| 39 | 1h | 112 | LEU | 2.8 |
| 6 | 2G | 50 | ALA | 2.8 |
| 21 | 1Z | 136 | PHE | 2.8 |
| 1 | 1A | 2897 | U | 2.8 |
| 56 | 1y | 47 | U | 2.8 |
| 24 | 12 | 70 | GLN | 2.8 |
| 32 | 1a | 1447 | A | 2.8 |
| 32 | 2a | 1447 | A | 2.8 |
| 56 | 2y | 9 | A | 2.8 |
| 1 | 1A | 2794 | C | 2.8 |
| 6 | 2G | 182 | LYS | 2.8 |
| 21 | 2Z | 137 | ILE | 2.8 |
| 33 | 2b | 127 | ILE | 2.8 |
| 1 | 1A | 2148 | G | 2.8 |
| 1 | 2A | 652(U) | G | 2.8 |
| 1 | 2A | 879 | G | 2.8 |
| 1 | 2A | 1171 | G | 2.8 |
| 1 | 2A | 2104 | G | 2.8 |
| 38 | 2g | 83 | ALA | 2.8 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 51 | 2t | 98 | PRO | 2.8 |
| 37 | 2f | 92 | LYS | 2.8 |
| 1 | 1A | 2126 | A | 2.8 |
| 53 | 1v | 14 | A | 2.8 |
| 53 | 2v | 14 | A | 2.8 |
| 1 | 1A | 2177 | C | 2.8 |
| 56 | 2y | 13 | C | 2.8 |
| 56 | 2y | 43 | C | 2.8 |
| 56 | 2y | 48 | C | 2.8 |
| 56 | 2y | 74 | C | 2.8 |
| 25 | 23 | 25 | ALA | 2.8 |
| 40 | 2i | 62 | TYR | 2.8 |
| 56 | 1y | 10 | G | 2.8 |
| 42 | 1k | 13 | GLN | 2.7 |
| 1 | 1A | 1065 | U | 2.7 |
| 1 | 1A | 2113 | U | 2.7 |
| 1 | 1A | 2895 | U | 2.7 |
| 54 | 1w | 16 | U | 2.7 |
| 56 | 2y | 47 | U | 2.7 |
| 21 | 2Z | 163 | LEU | 2.7 |
| 39 | 2h | 112 | LEU | 2.7 |
| 56 | 2y | 21 | A | 2.7 |
| 26 | 24 | 65 | ASP | 2.7 |
| 21 | 2Z | 104 | PHE | 2.7 |
| 26 | 14 | 49 | PHE | 2.7 |
| 32 | 1a | 1038 | C | 2.7 |
| 33 | 2b | 136 | VAL | 2.7 |
| 40 | 2i | 14 | VAL | 2.7 |
| 41 | 2j | 34 | VAL | 2.7 |
| 56 | 1y | 62 | C | 2.7 |
| 1 | 2A | 100 | G | 2.7 |
| 1 | 2A | 880 | G | 2.7 |
| 1 | 2A | 2792 | G | 2.7 |
| 56 | 2y | 27 | G | 2.7 |
| 39 | 1h | 2 | LEU | 2.7 |
| 33 | 1b | 93 | VAL | 2.7 |
| 34 | 2c | 62 | ASP | 2.7 |
| 38 | 1g | 32 | ARG | 2.7 |
| 38 | 2g | 7 | ALA | 2.7 |
| 26 | 14 | 59 | PHE | 2.7 |
| 1 | 2A | 2158 | A | 2.7 |
| 32 | 2a | 1001 | A | 2.7 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 35 | 1d | 172 | PRO | 2.7 |
| 56 | 2y | 35 | A | 2.7 |
| 12 | 2Q | 22 | LYS | 2.7 |
| 34 | 2c | 193 | TYR | 2.7 |
| 1 | 1A | 2179 | C | 2.7 |
| 32 | 1a | 1039 | C | 2.7 |
| 32 | 2a | 1037 | C | 2.7 |
| 56 | 1y | 13 | C | 2.7 |
| 7 | 2H | 136 | ILE | 2.7 |
| 40 | 1i | 19 | LEU | 2.7 |
| 1 | 1A | 2190 | G | 2.7 |
| 1 | 2A | 2141 | G | 2.7 |
| 1 | 2A | 2805 | G | 2.7 |
| 33 | 1b | 227 | GLY | 2.7 |
| 34 | 1c | 13 | GLY | 2.7 |
| 56 | 1y | 5 | G | 2.7 |
| 56 | 2y | 34 | G | 2.7 |
| 33 | 2b | 7 | VAL | 2.7 |
| 7 | 2H | 12 | PRO | 2.7 |
| 7 | 2H | 117 | PRO | 2.7 |
| 7 | 2H | 128 | PRO | 2.7 |
| 32 | 1a | 161 | A | 2.7 |
| 1 | 2A | 889 | C | 2.7 |
| 32 | 2a | 1325 | C | 2.7 |
| 35 | 1d | 87 | GLY | 2.7 |
| 35 | 1d | 167 | GLY | 2.7 |
| 6 | 2G | 29 | TRP | 2.7 |
| 38 | 1g | 84 | ASN | 2.7 |
| 41 | 2j | 76 | ASN | 2.7 |
| 31 | 29 | 16 | VAL | 2.7 |
| 47 | 2p | 68 | ASP | 2.7 |
| 1 | 1A | 11 | G | 2.6 |
| 1 | 1A | 2157 | G | 2.6 |
| 1 | 2A | 1114 | G | 2.6 |
| 1 | 2A | 2793 | G | 2.6 |
| 32 | 2a | 1094 | G | 2.6 |
| 56 | 1y | 19 | G | 2.6 |
| 56 | 1y | 63 | G | 2.6 |
| 56 | 1y | 65 | G | 2.6 |
| 56 | 2y | 69 | G | 2.6 |
| 1 | 1A | 2808 | U | 2.6 |
| 32 | 1a | 1040 | U | 2.6 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 56 | 2y | 33 | U | 2.6 |
| 33 | 1b | 121 | LEU | 2.6 |
| 23 | 21 | 28 | GLY | 2.6 |
| 1 | 1A | 2139 | C | 2.6 |
| 10 | 2O | 29 | ASN | 2.6 |
| 9 | 2N | 140 | VAL | 2.6 |
| 21 | 2Z | 141 | VAL | 2.6 |
| 33 | 1b | 17 | PHE | 2.6 |
| 35 | 1d | 149 | ALA | 2.6 |
| 7 | 2H | 21 | PRO | 2.6 |
| 21 | 2Z | 170 | THR | 2.6 |
| 21 | 2Z | 148 | ASP | 2.6 |
| 41 | 2j | 82 | ILE | 2.6 |
| 1 | 1A | 2154 | G | 2.6 |
| 1 | 2A | 1115 | G | 2.6 |
| 1 | 2A | 2157 | G | 2.6 |
| 56 | 1y | 6 | G | 2.6 |
| 56 | 2y | 66 | U | 2.6 |
| 41 | 2j | 65 | LEU | 2.6 |
| 33 | 1b | 19 | HIS | 2.6 |
| 41 | 2j | 10 | GLY | 2.6 |
| 1 | 1A | 2176 | A | 2.6 |
| 56 | 1y | 7 | A | 2.6 |
| 33 | 1b | 136 | VAL | 2.6 |
| 57 | 2z | 4 | SER | 2.6 |
| 1 | 1A | 2142 | C | 2.6 |
| 1 | 1A | 2146 | C | 2.6 |
| 6 | 2G | 147 | ASP | 2.6 |
| 26 | 24 | 68 | ARG | 2.6 |
| 45 | 2n | 3 | ARG | 2.6 |
| 9 | 2N | 10 | GLU | 2.6 |
| 7 | 2H | 48 | GLY | 2.6 |
| 10 | 2O | 27 | GLY | 2.6 |
| 44 | 1m | 100 | GLY | 2.6 |
| 1 | 2A | 2101 | G | 2.6 |
| 32 | 2a | 1131 | G | 2.6 |
| 33 | 1b | 7 | VAL | 2.6 |
| 40 | 1i | 15 | ALA | 2.6 |
| 42 | 1k | 14 | VAL | 2.6 |
| 1 | 1A | 1092 | C | 2.6 |
| 32 | 1a | 848 | C | 2.6 |
| 33 | 2b | 221 | LEU | 2.6 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|---------|------|------|
| 45 | 2n | 6 | LEU | 2.6 |
| 54 | 1w | 72 | C | 2.6 |
| 21 | 2Z | 72 | ARG | 2.6 |
| 44 | 1m | 125 | ARG | 2.6 |
| 8 | 2I | 87 | LYS | 2.6 |
| 44 | 2m | 13 | LYS | 2.6 |
| 7 | 2H | 47 | GLU | 2.6 |
| 35 | 1d | 192 | GLU | 2.6 |
| 51 | 1t | 103 | GLY | 2.6 |
| 32 | 1a | 841 | U | 2.6 |
| 33 | 1b | 15 | VAL | 2.6 |
| 26 | 24 | 49 | PHE | 2.6 |
| 44 | 2m | 42 | ALA | 2.6 |
| 1 | 1A | 271(M) | G | 2.5 |
| 1 | 1A | 1055 | G | 2.5 |
| 41 | 1j | 86 | MET | 2.5 |
| 1 | 1A | 1054 | A | 2.5 |
| 32 | 1a | 1001 | A | 2.5 |
| 32 | 1a | 1005 | A | 2.5 |
| 32 | 2a | 1030(D) | A | 2.5 |
| 33 | 2b | 10 | LEU | 2.5 |
| 56 | 2y | 26 | A | 2.5 |
| 56 | 2y | 73 | A | 2.5 |
| 6 | 1G | 51 | ARG | 2.5 |
| 35 | 1d | 191 | ARG | 2.5 |
| 43 | 1l | 19 | ARG | 2.5 |
| 8 | 2I | 135 | GLU | 2.5 |
| 33 | 1b | 9 | GLU | 2.5 |
| 1 | 1A | 154(A) | C | 2.5 |
| 32 | 1a | 1137 | C | 2.5 |
| 32 | 2a | 1028 | C | 2.5 |
| 32 | 2a | 1116 | C | 2.5 |
| 50 | 1s | 68 | GLY | 2.5 |
| 7 | 2H | 43 | VAL | 2.5 |
| 40 | 2i | 41 | VAL | 2.5 |
| 36 | 2e | 20 | GLN | 2.5 |
| 32 | 2a | 1148 | U | 2.5 |
| 7 | 2H | 175 | LYS | 2.5 |
| 20 | 2Y | 34 | LYS | 2.5 |
| 23 | 21 | 26 | ARG | 2.5 |
| 40 | 2i | 66 | ARG | 2.5 |
| 46 | 2o | 88 | ARG | 2.5 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 33 | 2b | 16 | HIS | 2.5 |
| 1 | 2A | 2131 | G | 2.5 |
| 56 | 2y | 10 | G | 2.5 |
| 7 | 2H | 83 | TYR | 2.5 |
| 8 | 2I | 89 | TYR | 2.5 |
| 33 | 1b | 129 | GLU | 2.5 |
| 56 | 1y | 73 | A | 2.5 |
| 20 | 2Y | 58 | GLY | 2.5 |
| 41 | 2j | 77 | PRO | 2.5 |
| 33 | 1b | 123 | ALA | 2.5 |
| 36 | 2e | 45 | PHE | 2.5 |
| 1 | 1A | 2188 | C | 2.5 |
| 32 | 1a | 219 | C | 2.5 |
| 32 | 2a | 1007 | C | 2.5 |
| 56 | 1y | 3 | C | 2.5 |
| 1 | 1A | 1175 | U | 2.5 |
| 7 | 2H | 88 | LEU | 2.5 |
| 33 | 1b | 10 | LEU | 2.5 |
| 36 | 2e | 5 | ASP | 2.5 |
| 32 | 1a | 1000 | U | 2.5 |
| 26 | 24 | 54 | GLY | 2.5 |
| 50 | 2s | 68 | GLY | 2.5 |
| 1 | 1A | 10 | G | 2.5 |
| 1 | 1A | 881 | G | 2.5 |
| 1 | 1A | 1086 | A | 2.5 |
| 1 | 1A | 2158 | A | 2.5 |
| 21 | 2Z | 105 | VAL | 2.5 |
| 32 | 2a | 1041 | A | 2.5 |
| 32 | 2a | 1224 | G | 2.5 |
| 40 | 2i | 44 | VAL | 2.5 |
| 56 | 2y | 1 | G | 2.5 |
| 33 | 2b | 123 | ALA | 2.5 |
| 38 | 1g | 83 | ALA | 2.5 |
| 40 | 1i | 106 | ALA | 2.5 |
| 21 | 2Z | 144 | LEU | 2.5 |
| 21 | 2Z | 171 | ILE | 2.5 |
| 33 | 2b | 200 | ILE | 2.5 |
| 44 | 1m | 25 | ILE | 2.5 |
| 1 | 2A | 1040 | C | 2.5 |
| 1 | 2A | 1041 | C | 2.5 |
| 40 | 1i | 75 | ASP | 2.5 |
| 45 | 2n | 61 | TRP | 2.5 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|--------|------|------|
| 56 | 1y | 43 | C | 2.5 |
| 56 | 2y | 2 | C | 2.5 |
| 1 | 1A | 2167 | U | 2.5 |
| 32 | 2a | 961 | U | 2.5 |
| 40 | 2i | 12 | GLU | 2.5 |
| 7 | 2H | 10 | PRO | 2.5 |
| 33 | 1b | 232 | PRO | 2.5 |
| 38 | 2g | 154 | TYR | 2.5 |
| 24 | 22 | 1 | MET | 2.5 |
| 4 | 2E | 204 | ALA | 2.5 |
| 34 | 2c | 71 | ALA | 2.5 |
| 40 | 2i | 43 | ALA | 2.5 |
| 3 | 2D | 275 | LYS | 2.4 |
| 33 | 2b | 132 | LYS | 2.4 |
| 48 | 1q | 100 | LYS | 2.4 |
| 1 | 1A | 278 | A | 2.4 |
| 1 | 1A | 2629 | A | 2.4 |
| 32 | 1a | 195 | A | 2.4 |
| 56 | 1y | 21 | A | 2.4 |
| 1 | 1A | 271(D) | G | 2.4 |
| 1 | 1A | 545 | G | 2.4 |
| 32 | 2a | 1220 | G | 2.4 |
| 35 | 1d | 134 | ASP | 2.4 |
| 6 | 2G | 48 | GLU | 2.4 |
| 33 | 2b | 129 | GLU | 2.4 |
| 1 | 2A | 1178 | C | 2.4 |
| 1 | 2A | 2145 | C | 2.4 |
| 56 | 2y | 40 | C | 2.4 |
| 56 | 2y | 49 | C | 2.4 |
| 1 | 1A | 271(K) | U | 2.4 |
| 1 | 1A | 1083 | U | 2.4 |
| 32 | 1a | 173 | U | 2.4 |
| 32 | 1a | 182 | U | 2.4 |
| 41 | 2j | 31 | GLY | 2.4 |
| 50 | 1s | 8 | GLY | 2.4 |
| 56 | 2y | 60 | U | 2.4 |
| 35 | 1d | 29 | PRO | 2.4 |
| 33 | 1b | 236 | TYR | 2.4 |
| 20 | 2Y | 57 | GLN | 2.4 |
| 45 | 2n | 18 | VAL | 2.4 |
| 33 | 2b | 77 | ALA | 2.4 |
| 38 | 2g | 40 | ALA | 2.4 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 41 | 2j | 100 | THR | 2.4 |
| 1 | 1A | 1045 | A | 2.4 |
| 1 | 1A | 1103 | A | 2.4 |
| 1 | 2A | 887 | A | 2.4 |
| 1 | 2A | 900 | A | 2.4 |
| 35 | 1d | 173 | TRP | 2.4 |
| 56 | 2y | 58 | A | 2.4 |
| 1 | 2A | 2751 | G | 2.4 |
| 54 | 2w | 19 | G | 2.4 |
| 56 | 1y | 18 | G | 2.4 |
| 56 | 1y | 69 | G | 2.4 |
| 45 | 2n | 38 | GLY | 2.4 |
| 1 | 1A | 1509 | C | 2.4 |
| 1 | 1A | 2140 | C | 2.4 |
| 1 | 2A | 2146 | C | 2.4 |
| 24 | 22 | 70 | GLN | 2.4 |
| 26 | 24 | 67 | TYR | 2.4 |
| 32 | 1a | 1008 | C | 2.4 |
| 33 | 1b | 165 | VAL | 2.4 |
| 1 | 1A | 362 | U | 2.4 |
| 1 | 1A | 895 | U | 2.4 |
| 32 | 1a | 203 | U | 2.4 |
| 32 | 2a | 1025 | U | 2.4 |
| 34 | 1c | 193 | TYR | 2.4 |
| 34 | 2c | 92 | ALA | 2.4 |
| 54 | 2w | 47 | U | 2.4 |
| 40 | 1i | 10 | ARG | 2.4 |
| 6 | 2G | 53 | LEU | 2.4 |
| 21 | 2Z | 125 | LEU | 2.4 |
| 41 | 2j | 90 | LEU | 2.4 |
| 45 | 2n | 13 | THR | 2.4 |
| 48 | 1q | 98 | LEU | 2.4 |
| 50 | 2s | 71 | LEU | 2.4 |
| 23 | 21 | 27 | GLU | 2.4 |
| 1 | 1A | 899 | A | 2.4 |
| 1 | 2A | 890 | A | 2.4 |
| 1 | 2A | 1847 | A | 2.4 |
| 32 | 2a | 1250 | A | 2.4 |
| 47 | 1p | 12 | LYS | 2.4 |
| 53 | 1v | 15 | A | 2.4 |
| 12 | 2Q | 15 | GLY | 2.4 |
| 44 | 1m | 26 | GLY | 2.4 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|---------|------|------|
| 1 | 1A | 1071 | G | 2.4 |
| 1 | 2A | 2833 | G | 2.4 |
| 32 | 2a | 1124 | G | 2.4 |
| 33 | 2b | 207 | ALA | 2.4 |
| 1 | 2A | 272(A) | U | 2.4 |
| 34 | 2c | 84 | ILE | 2.4 |
| 35 | 1d | 5 | ILE | 2.4 |
| 40 | 2i | 64 | THR | 2.4 |
| 44 | 1m | 105 | THR | 2.4 |
| 1 | 2A | 2177 | C | 2.4 |
| 1 | 2A | 2183 | C | 2.4 |
| 1 | 2A | 2789 | C | 2.4 |
| 32 | 2a | 470 | C | 2.4 |
| 32 | 2a | 1363 | C | 2.4 |
| 33 | 1b | 231 | GLU | 2.4 |
| 40 | 2i | 105 | ASP | 2.4 |
| 3 | 2D | 38 | LYS | 2.4 |
| 35 | 1d | 169 | LYS | 2.4 |
| 12 | 1Q | 60 | ARG | 2.4 |
| 41 | 2j | 79 | ARG | 2.4 |
| 44 | 2m | 54 | VAL | 2.4 |
| 45 | 2n | 12 | ARG | 2.4 |
| 52 | 1u | 6 | ARG | 2.4 |
| 1 | 1A | 229 | A | 2.4 |
| 1 | 1A | 878 | A | 2.4 |
| 16 | 2U | 106 | PHE | 2.4 |
| 40 | 1i | 7 | THR | 2.3 |
| 22 | 10 | 3 | HIS | 2.3 |
| 8 | 2I | 74 | ASN | 2.3 |
| 1 | 1A | 1176 | G | 2.3 |
| 1 | 1A | 2118 | U | 2.3 |
| 1 | 2A | 1170 | G | 2.3 |
| 1 | 2A | 2166 | G | 2.3 |
| 1 | 2A | 2191 | G | 2.3 |
| 56 | 1y | 33 | U | 2.3 |
| 56 | 2y | 52 | G | 2.3 |
| 41 | 1j | 83 | GLU | 2.3 |
| 1 | 1A | 889 | C | 2.3 |
| 1 | 2A | 2142 | C | 2.3 |
| 32 | 1a | 1030(B) | C | 2.3 |
| 32 | 2a | 1019 | C | 2.3 |
| 50 | 1s | 4 | SER | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|--------|------|------|
| 56 | 1y | 48 | C | 2.3 |
| 56 | 2y | 56 | C | 2.3 |
| 52 | 1u | 19 | GLY | 2.3 |
| 11 | 2P | 90 | ARG | 2.3 |
| 12 | 2Q | 60 | ARG | 2.3 |
| 47 | 1p | 71 | ARG | 2.3 |
| 7 | 2H | 79 | VAL | 2.3 |
| 29 | 27 | 46 | VAL | 2.3 |
| 26 | 24 | 59 | PHE | 2.3 |
| 29 | 27 | 45 | ALA | 2.3 |
| 40 | 2i | 15 | ALA | 2.3 |
| 7 | 2H | 121 | ILE | 2.3 |
| 1 | 1A | 887 | A | 2.3 |
| 1 | 1A | 1067 | A | 2.3 |
| 2 | 2B | 59 | A | 2.3 |
| 30 | 28 | 29 | LYS | 2.3 |
| 32 | 2a | 204 | U | 2.3 |
| 1 | 2A | 652(C) | G | 2.3 |
| 1 | 2A | 1039 | G | 2.3 |
| 32 | 1a | 79 | G | 2.3 |
| 32 | 1a | 183 | G | 2.3 |
| 56 | 1y | 53 | G | 2.3 |
| 1 | 2A | 2105 | C | 2.3 |
| 32 | 1a | 1037 | C | 2.3 |
| 32 | 2a | 1326 | C | 2.3 |
| 35 | 1d | 62 | GLN | 2.3 |
| 41 | 2j | 28 | ARG | 2.3 |
| 44 | 1m | 24 | GLY | 2.3 |
| 56 | 1y | 25 | C | 2.3 |
| 56 | 2y | 25 | C | 2.3 |
| 7 | 2H | 11 | VAL | 2.3 |
| 7 | 2H | 15 | VAL | 2.3 |
| 7 | 2H | 44 | VAL | 2.3 |
| 7 | 2H | 50 | VAL | 2.3 |
| 7 | 2H | 114 | VAL | 2.3 |
| 40 | 2i | 65 | VAL | 2.3 |
| 19 | 1X | 95 | LEU | 2.3 |
| 40 | 2i | 45 | ALA | 2.3 |
| 41 | 1j | 40 | LEU | 2.3 |
| 44 | 1m | 5 | ALA | 2.3 |
| 49 | 2r | 20 | ALA | 2.3 |
| 7 | 2H | 9 | ILE | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 34 | 2c | 182 | ILE | 2.3 |
| 26 | 14 | 32 | TYR | 2.3 |
| 36 | 2e | 133 | TYR | 2.3 |
| 45 | 2n | 22 | THR | 2.3 |
| 6 | 1G | 35 | GLU | 2.3 |
| 8 | 2I | 70 | GLU | 2.3 |
| 48 | 2q | 100 | LYS | 2.3 |
| 44 | 2m | 12 | ASN | 2.3 |
| 53 | 2v | 15 | A | 2.3 |
| 20 | 2Y | 53 | PRO | 2.3 |
| 38 | 2g | 5 | ARG | 2.3 |
| 42 | 2k | 91 | ARG | 2.3 |
| 34 | 1c | 171 | GLY | 2.3 |
| 42 | 2k | 86 | GLY | 2.3 |
| 1 | 2A | 1026 | U | 2.3 |
| 1 | 2A | 2132 | U | 2.3 |
| 32 | 1a | 164 | U | 2.3 |
| 32 | 2a | 1000 | U | 2.3 |
| 7 | 1H | 171 | LEU | 2.3 |
| 38 | 2g | 16 | LEU | 2.3 |
| 33 | 2b | 218 | ALA | 2.3 |
| 42 | 2k | 15 | ALA | 2.3 |
| 1 | 1A | 1080 | C | 2.3 |
| 1 | 1A | 1099 | G | 2.3 |
| 1 | 1A | 2100 | G | 2.3 |
| 1 | 1A | 2105 | C | 2.3 |
| 1 | 1A | 2805 | G | 2.3 |
| 1 | 2A | 2181 | G | 2.3 |
| 1 | 2A | 2188 | C | 2.3 |
| 32 | 1a | 218 | C | 2.3 |
| 32 | 2a | 999 | C | 2.3 |
| 56 | 1y | 72 | C | 2.3 |
| 56 | 2y | 71 | G | 2.3 |
| 36 | 2e | 10 | MET | 2.3 |
| 4 | 2E | 73 | GLU | 2.3 |
| 42 | 1k | 117 | ASN | 2.3 |
| 34 | 2c | 79 | ARG | 2.3 |
| 1 | 1A | 548 | A | 2.3 |
| 1 | 1A | 1085 | A | 2.3 |
| 36 | 1e | 85 | GLY | 2.3 |
| 40 | 2i | 39 | GLY | 2.3 |
| 52 | 2u | 16 | GLY | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|--------|------|------|
| 56 | 1y | 26 | A | 2.3 |
| 56 | 1y | 64 | A | 2.3 |
| 8 | 2I | 68 | LEU | 2.3 |
| 16 | 2U | 8 | VAL | 2.3 |
| 26 | 24 | 50 | VAL | 2.3 |
| 33 | 1b | 215 | LEU | 2.3 |
| 34 | 2c | 195 | VAL | 2.3 |
| 32 | 1a | 65 | U | 2.2 |
| 56 | 1y | 66 | U | 2.2 |
| 8 | 1I | 41 | GLU | 2.2 |
| 35 | 1d | 179 | GLU | 2.2 |
| 6 | 2G | 146 | TYR | 2.2 |
| 1 | 1A | 1075 | C | 2.2 |
| 1 | 2A | 893 | C | 2.2 |
| 1 | 2A | 2163 | C | 2.2 |
| 32 | 1a | 1030 | C | 2.2 |
| 54 | 2w | 2 | C | 2.2 |
| 1 | 1A | 652(C) | G | 2.2 |
| 1 | 2A | 2186 | G | 2.2 |
| 32 | 1a | 93 | G | 2.2 |
| 54 | 2w | 71 | G | 2.2 |
| 35 | 1d | 65 | ARG | 2.2 |
| 21 | 2Z | 158 | PRO | 2.2 |
| 21 | 2Z | 167 | PRO | 2.2 |
| 21 | 2Z | 142 | SER | 2.2 |
| 26 | 14 | 50 | VAL | 2.2 |
| 35 | 1d | 88 | VAL | 2.2 |
| 41 | 2j | 40 | LEU | 2.2 |
| 50 | 2s | 15 | LEU | 2.2 |
| 1 | 2A | 6 | A | 2.2 |
| 20 | 2Y | 44 | ILE | 2.2 |
| 32 | 1a | 1286 | A | 2.2 |
| 34 | 2c | 77 | ILE | 2.2 |
| 34 | 2c | 137 | ALA | 2.2 |
| 38 | 1g | 2 | ALA | 2.2 |
| 51 | 2t | 97 | ALA | 2.2 |
| 56 | 1y | 9 | A | 2.2 |
| 56 | 1y | 58 | A | 2.2 |
| 32 | 2a | 1219 | U | 2.2 |
| 35 | 2d | 192 | GLU | 2.2 |
| 33 | 2b | 31 | TYR | 2.2 |
| 5 | 2F | 169 | ASN | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 5 | 2F | 171 | PRO | 2.2 |
| 34 | 2c | 109 | PRO | 2.2 |
| 1 | 2A | 2178 | C | 2.2 |
| 1 | 2A | 2185 | C | 2.2 |
| 56 | 2y | 4 | C | 2.2 |
| 1 | 1A | 1091 | G | 2.2 |
| 1 | 2A | 2156 | G | 2.2 |
| 1 | 2A | 2182 | G | 2.2 |
| 1 | 2A | 2807 | G | 2.2 |
| 32 | 1a | 1138 | G | 2.2 |
| 41 | 1j | 90 | LEU | 2.2 |
| 42 | 2k | 103 | LEU | 2.2 |
| 20 | 2Y | 49 | VAL | 2.2 |
| 42 | 2k | 105 | VAL | 2.2 |
| 34 | 2c | 128 | PHE | 2.2 |
| 1 | 1A | 2790 | A | 2.2 |
| 32 | 1a | 171 | A | 2.2 |
| 34 | 2c | 95 | THR | 2.2 |
| 40 | 1i | 64 | THR | 2.2 |
| 3 | 2D | 263 | ARG | 2.2 |
| 32 | 1a | 1446 | U | 2.2 |
| 38 | 2g | 4 | ARG | 2.2 |
| 41 | 2j | 5 | ARG | 2.2 |
| 33 | 1b | 131 | PRO | 2.2 |
| 33 | 1b | 154 | LEU | 2.2 |
| 39 | 2h | 130 | GLY | 2.2 |
| 40 | 1i | 91 | ASP | 2.2 |
| 42 | 2k | 36 | ASP | 2.2 |
| 51 | 2t | 10 | LEU | 2.2 |
| 34 | 2c | 116 | VAL | 2.2 |
| 48 | 2q | 23 | VAL | 2.2 |
| 1 | 2A | 1509 | C | 2.2 |
| 6 | 1G | 52 | ILE | 2.2 |
| 41 | 1j | 74 | ILE | 2.2 |
| 1 | 1A | 1062 | G | 2.2 |
| 1 | 1A | 1173 | G | 2.2 |
| 1 | 2A | 1042 | G | 2.2 |
| 1 | 2A | 1112 | G | 2.2 |
| 1 | 2A | 2184 | G | 2.2 |
| 32 | 1a | 77 | G | 2.2 |
| 32 | 2a | 1181 | G | 2.2 |
| 56 | 1y | 70 | G | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 41 | 2j | 15 | THR | 2.2 |
| 41 | 2j | 42 | THR | 2.2 |
| 35 | 1d | 3 | ARG | 2.2 |
| 7 | 2H | 36 | PRO | 2.2 |
| 32 | 2a | 1256 | A | 2.2 |
| 34 | 2c | 23 | TYR | 2.2 |
| 1 | 1A | 2102 | U | 2.2 |
| 7 | 2H | 33 | LEU | 2.2 |
| 40 | 2i | 91 | ASP | 2.2 |
| 7 | 2H | 49 | VAL | 2.2 |
| 14 | 2S | 31 | SER | 2.2 |
| 21 | 2Z | 139 | VAL | 2.2 |
| 21 | 2Z | 149 | SER | 2.2 |
| 40 | 2i | 108 | VAL | 2.2 |
| 33 | 2b | 97 | TRP | 2.1 |
| 40 | 2i | 94 | ALA | 2.1 |
| 1 | 1A | 645 | C | 2.1 |
| 1 | 1A | 893 | C | 2.1 |
| 1 | 2A | 2143 | C | 2.1 |
| 23 | 11 | 26 | ARG | 2.1 |
| 32 | 1a | 1043 | C | 2.1 |
| 32 | 2a | 1043 | C | 2.1 |
| 1 | 1A | 1056 | G | 2.1 |
| 1 | 1A | 2147 | G | 2.1 |
| 1 | 1A | 2793 | G | 2.1 |
| 1 | 2A | 2891 | G | 2.1 |
| 21 | 2Z | 159 | PRO | 2.1 |
| 32 | 1a | 78 | G | 2.1 |
| 32 | 2a | 1022 | G | 2.1 |
| 41 | 1j | 39 | PRO | 2.1 |
| 55 | 1x | 46 | G | 2.1 |
| 33 | 1b | 187 | LEU | 2.1 |
| 1 | 1A | 8 | A | 2.1 |
| 1 | 1A | 1174 | A | 2.1 |
| 32 | 2a | 171 | A | 2.1 |
| 40 | 2i | 67 | GLY | 2.1 |
| 50 | 2s | 26 | GLY | 2.1 |
| 1 | 2A | 1113 | U | 2.1 |
| 7 | 2H | 45 | VAL | 2.1 |
| 32 | 1a | 204 | U | 2.1 |
| 35 | 2d | 158 | ILE | 2.1 |
| 40 | 1i | 14 | VAL | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|--------|------|------|
| 35 | 1d | 195 | ALA | 2.1 |
| 6 | 1G | 48 | GLU | 2.1 |
| 7 | 2H | 101 | ARG | 2.1 |
| 12 | 2Q | 5 | ARG | 2.1 |
| 35 | 2d | 3 | ARG | 2.1 |
| 41 | 2j | 66 | ARG | 2.1 |
| 9 | 2N | 118 | LYS | 2.1 |
| 20 | 1Y | 53 | PRO | 2.1 |
| 40 | 2i | 95 | LYS | 2.1 |
| 1 | 1A | 1053 | C | 2.1 |
| 1 | 2A | 652(T) | C | 2.1 |
| 32 | 2a | 1128 | C | 2.1 |
| 56 | 1y | 4 | C | 2.1 |
| 11 | 2P | 1 | MET | 2.1 |
| 41 | 1j | 78 | ASN | 2.1 |
| 1 | 1A | 2182 | G | 2.1 |
| 20 | 2Y | 45 | VAL | 2.1 |
| 26 | 24 | 56 | VAL | 2.1 |
| 47 | 1p | 68 | ASP | 2.1 |
| 21 | 2Z | 88 | PHE | 2.1 |
| 38 | 2g | 77 | SER | 2.1 |
| 42 | 2k | 16 | SER | 2.1 |
| 47 | 1p | 80 | PHE | 2.1 |
| 1 | 1A | 890 | A | 2.1 |
| 1 | 1A | 1046 | A | 2.1 |
| 32 | 2a | 197 | A | 2.1 |
| 32 | 2a | 978 | A | 2.1 |
| 50 | 2s | 24 | ALA | 2.1 |
| 6 | 1G | 137 | GLU | 2.1 |
| 56 | 1y | 50 | U | 2.1 |
| 44 | 2m | 99 | ARG | 2.1 |
| 23 | 2l | 81 | LYS | 2.1 |
| 43 | 2l | 91 | LYS | 2.1 |
| 41 | 1j | 76 | ASN | 2.1 |
| 33 | 1b | 40 | HIS | 2.1 |
| 33 | 2b | 228 | GLY | 2.1 |
| 35 | 1d | 138 | TYR | 2.1 |
| 1 | 1A | 2185 | C | 2.1 |
| 15 | 2T | 28 | VAL | 2.1 |
| 32 | 1a | 92 | C | 2.1 |
| 32 | 2a | 1118 | C | 2.1 |
| 41 | 2j | 49 | VAL | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 5 | 2F | 168 | ARG | 2.1 |
| 7 | 1H | 156 | ALA | 2.1 |
| 7 | 2H | 96 | ALA | 2.1 |
| 33 | 2b | 126 | GLU | 2.1 |
| 34 | 2c | 206 | GLU | 2.1 |
| 36 | 2e | 21 | ALA | 2.1 |
| 40 | 2i | 10 | ARG | 2.1 |
| 51 | 1t | 97 | ALA | 2.1 |
| 1 | 1A | 2792 | G | 2.1 |
| 32 | 2a | 998 | G | 2.1 |
| 32 | 2a | 1021 | G | 2.1 |
| 32 | 1a | 368 | U | 2.1 |
| 41 | 2j | 80 | LYS | 2.1 |
| 56 | 1y | 23 | A | 2.1 |
| 56 | 2y | 51 | U | 2.1 |
| 7 | 2H | 8 | PRO | 2.1 |
| 7 | 2H | 41 | MET | 2.1 |
| 38 | 2g | 86 | GLN | 2.1 |
| 21 | 2Z | 157 | LEU | 2.1 |
| 35 | 1d | 21 | LEU | 2.1 |
| 7 | 1H | 158 | HIS | 2.1 |
| 7 | 2H | 82 | GLY | 2.1 |
| 7 | 2H | 135 | GLY | 2.1 |
| 34 | 1c | 2 | GLY | 2.1 |
| 41 | 1j | 93 | GLY | 2.1 |
| 21 | 2Z | 96 | VAL | 2.1 |
| 36 | 2e | 51 | VAL | 2.1 |
| 6 | 2G | 45 | GLU | 2.0 |
| 21 | 2Z | 145 | GLU | 2.0 |
| 33 | 1b | 12 | GLU | 2.0 |
| 33 | 2b | 137 | ARG | 2.0 |
| 34 | 1c | 79 | ARG | 2.0 |
| 35 | 1d | 132 | ARG | 2.0 |
| 33 | 1b | 188 | ALA | 2.0 |
| 40 | 2i | 2 | GLU | 2.0 |
| 47 | 1p | 42 | ARG | 2.0 |
| 31 | 29 | 6 | SER | 2.0 |
| 1 | 1A | 2143 | C | 2.0 |
| 20 | 2Y | 33 | LYS | 2.0 |
| 56 | 2y | 11 | C | 2.0 |
| 41 | 2j | 92 | THR | 2.0 |
| 46 | 1o | 19 | PRO | 2.0 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|--------|------|------|
| 1 | 2A | 2180 | U | 2.0 |
| 5 | 2F | 170 | LEU | 2.0 |
| 35 | 1d | 11 | LEU | 2.0 |
| 35 | 1d | 120 | LEU | 2.0 |
| 38 | 2g | 12 | LEU | 2.0 |
| 40 | 2i | 50 | LEU | 2.0 |
| 40 | 2i | 56 | LEU | 2.0 |
| 45 | 2n | 39 | LEU | 2.0 |
| 46 | 1o | 57 | LEU | 2.0 |
| 32 | 1a | 181 | G | 2.0 |
| 54 | 1w | 71 | G | 2.0 |
| 56 | 2y | 28 | G | 2.0 |
| 7 | 2H | 31 | GLY | 2.0 |
| 21 | 2Z | 12 | GLY | 2.0 |
| 21 | 2Z | 147 | GLY | 2.0 |
| 34 | 1c | 81 | GLY | 2.0 |
| 40 | 2i | 8 | GLY | 2.0 |
| 41 | 1j | 75 | ILE | 2.0 |
| 11 | 2P | 91 | PHE | 2.0 |
| 33 | 2b | 70 | PHE | 2.0 |
| 34 | 2c | 88 | ARG | 2.0 |
| 44 | 1m | 102 | ARG | 2.0 |
| 34 | 1c | 82 | GLU | 2.0 |
| 3 | 1D | 38 | LYS | 2.0 |
| 7 | 2H | 150 | ALA | 2.0 |
| 33 | 1b | 22 | LYS | 2.0 |
| 33 | 1b | 132 | LYS | 2.0 |
| 41 | 2j | 14 | LYS | 2.0 |
| 21 | 2Z | 92 | SER | 2.0 |
| 47 | 2p | 48 | TRP | 2.0 |
| 1 | 1A | 34 | C | 2.0 |
| 1 | 1A | 271(Z) | C | 2.0 |
| 1 | 2A | 1043 | C | 2.0 |
| 1 | 2A | 2103 | C | 2.0 |
| 32 | 2a | 1008 | C | 2.0 |
| 32 | 2a | 1452 | C | 2.0 |
| 33 | 1b | 213 | LEU | 2.0 |
| 34 | 2c | 87 | LEU | 2.0 |
| 1 | 2A | 2808 | U | 2.0 |
| 5 | 2F | 208 | GLY | 2.0 |
| 34 | 2c | 159 | GLY | 2.0 |
| 41 | 1j | 10 | GLY | 2.0 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | 2A | 229 | A | 2.0 |
| 22 | 20 | 55 | ARG | 2.0 |
| 29 | 17 | 46 | VAL | 2.0 |
| 33 | 1b | 137 | ARG | 2.0 |
| 35 | 2d | 132 | ARG | 2.0 |
| 36 | 2e | 27 | ARG | 2.0 |
| 45 | 1n | 3 | ARG | 2.0 |
| 45 | 2n | 34 | TYR | 2.0 |

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

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | 4SU | 2y | 8 | 20/21 | 0.45 | 0.20 | 84,89,100,114 | 0 |
| 56 | G7M | 2y | 46 | 24/25 | 0.47 | 0.18 | 75,85,92,101 | 0 |
| 56 | 5MU | 2y | 54 | 21/22 | 0.48 | 0.17 | 78,86,96,113 | 0 |
| 56 | 5MU | 1y | 54 | 21/22 | 0.51 | 0.18 | 77,85,93,112 | 0 |
| 56 | G7M | 1y | 46 | 24/25 | 0.52 | 0.19 | 81,86,94,100 | 0 |
| 56 | 4SU | 1y | 8 | 20/21 | 0.57 | 0.18 | 83,88,92,103 | 0 |
| 56 | PSU | 1y | 55 | 20/21 | 0.66 | 0.18 | 83,87,96,107 | 0 |
| 56 | MIA | 1y | 37 | 22/30 | 0.67 | 0.18 | 74,79,86,90 | 0 |
| 56 | PSU | 2y | 39 | 20/21 | 0.67 | 0.16 | 76,80,88,100 | 0 |
| 56 | MIA | 2y | 37 | 22/30 | 0.68 | 0.17 | 65,84,90,108 | 0 |
| 56 | PSU | 2y | 32 | 20/21 | 0.71 | 0.16 | 79,83,88,104 | 0 |
| 56 | PSU | 2y | 55 | 20/21 | 0.74 | 0.14 | 79,86,95,97 | 0 |
| 54 | G7M | 1w | 46 | 24/25 | 0.77 | 0.14 | 58,66,85,96 | 0 |
| 56 | PSU | 1y | 39 | 20/21 | 0.80 | 0.13 | 68,76,80,85 | 0 |
| 54 | G7M | 2w | 46 | 24/25 | 0.82 | 0.12 | 69,73,87,98 | 0 |
| 56 | PSU | 1y | 32 | 20/21 | 0.82 | 0.14 | 72,76,84,94 | 0 |
| 54 | PSU | 2w | 55 | 20/21 | 0.86 | 0.13 | 63,68,77,78 | 0 |
| 54 | 4SU | 2w | 8 | 20/21 | 0.88 | 0.11 | 68,73,76,88 | 0 |
| 55 | PSU | 2x | 55 | 20/21 | 0.91 | 0.11 | 54,58,63,65 | 0 |
| 54 | 5MU | 2w | 54 | 21/22 | 0.91 | 0.11 | 55,61,67,72 | 0 |
| 54 | PSU | 1w | 55 | 20/21 | 0.91 | 0.11 | 42,57,69,69 | 0 |
| 55 | 4SU | 2x | 8 | 20/21 | 0.91 | 0.12 | 55,64,69,81 | 0 |
| 54 | PSU | 2w | 32 | 20/21 | 0.92 | 0.12 | 47,58,63,66 | 0 |
| 55 | 5MU | 2x | 54 | 21/22 | 0.92 | 0.15 | 55,61,63,65 | 0 |
| 32 | 2MG | 2a | 1207 | 24/25 | 0.92 | 0.10 | 53,61,65,68 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 43 | 0TD | 2l | 92 | 10/11 | 0.92 | 0.16 | 45,53,56,61 | 0 |
| 55 | 5MU | 1x | 54 | 21/22 | 0.92 | 0.13 | 48,54,59,60 | 0 |
| 43 | 0TD | 1l | 92 | 10/11 | 0.93 | 0.11 | 35,41,45,48 | 0 |
| 32 | 5MC | 2a | 1400 | 21/22 | 0.93 | 0.11 | 43,50,55,58 | 0 |
| 32 | PSU | 2a | 516 | 20/21 | 0.93 | 0.09 | 46,56,61,62 | 0 |
| 54 | PSU | 1w | 32 | 20/21 | 0.94 | 0.09 | 38,41,47,49 | 0 |
| 55 | PSU | 1x | 55 | 20/21 | 0.94 | 0.09 | 38,46,56,61 | 0 |
| 32 | G7M | 2a | 527 | 24/25 | 0.94 | 0.10 | 47,52,59,60 | 0 |
| 32 | M2G | 2a | 966 | 25/26 | 0.94 | 0.10 | 43,48,60,65 | 0 |
| 55 | 5MC | 2x | 32 | 21/22 | 0.94 | 0.11 | 45,52,57,59 | 0 |
| 32 | 5MC | 2a | 967 | 21/22 | 0.94 | 0.10 | 45,52,60,61 | 0 |
| 54 | MIA | 2w | 37 | 25/30 | 0.94 | 0.09 | 29,50,59,65 | 0 |
| 55 | 5MC | 1x | 32 | 21/22 | 0.95 | 0.10 | 37,43,47,57 | 0 |
| 54 | 4SU | 1w | 8 | 20/21 | 0.95 | 0.09 | 55,63,67,67 | 0 |
| 32 | 5MC | 1a | 967 | 21/22 | 0.95 | 0.09 | 35,40,49,53 | 0 |
| 1 | 5MU | 2A | 1915 | 21/22 | 0.95 | 0.09 | 40,47,52,53 | 0 |
| 1 | PSU | 2A | 1917 | 20/21 | 0.95 | 0.08 | 46,50,57,66 | 0 |
| 1 | 5MC | 2A | 1942 | 21/22 | 0.95 | 0.11 | 39,46,50,59 | 0 |
| 32 | 2MG | 1a | 1207 | 24/25 | 0.95 | 0.08 | 41,53,57,57 | 0 |
| 54 | 5MU | 1w | 54 | 21/22 | 0.95 | 0.10 | 38,46,51,52 | 0 |
| 1 | PSU | 1A | 1917 | 20/21 | 0.95 | 0.10 | 34,38,46,47 | 0 |
| 55 | 4SU | 1x | 8 | 20/21 | 0.95 | 0.10 | 45,49,55,58 | 0 |
| 1 | 5MU | 1A | 1915 | 21/22 | 0.96 | 0.09 | 29,38,41,43 | 0 |
| 32 | 4OC | 2a | 1402 | 22/23 | 0.96 | 0.08 | 37,44,47,49 | 0 |
| 32 | 5MC | 2a | 1407 | 21/22 | 0.96 | 0.07 | 33,39,42,45 | 0 |
| 32 | UR3 | 2a | 1498 | 21/22 | 0.96 | 0.09 | 37,41,46,49 | 0 |
| 55 | 31H | 2x | 76 | 32/33 | 0.96 | 0.09 | 27,32,37,40 | 0 |
| 1 | 5MC | 2A | 1962 | 21/22 | 0.96 | 0.09 | 35,41,48,56 | 0 |
| 1 | OMU | 2A | 2552 | 21/22 | 0.96 | 0.08 | 29,34,39,41 | 0 |
| 1 | PSU | 2A | 1911 | 20/21 | 0.96 | 0.08 | 36,44,48,53 | 0 |
| 32 | G7M | 1a | 527 | 24/25 | 0.96 | 0.07 | 32,37,41,44 | 0 |
| 32 | M2G | 1a | 966 | 25/26 | 0.96 | 0.08 | 34,39,46,48 | 0 |
| 1 | OMC | 2A | 1920 | 21/22 | 0.96 | 0.09 | 40,45,49,52 | 0 |
| 1 | 5MU | 2A | 1939 | 21/22 | 0.96 | 0.08 | 29,32,37,38 | 0 |
| 32 | PSU | 1a | 516 | 20/21 | 0.97 | 0.07 | 32,41,45,46 | 0 |
| 32 | MA6 | 2a | 1518 | 24/25 | 0.97 | 0.08 | 35,43,48,49 | 0 |
| 32 | MA6 | 2a | 1519 | 24/25 | 0.97 | 0.09 | 31,43,47,49 | 0 |
| 32 | 5MC | 1a | 1400 | 21/22 | 0.97 | 0.10 | 32,36,40,42 | 0 |
| 54 | MIA | 1w | 37 | 29/30 | 0.97 | 0.08 | 25,37,48,53 | 0 |
| 32 | 4OC | 1a | 1402 | 22/23 | 0.97 | 0.07 | 26,31,35,40 | 0 |
| 55 | 31H | 1x | 76 | 32/33 | 0.97 | 0.07 | 10,14,18,23 | 10 |
| 54 | PSU | 2w | 39 | 20/21 | 0.97 | 0.08 | 37,49,59,61 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 32 | 5MC | 1a | 1407 | 21/22 | 0.97 | 0.09 | 26,32,35,40 | 0 |
| 32 | 5MC | 2a | 1404 | 21/22 | 0.97 | 0.07 | 34,37,40,42 | 0 |
| 1 | 5MC | 1A | 1942 | 21/22 | 0.97 | 0.08 | 23,28,31,35 | 0 |
| 54 | F3N | 2w | 76 | 33/34 | 0.97 | 0.09 | 22,31,36,37 | 0 |
| 1 | 2MA | 2A | 2503 | 23/24 | 0.98 | 0.07 | 19,28,33,33 | 0 |
| 1 | PSU | 1A | 1911 | 20/21 | 0.98 | 0.07 | 26,35,39,42 | 0 |
| 1 | PSU | 2A | 2605 | 20/21 | 0.98 | 0.06 | 24,26,30,30 | 0 |
| 1 | 5MC | 1A | 1962 | 21/22 | 0.98 | 0.06 | 20,26,30,34 | 0 |
| 32 | 5MC | 1a | 1404 | 21/22 | 0.98 | 0.06 | 23,27,30,35 | 0 |
| 54 | PSU | 1w | 39 | 20/21 | 0.98 | 0.07 | 28,39,42,45 | 0 |
| 1 | 2MA | 1A | 2503 | 23/24 | 0.98 | 0.05 | 10,15,18,20 | 0 |
| 32 | UR3 | 1a | 1498 | 21/22 | 0.98 | 0.06 | 22,32,34,40 | 0 |
| 32 | MA6 | 1a | 1519 | 24/25 | 0.98 | 0.07 | 24,28,30,31 | 0 |
| 54 | F3N | 1w | 76 | 33/34 | 0.98 | 0.07 | 10,14,18,25 | 0 |
| 1 | OMC | 1A | 1920 | 21/22 | 0.98 | 0.07 | 27,33,37,39 | 0 |
| 1 | OMG | 2A | 2251 | 24/25 | 0.98 | 0.06 | 24,27,32,39 | 0 |
| 1 | PSU | 1A | 2605 | 20/21 | 0.99 | 0.05 | 13,16,21,23 | 0 |
| 1 | OMG | 1A | 2251 | 24/25 | 0.99 | 0.05 | 11,15,18,18 | 0 |
| 1 | 5MU | 1A | 1939 | 21/22 | 0.99 | 0.05 | 14,19,23,27 | 0 |
| 32 | MA6 | 1a | 1518 | 24/25 | 0.99 | 0.06 | 19,27,30,31 | 0 |
| 1 | OMU | 1A | 2552 | 21/22 | 0.99 | 0.05 | 15,18,21,24 | 0 |

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58 | MG | 2A | 3686 | 1/1 | 0.28 | 0.25 | 77,77,77,77 | 0 |
| 58 | MG | 2A | 3253 | 1/1 | 0.41 | 0.15 | 76,76,76,76 | 0 |
| 58 | MG | 2A | 3272 | 1/1 | 0.42 | 0.32 | 78,78,78,78 | 0 |
| 58 | MG | 2B | 219 | 1/1 | 0.47 | 0.27 | 78,78,78,78 | 0 |
| 58 | MG | 18 | 105 | 1/1 | 0.48 | 0.24 | 70,70,70,70 | 0 |
| 58 | MG | 1A | 3988 | 1/1 | 0.60 | 0.17 | 66,66,66,66 | 0 |
| 58 | MG | 2a | 1626 | 1/1 | 0.62 | 0.26 | 65,65,65,65 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58 | MG | 2a | 1780 | 1/1 | 0.62 | 0.21 | 66,66,66,66 | 0 |
| 58 | MG | 2w | 102 | 1/1 | 0.62 | 0.16 | 73,73,73,73 | 0 |
| 58 | MG | 2a | 1631 | 1/1 | 0.63 | 0.16 | 78,78,78,78 | 0 |
| 58 | MG | 1A | 4094 | 1/1 | 0.64 | 0.18 | 71,71,71,71 | 0 |
| 58 | MG | 1a | 1741 | 1/1 | 0.64 | 0.20 | 67,67,67,67 | 0 |
| 58 | MG | 1B | 222 | 1/1 | 0.65 | 0.18 | 57,57,57,57 | 0 |
| 58 | MG | 2A | 3810 | 1/1 | 0.65 | 0.26 | 62,62,62,62 | 0 |
| 58 | MG | 2a | 1749 | 1/1 | 0.65 | 0.17 | 66,66,66,66 | 0 |
| 58 | MG | 2A | 3850 | 1/1 | 0.65 | 0.38 | 65,65,65,65 | 0 |
| 58 | MG | 2a | 1817 | 1/1 | 0.65 | 0.25 | 66,66,66,66 | 0 |
| 58 | MG | 1y | 101 | 1/1 | 0.65 | 0.15 | 78,78,78,78 | 0 |
| 58 | MG | 1D | 311 | 1/1 | 0.66 | 0.24 | 59,59,59,59 | 0 |
| 58 | MG | 2A | 3608 | 1/1 | 0.67 | 0.23 | 73,73,73,73 | 0 |
| 58 | MG | 2a | 1810 | 1/1 | 0.67 | 0.16 | 76,76,76,76 | 0 |
| 58 | MG | 1A | 3478 | 1/1 | 0.68 | 0.14 | 52,52,52,52 | 0 |
| 58 | MG | 2A | 3701 | 1/1 | 0.68 | 0.16 | 69,69,69,69 | 0 |
| 58 | MG | 1a | 1779 | 1/1 | 0.68 | 0.14 | 48,48,48,48 | 0 |
| 58 | MG | 2A | 3681 | 1/1 | 0.69 | 0.20 | 58,58,58,58 | 0 |
| 58 | MG | 1A | 4038 | 1/1 | 0.69 | 0.18 | 49,49,49,49 | 0 |
| 58 | MG | 1O | 205 | 1/1 | 0.69 | 0.26 | 62,62,62,62 | 0 |
| 58 | MG | 2A | 3176 | 1/1 | 0.69 | 0.32 | 60,60,60,60 | 0 |
| 58 | MG | 2a | 1745 | 1/1 | 0.69 | 0.15 | 71,71,71,71 | 0 |
| 58 | MG | 2y | 104 | 1/1 | 0.69 | 0.28 | 80,80,80,80 | 0 |
| 58 | MG | 1a | 1714 | 1/1 | 0.70 | 0.30 | 57,57,57,57 | 0 |
| 58 | MG | 2A | 3291 | 1/1 | 0.70 | 0.23 | 64,64,64,64 | 0 |
| 58 | MG | 1A | 3793 | 1/1 | 0.70 | 0.21 | 72,72,72,72 | 0 |
| 58 | MG | 29 | 101 | 1/1 | 0.71 | 0.57 | 63,63,63,63 | 0 |
| 58 | MG | 1A | 3684 | 1/1 | 0.71 | 0.25 | 67,67,67,67 | 0 |
| 58 | MG | 2A | 3344 | 1/1 | 0.72 | 0.15 | 72,72,72,72 | 0 |
| 58 | MG | 2A | 3361 | 1/1 | 0.72 | 0.26 | 70,70,70,70 | 0 |
| 58 | MG | 1A | 3750 | 1/1 | 0.72 | 0.18 | 60,60,60,60 | 0 |
| 58 | MG | 2a | 1796 | 1/1 | 0.72 | 0.20 | 69,69,69,69 | 0 |
| 58 | MG | 1A | 4023 | 1/1 | 0.73 | 0.20 | 55,55,55,55 | 0 |
| 58 | MG | 2A | 3390 | 1/1 | 0.73 | 0.18 | 62,62,62,62 | 0 |
| 58 | MG | 2A | 3404 | 1/1 | 0.73 | 0.17 | 64,64,64,64 | 0 |
| 58 | MG | 2a | 1779 | 1/1 | 0.73 | 0.16 | 68,68,68,68 | 0 |
| 58 | MG | 10 | 107 | 1/1 | 0.73 | 0.31 | 59,59,59,59 | 0 |
| 58 | MG | 1A | 4100 | 1/1 | 0.74 | 0.14 | 60,60,60,60 | 0 |
| 58 | MG | 2A | 3373 | 1/1 | 0.74 | 0.22 | 76,76,76,76 | 0 |
| 58 | MG | 2A | 3710 | 1/1 | 0.74 | 0.17 | 50,50,50,50 | 0 |
| 58 | MG | 2A | 3768 | 1/1 | 0.74 | 0.18 | 48,48,48,48 | 0 |
| 58 | MG | 2A | 3769 | 1/1 | 0.74 | 0.23 | 58,58,58,58 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58 | MG | 2A | 3800 | 1/1 | 0.74 | 0.15 | 52,52,52,52 | 0 |
| 58 | MG | 2A | 3266 | 1/1 | 0.74 | 0.14 | 70,70,70,70 | 0 |
| 58 | MG | 1A | 3803 | 1/1 | 0.74 | 0.20 | 54,54,54,54 | 0 |
| 58 | MG | 2A | 3118 | 1/1 | 0.74 | 0.17 | 47,47,47,47 | 0 |
| 58 | MG | 2r | 101 | 1/1 | 0.74 | 0.13 | 65,65,65,65 | 0 |
| 58 | MG | 1a | 1769 | 1/1 | 0.74 | 0.15 | 70,70,70,70 | 0 |
| 58 | MG | 2w | 103 | 1/1 | 0.74 | 0.19 | 73,73,73,73 | 0 |
| 58 | MG | 2a | 1610 | 1/1 | 0.74 | 0.11 | 54,54,54,54 | 0 |
| 58 | MG | 2A | 3340 | 1/1 | 0.75 | 0.18 | 58,58,58,58 | 0 |
| 58 | MG | 2l | 201 | 1/1 | 0.75 | 0.25 | 63,63,63,63 | 0 |
| 58 | MG | 2A | 3724 | 1/1 | 0.75 | 0.17 | 69,69,69,69 | 0 |
| 58 | MG | 2A | 3752 | 1/1 | 0.76 | 0.18 | 61,61,61,61 | 0 |
| 58 | MG | 2A | 3690 | 1/1 | 0.76 | 0.14 | 46,46,46,46 | 0 |
| 58 | MG | 1a | 1814 | 1/1 | 0.76 | 0.29 | 64,64,64,64 | 0 |
| 58 | MG | 2A | 3281 | 1/1 | 0.76 | 0.19 | 66,66,66,66 | 0 |
| 58 | MG | 2A | 3074 | 1/1 | 0.76 | 0.24 | 66,66,66,66 | 0 |
| 58 | MG | 2A | 3838 | 1/1 | 0.76 | 0.16 | 33,33,33,33 | 0 |
| 58 | MG | 2a | 1708 | 1/1 | 0.77 | 0.20 | 59,59,59,59 | 0 |
| 58 | MG | 1a | 1705 | 1/1 | 0.77 | 0.19 | 51,51,51,51 | 0 |
| 58 | MG | 2j | 201 | 1/1 | 0.77 | 0.14 | 64,64,64,64 | 0 |
| 58 | MG | 2A | 3761 | 1/1 | 0.77 | 0.12 | 42,42,42,42 | 0 |
| 58 | MG | 2A | 3302 | 1/1 | 0.77 | 0.17 | 55,55,55,55 | 0 |
| 58 | MG | 1A | 4093 | 1/1 | 0.77 | 0.21 | 55,55,55,55 | 0 |
| 58 | MG | 2B | 202 | 1/1 | 0.77 | 0.19 | 69,69,69,69 | 0 |
| 58 | MG | 2a | 1804 | 1/1 | 0.77 | 0.22 | 64,64,64,64 | 0 |
| 58 | MG | 2A | 3755 | 1/1 | 0.78 | 0.13 | 33,33,33,33 | 0 |
| 58 | MG | 1a | 1761 | 1/1 | 0.78 | 0.15 | 51,51,51,51 | 0 |
| 58 | MG | 1A | 3688 | 1/1 | 0.78 | 0.12 | 49,49,49,49 | 0 |
| 58 | MG | 2A | 3238 | 1/1 | 0.78 | 0.14 | 70,70,70,70 | 0 |
| 58 | MG | 2A | 3775 | 1/1 | 0.78 | 0.17 | 71,71,71,71 | 0 |
| 58 | MG | 2a | 1835 | 1/1 | 0.78 | 0.22 | 51,51,51,51 | 0 |
| 58 | MG | 2e | 201 | 1/1 | 0.78 | 0.10 | 59,59,59,59 | 0 |
| 58 | MG | 2A | 3778 | 1/1 | 0.78 | 0.23 | 51,51,51,51 | 0 |
| 58 | MG | 1A | 3773 | 1/1 | 0.78 | 0.12 | 16,16,16,16 | 0 |
| 58 | MG | 2A | 3307 | 1/1 | 0.78 | 0.22 | 61,61,61,61 | 0 |
| 58 | MG | 2A | 3556 | 1/1 | 0.78 | 0.17 | 59,59,59,59 | 0 |
| 58 | MG | 2a | 1757 | 1/1 | 0.78 | 0.16 | 68,68,68,68 | 0 |
| 58 | MG | 2w | 105 | 1/1 | 0.78 | 0.12 | 61,61,61,61 | 0 |
| 58 | MG | 2A | 3097 | 1/1 | 0.78 | 0.14 | 61,61,61,61 | 0 |
| 58 | MG | 2A | 3582 | 1/1 | 0.79 | 0.24 | 70,70,70,70 | 0 |
| 58 | MG | 1A | 3549 | 1/1 | 0.79 | 0.15 | 53,53,53,53 | 0 |
| 58 | MG | 2A | 3658 | 1/1 | 0.79 | 0.17 | 41,41,41,41 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58 | MG | 1A | 4010 | 1/1 | 0.79 | 0.11 | 73,73,73,73 | 0 |
| 58 | MG | 2E | 301 | 1/1 | 0.79 | 0.21 | 57,57,57,57 | 0 |
| 58 | MG | 1A | 3951 | 1/1 | 0.79 | 0.13 | 57,57,57,57 | 0 |
| 58 | MG | 2y | 101 | 1/1 | 0.79 | 0.18 | 79,79,79,79 | 0 |
| 58 | MG | 2A | 3576 | 1/1 | 0.79 | 0.14 | 43,43,43,43 | 0 |
| 58 | MG | 2A | 3101 | 1/1 | 0.80 | 0.23 | 64,64,64,64 | 0 |
| 58 | MG | 1A | 3062 | 1/1 | 0.80 | 0.13 | 56,56,56,56 | 0 |
| 58 | MG | 1A | 3199 | 1/1 | 0.80 | 0.22 | 44,44,44,44 | 0 |
| 58 | MG | 2A | 3773 | 1/1 | 0.80 | 0.15 | 38,38,38,38 | 0 |
| 58 | MG | 1a | 1797 | 1/1 | 0.80 | 0.12 | 55,55,55,55 | 0 |
| 58 | MG | 1A | 3212 | 1/1 | 0.80 | 0.24 | 66,66,66,66 | 0 |
| 58 | MG | 2a | 1696 | 1/1 | 0.80 | 0.19 | 64,64,64,64 | 0 |
| 58 | MG | 2a | 1698 | 1/1 | 0.80 | 0.17 | 47,47,47,47 | 0 |
| 58 | MG | 1t | 201 | 1/1 | 0.80 | 0.12 | 51,51,51,51 | 0 |
| 58 | MG | 1x | 105 | 1/1 | 0.80 | 0.21 | 59,59,59,59 | 0 |
| 58 | MG | 1B | 230 | 1/1 | 0.80 | 0.17 | 69,69,69,69 | 0 |
| 58 | MG | 1A | 3426 | 1/1 | 0.80 | 0.33 | 58,58,58,58 | 0 |
| 58 | MG | 2A | 3869 | 1/1 | 0.80 | 0.14 | 52,52,52,52 | 0 |
| 58 | MG | 1A | 3740 | 1/1 | 0.80 | 0.11 | 51,51,51,51 | 0 |
| 58 | MG | 2A | 3597 | 1/1 | 0.81 | 0.20 | 62,62,62,62 | 0 |
| 58 | MG | 1A | 3665 | 1/1 | 0.81 | 0.14 | 47,47,47,47 | 0 |
| 58 | MG | 1A | 3548 | 1/1 | 0.81 | 0.50 | 52,52,52,52 | 0 |
| 58 | MG | 1A | 3831 | 1/1 | 0.81 | 0.12 | 38,38,38,38 | 0 |
| 58 | MG | 2A | 3682 | 1/1 | 0.81 | 0.21 | 60,60,60,60 | 0 |
| 58 | MG | 1A | 4046 | 1/1 | 0.81 | 0.10 | 44,44,44,44 | 0 |
| 58 | MG | 2A | 3846 | 1/1 | 0.81 | 0.13 | 60,60,60,60 | 0 |
| 58 | MG | 2a | 1795 | 1/1 | 0.81 | 0.15 | 64,64,64,64 | 0 |
| 58 | MG | 2A | 3848 | 1/1 | 0.81 | 0.14 | 61,61,61,61 | 0 |
| 58 | MG | 2A | 3221 | 1/1 | 0.81 | 0.16 | 49,49,49,49 | 0 |
| 58 | MG | 2A | 3860 | 1/1 | 0.81 | 0.22 | 56,56,56,56 | 0 |
| 58 | MG | 1Y | 202 | 1/1 | 0.81 | 0.09 | 57,57,57,57 | 0 |
| 58 | MG | 2a | 1818 | 1/1 | 0.81 | 0.16 | 63,63,63,63 | 0 |
| 58 | MG | 2a | 1820 | 1/1 | 0.81 | 0.20 | 66,66,66,66 | 0 |
| 58 | MG | 2A | 3871 | 1/1 | 0.81 | 0.11 | 62,62,62,62 | 0 |
| 58 | MG | 2A | 3708 | 1/1 | 0.81 | 0.11 | 29,29,29,29 | 0 |
| 58 | MG | 1A | 3848 | 1/1 | 0.81 | 0.12 | 41,41,41,41 | 0 |
| 58 | MG | 1A | 3585 | 1/1 | 0.81 | 0.18 | 66,66,66,66 | 0 |
| 58 | MG | 2A | 3411 | 1/1 | 0.81 | 0.11 | 49,49,49,49 | 0 |
| 58 | MG | 1A | 3774 | 1/1 | 0.81 | 0.13 | 54,54,54,54 | 0 |
| 58 | MG | 2a | 1616 | 1/1 | 0.81 | 0.14 | 60,60,60,60 | 0 |
| 58 | MG | 2A | 3575 | 1/1 | 0.81 | 0.18 | 64,64,64,64 | 0 |
| 58 | MG | 1B | 208 | 1/1 | 0.81 | 0.13 | 60,60,60,60 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58 | MG | 1a | 1733 | 1/1 | 0.81 | 0.15 | 50,50,50,50 | 0 |
| 58 | MG | 2A | 3645 | 1/1 | 0.82 | 0.19 | 46,46,46,46 | 0 |
| 58 | MG | 16 | 102 | 1/1 | 0.82 | 0.12 | 40,40,40,40 | 0 |
| 58 | MG | 1A | 4009 | 1/1 | 0.82 | 0.11 | 62,62,62,62 | 0 |
| 58 | MG | 1B | 203 | 1/1 | 0.82 | 0.25 | 51,51,51,51 | 0 |
| 58 | MG | 2A | 3088 | 1/1 | 0.82 | 0.26 | 62,62,62,62 | 0 |
| 58 | MG | 1A | 3836 | 1/1 | 0.82 | 0.12 | 57,57,57,57 | 0 |
| 58 | MG | 1B | 212 | 1/1 | 0.82 | 0.27 | 46,46,46,46 | 0 |
| 58 | MG | 1A | 3841 | 1/1 | 0.82 | 0.16 | 50,50,50,50 | 0 |
| 58 | MG | 2a | 1808 | 1/1 | 0.82 | 0.12 | 51,51,51,51 | 0 |
| 58 | MG | 2A | 3709 | 1/1 | 0.82 | 0.22 | 62,62,62,62 | 0 |
| 58 | MG | 1A | 4034 | 1/1 | 0.82 | 0.13 | 35,35,35,35 | 0 |
| 58 | MG | 2A | 3720 | 1/1 | 0.82 | 0.14 | 44,44,44,44 | 0 |
| 58 | MG | 1A | 3421 | 1/1 | 0.82 | 0.17 | 54,54,54,54 | 0 |
| 58 | MG | 2A | 3234 | 1/1 | 0.82 | 0.15 | 50,50,50,50 | 0 |
| 58 | MG | 1A | 3506 | 1/1 | 0.82 | 0.18 | 63,63,63,63 | 0 |
| 58 | MG | 1a | 1790 | 1/1 | 0.82 | 0.15 | 74,74,74,74 | 0 |
| 58 | MG | 2A | 3257 | 1/1 | 0.82 | 0.14 | 55,55,55,55 | 0 |
| 58 | MG | 1W | 208 | 1/1 | 0.82 | 0.18 | 33,33,33,33 | 0 |
| 58 | MG | 2a | 1649 | 1/1 | 0.82 | 0.19 | 70,70,70,70 | 0 |
| 58 | MG | 2a | 1651 | 1/1 | 0.82 | 0.13 | 50,50,50,50 | 0 |
| 58 | MG | 1A | 3957 | 1/1 | 0.82 | 0.20 | 69,69,69,69 | 0 |
| 58 | MG | 1A | 3330 | 1/1 | 0.82 | 0.16 | 55,55,55,55 | 0 |
| 58 | MG | 2A | 3629 | 1/1 | 0.82 | 0.11 | 52,52,52,52 | 0 |
| 58 | MG | 2A | 3488 | 1/1 | 0.83 | 0.16 | 63,63,63,63 | 0 |
| 58 | MG | 2A | 3491 | 1/1 | 0.83 | 0.17 | 58,58,58,58 | 0 |
| 58 | MG | 1a | 1747 | 1/1 | 0.83 | 0.17 | 60,60,60,60 | 0 |
| 58 | MG | 1S | 203 | 1/1 | 0.83 | 0.09 | 61,61,61,61 | 0 |
| 58 | MG | 2a | 1704 | 1/1 | 0.83 | 0.14 | 52,52,52,52 | 0 |
| 58 | MG | 1U | 211 | 1/1 | 0.83 | 0.69 | 64,64,64,64 | 0 |
| 58 | MG | 1A | 3568 | 1/1 | 0.83 | 0.36 | 48,48,48,48 | 0 |
| 58 | MG | 2a | 1748 | 1/1 | 0.83 | 0.19 | 75,75,75,75 | 0 |
| 58 | MG | 1Y | 201 | 1/1 | 0.83 | 0.18 | 58,58,58,58 | 0 |
| 58 | MG | 1A | 3489 | 1/1 | 0.83 | 0.12 | 53,53,53,53 | 0 |
| 58 | MG | 2A | 3616 | 1/1 | 0.83 | 0.14 | 31,31,31,31 | 0 |
| 58 | MG | 1A | 3089 | 1/1 | 0.83 | 0.10 | 30,30,30,30 | 0 |
| 58 | MG | 11 | 103 | 1/1 | 0.83 | 0.23 | 56,56,56,56 | 0 |
| 58 | MG | 1A | 3544 | 1/1 | 0.83 | 0.32 | 56,56,56,56 | 0 |
| 58 | MG | 2A | 3670 | 1/1 | 0.83 | 0.21 | 55,55,55,55 | 0 |
| 58 | MG | 2A | 3853 | 1/1 | 0.83 | 0.16 | 60,60,60,60 | 0 |
| 58 | MG | 2A | 3295 | 1/1 | 0.83 | 0.16 | 56,56,56,56 | 0 |
| 58 | MG | 1B | 215 | 1/1 | 0.83 | 0.11 | 44,44,44,44 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58 | MG | 1a | 1625 | 1/1 | 0.83 | 0.26 | 61,61,61,61 | 0 |
| 58 | MG | 2A | 3877 | 1/1 | 0.83 | 0.11 | 71,71,71,71 | 0 |
| 58 | MG | 1A | 4043 | 1/1 | 0.83 | 0.11 | 27,27,27,27 | 0 |
| 58 | MG | 1a | 1713 | 1/1 | 0.83 | 0.20 | 39,39,39,39 | 0 |
| 58 | MG | 1A | 3459 | 1/1 | 0.83 | 0.23 | 41,41,41,41 | 0 |
| 58 | MG | 1A | 3828 | 1/1 | 0.83 | 0.09 | 25,25,25,25 | 0 |
| 58 | MG | 2a | 1609 | 1/1 | 0.83 | 0.12 | 64,64,64,64 | 0 |
| 58 | MG | 2A | 3172 | 1/1 | 0.83 | 0.11 | 71,71,71,71 | 0 |
| 58 | MG | 1A | 3260 | 1/1 | 0.83 | 0.09 | 57,57,57,57 | 0 |
| 58 | MG | 2a | 1625 | 1/1 | 0.83 | 0.14 | 63,63,63,63 | 0 |
| 58 | MG | 2A | 3405 | 1/1 | 0.83 | 0.18 | 56,56,56,56 | 0 |
| 58 | MG | 2A | 3204 | 1/1 | 0.83 | 0.31 | 66,66,66,66 | 0 |
| 58 | MG | 2A | 3444 | 1/1 | 0.84 | 0.11 | 68,68,68,68 | 0 |
| 58 | MG | 2A | 3472 | 1/1 | 0.84 | 0.14 | 67,67,67,67 | 0 |
| 58 | MG | 2a | 1632 | 1/1 | 0.84 | 0.41 | 71,71,71,71 | 0 |
| 58 | MG | 2a | 1633 | 1/1 | 0.84 | 0.20 | 60,60,60,60 | 0 |
| 58 | MG | 2A | 3477 | 1/1 | 0.84 | 0.26 | 68,68,68,68 | 0 |
| 58 | MG | 2A | 3767 | 1/1 | 0.84 | 0.15 | 48,48,48,48 | 0 |
| 58 | MG | 2a | 1655 | 1/1 | 0.84 | 0.13 | 66,66,66,66 | 0 |
| 58 | MG | 1A | 3725 | 1/1 | 0.84 | 0.19 | 48,48,48,48 | 0 |
| 58 | MG | 1A | 3505 | 1/1 | 0.84 | 0.15 | 49,49,49,49 | 0 |
| 58 | MG | 2A | 3070 | 1/1 | 0.84 | 0.24 | 47,47,47,47 | 0 |
| 58 | MG | 2A | 3268 | 1/1 | 0.84 | 0.19 | 56,56,56,56 | 0 |
| 58 | MG | 2A | 3271 | 1/1 | 0.84 | 0.11 | 52,52,52,52 | 0 |
| 58 | MG | 1A | 3474 | 1/1 | 0.84 | 0.21 | 52,52,52,52 | 0 |
| 58 | MG | 1A | 3837 | 1/1 | 0.84 | 0.11 | 30,30,30,30 | 0 |
| 58 | MG | 2A | 3822 | 1/1 | 0.84 | 0.11 | 42,42,42,42 | 0 |
| 58 | MG | 2a | 1762 | 1/1 | 0.84 | 0.11 | 76,76,76,76 | 0 |
| 58 | MG | 2A | 3283 | 1/1 | 0.84 | 0.28 | 54,54,54,54 | 0 |
| 58 | MG | 2A | 3286 | 1/1 | 0.84 | 0.23 | 58,58,58,58 | 0 |
| 58 | MG | 2a | 1793 | 1/1 | 0.84 | 0.15 | 56,56,56,56 | 0 |
| 58 | MG | 2A | 3626 | 1/1 | 0.84 | 0.15 | 55,55,55,55 | 0 |
| 58 | MG | 1a | 1751 | 1/1 | 0.84 | 0.08 | 50,50,50,50 | 0 |
| 58 | MG | 2A | 3293 | 1/1 | 0.84 | 0.11 | 53,53,53,53 | 0 |
| 58 | MG | 1A | 3476 | 1/1 | 0.84 | 0.27 | 66,66,66,66 | 0 |
| 58 | MG | 1A | 3401 | 1/1 | 0.84 | 0.22 | 64,64,64,64 | 0 |
| 58 | MG | 1A | 3924 | 1/1 | 0.84 | 0.17 | 68,68,68,68 | 0 |
| 58 | MG | 2A | 3872 | 1/1 | 0.84 | 0.13 | 62,62,62,62 | 0 |
| 58 | MG | 1A | 3358 | 1/1 | 0.84 | 0.21 | 58,58,58,58 | 0 |
| 58 | MG | 2A | 3191 | 1/1 | 0.84 | 0.12 | 52,52,52,52 | 0 |
| 58 | MG | 2A | 3195 | 1/1 | 0.84 | 0.17 | 62,62,62,62 | 0 |
| 58 | MG | 1a | 1687 | 1/1 | 0.84 | 0.17 | 62,62,62,62 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58 | MG | 2U | 202 | 1/1 | 0.84 | 0.08 | 40,40,40,40 | 0 |
| 58 | MG | 28 | 101 | 1/1 | 0.84 | 0.34 | 60,60,60,60 | 0 |
| 58 | MG | 2A | 3383 | 1/1 | 0.84 | 0.17 | 54,54,54,54 | 0 |
| 58 | MG | 2A | 3209 | 1/1 | 0.84 | 0.20 | 57,57,57,57 | 0 |
| 58 | MG | 1a | 1798 | 1/1 | 0.84 | 0.18 | 66,66,66,66 | 0 |
| 58 | MG | 2x | 105 | 1/1 | 0.84 | 0.40 | 58,58,58,58 | 0 |
| 58 | MG | 1A | 3711 | 1/1 | 0.84 | 0.14 | 31,31,31,31 | 0 |
| 58 | MG | 1A | 3805 | 1/1 | 0.84 | 0.12 | 47,47,47,47 | 0 |
| 58 | MG | 1A | 3368 | 1/1 | 0.85 | 0.10 | 42,42,42,42 | 0 |
| 58 | MG | 2A | 3697 | 1/1 | 0.85 | 0.13 | 57,57,57,57 | 0 |
| 58 | MG | 1A | 3970 | 1/1 | 0.85 | 0.15 | 34,34,34,34 | 0 |
| 58 | MG | 1A | 3527 | 1/1 | 0.85 | 0.29 | 61,61,61,61 | 0 |
| 58 | MG | 1A | 3475 | 1/1 | 0.85 | 0.17 | 46,46,46,46 | 0 |
| 58 | MG | 2A | 3393 | 1/1 | 0.85 | 0.21 | 61,61,61,61 | 0 |
| 58 | MG | 2A | 3401 | 1/1 | 0.85 | 0.12 | 57,57,57,57 | 0 |
| 58 | MG | 2A | 3721 | 1/1 | 0.85 | 0.11 | 43,43,43,43 | 0 |
| 58 | MG | 1A | 3274 | 1/1 | 0.85 | 0.23 | 62,62,62,62 | 0 |
| 58 | MG | 2A | 3733 | 1/1 | 0.85 | 0.16 | 59,59,59,59 | 0 |
| 58 | MG | 1A | 3334 | 1/1 | 0.85 | 0.09 | 41,41,41,41 | 0 |
| 58 | MG | 2a | 1661 | 1/1 | 0.85 | 0.15 | 55,55,55,55 | 0 |
| 58 | MG | 1A | 3554 | 1/1 | 0.85 | 0.17 | 60,60,60,60 | 0 |
| 58 | MG | 1A | 3840 | 1/1 | 0.85 | 0.13 | 43,43,43,43 | 0 |
| 58 | MG | 1W | 202 | 1/1 | 0.85 | 0.17 | 40,40,40,40 | 0 |
| 58 | MG | 1A | 3566 | 1/1 | 0.85 | 0.08 | 44,44,44,44 | 0 |
| 58 | MG | 2a | 1726 | 1/1 | 0.85 | 0.14 | 65,65,65,65 | 0 |
| 58 | MG | 1A | 3842 | 1/1 | 0.85 | 0.12 | 42,42,42,42 | 0 |
| 58 | MG | 1A | 4058 | 1/1 | 0.85 | 0.11 | 13,13,13,13 | 0 |
| 58 | MG | 2A | 3493 | 1/1 | 0.85 | 0.12 | 44,44,44,44 | 0 |
| 58 | MG | 2A | 3504 | 1/1 | 0.85 | 0.19 | 57,57,57,57 | 0 |
| 58 | MG | 2A | 3519 | 1/1 | 0.85 | 0.18 | 57,57,57,57 | 0 |
| 58 | MG | 1A | 4068 | 1/1 | 0.85 | 0.11 | 41,41,41,41 | 0 |
| 58 | MG | 2A | 3817 | 1/1 | 0.85 | 0.13 | 51,51,51,51 | 0 |
| 58 | MG | 1A | 4090 | 1/1 | 0.85 | 0.25 | 46,46,46,46 | 0 |
| 58 | MG | 2a | 1794 | 1/1 | 0.85 | 0.16 | 42,42,42,42 | 0 |
| 58 | MG | 2A | 3275 | 1/1 | 0.85 | 0.10 | 55,55,55,55 | 0 |
| 58 | MG | 1A | 3356 | 1/1 | 0.85 | 0.15 | 53,53,53,53 | 0 |
| 58 | MG | 1A | 3856 | 1/1 | 0.85 | 0.16 | 59,59,59,59 | 0 |
| 58 | MG | 1a | 1605 | 1/1 | 0.85 | 0.13 | 62,62,62,62 | 0 |
| 58 | MG | 2a | 1809 | 1/1 | 0.85 | 0.19 | 58,58,58,58 | 0 |
| 58 | MG | 1A | 3303 | 1/1 | 0.85 | 0.29 | 52,52,52,52 | 0 |
| 58 | MG | 1a | 1641 | 1/1 | 0.85 | 0.16 | 60,60,60,60 | 0 |
| 58 | MG | 2A | 3096 | 1/1 | 0.85 | 0.15 | 61,61,61,61 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58 | MG | 1a | 1645 | 1/1 | 0.85 | 0.11 | 55,55,55,55 | 0 |
| 58 | MG | 2a | 1827 | 1/1 | 0.85 | 0.26 | 66,66,66,66 | 0 |
| 58 | MG | 2A | 3655 | 1/1 | 0.85 | 0.20 | 44,44,44,44 | 0 |
| 58 | MG | 2d | 301 | 1/1 | 0.85 | 0.32 | 61,61,61,61 | 0 |
| 58 | MG | 2A | 3303 | 1/1 | 0.85 | 0.33 | 56,56,56,56 | 0 |
| 58 | MG | 2A | 3879 | 1/1 | 0.85 | 0.15 | 49,49,49,49 | 0 |
| 58 | MG | 2A | 3883 | 1/1 | 0.85 | 0.16 | 59,59,59,59 | 0 |
| 58 | MG | 2A | 3660 | 1/1 | 0.85 | 0.12 | 62,62,62,62 | 0 |
| 58 | MG | 1A | 3943 | 1/1 | 0.85 | 0.14 | 51,51,51,51 | 0 |
| 58 | MG | 2A | 3675 | 1/1 | 0.85 | 0.15 | 46,46,46,46 | 0 |
| 58 | MG | 1a | 1688 | 1/1 | 0.85 | 0.20 | 52,52,52,52 | 0 |
| 58 | MG | 2A | 3342 | 1/1 | 0.85 | 0.30 | 68,68,68,68 | 0 |
| 58 | MG | 1A | 3589 | 1/1 | 0.85 | 0.49 | 54,54,54,54 | 0 |
| 58 | MG | 2y | 103 | 1/1 | 0.85 | 0.21 | 70,70,70,70 | 0 |
| 58 | MG | 2a | 1602 | 1/1 | 0.85 | 0.14 | 68,68,68,68 | 0 |
| 58 | MG | 2a | 1666 | 1/1 | 0.86 | 0.20 | 53,53,53,53 | 0 |
| 58 | MG | 1A | 3995 | 1/1 | 0.86 | 0.08 | 25,25,25,25 | 0 |
| 58 | MG | 1A | 3839 | 1/1 | 0.86 | 0.13 | 45,45,45,45 | 0 |
| 58 | MG | 2A | 3403 | 1/1 | 0.86 | 0.16 | 65,65,65,65 | 0 |
| 58 | MG | 1A | 3555 | 1/1 | 0.86 | 0.08 | 51,51,51,51 | 0 |
| 58 | MG | 2A | 3212 | 1/1 | 0.86 | 0.12 | 64,64,64,64 | 0 |
| 58 | MG | 2A | 3218 | 1/1 | 0.86 | 0.14 | 53,53,53,53 | 0 |
| 58 | MG | 1a | 1644 | 1/1 | 0.86 | 0.15 | 47,47,47,47 | 0 |
| 58 | MG | 2A | 3465 | 1/1 | 0.86 | 0.14 | 62,62,62,62 | 0 |
| 58 | MG | 2a | 1755 | 1/1 | 0.86 | 0.11 | 68,68,68,68 | 0 |
| 58 | MG | 1B | 221 | 1/1 | 0.86 | 0.10 | 39,39,39,39 | 0 |
| 58 | MG | 2A | 3473 | 1/1 | 0.86 | 0.09 | 52,52,52,52 | 0 |
| 58 | MG | 2A | 3236 | 1/1 | 0.86 | 0.15 | 57,57,57,57 | 0 |
| 58 | MG | 2A | 3237 | 1/1 | 0.86 | 0.21 | 53,53,53,53 | 0 |
| 58 | MG | 2a | 1785 | 1/1 | 0.86 | 0.11 | 33,33,33,33 | 0 |
| 58 | MG | 1a | 1674 | 1/1 | 0.86 | 0.20 | 52,52,52,52 | 0 |
| 58 | MG | 2A | 3320 | 1/1 | 0.86 | 0.17 | 65,65,65,65 | 0 |
| 58 | MG | 2A | 3718 | 1/1 | 0.86 | 0.16 | 50,50,50,50 | 0 |
| 58 | MG | 2A | 3334 | 1/1 | 0.86 | 0.14 | 60,60,60,60 | 0 |
| 58 | MG | 2A | 3338 | 1/1 | 0.86 | 0.10 | 63,63,63,63 | 0 |
| 58 | MG | 2A | 3542 | 1/1 | 0.86 | 0.17 | 45,45,45,45 | 0 |
| 58 | MG | 2A | 3243 | 1/1 | 0.86 | 0.14 | 59,59,59,59 | 0 |
| 58 | MG | 2E | 311 | 1/1 | 0.86 | 0.14 | 57,57,57,57 | 0 |
| 58 | MG | 2T | 202 | 1/1 | 0.86 | 0.14 | 61,61,61,61 | 0 |
| 58 | MG | 2A | 3734 | 1/1 | 0.86 | 0.13 | 51,51,51,51 | 0 |
| 58 | MG | 2A | 3736 | 1/1 | 0.86 | 0.10 | 37,37,37,37 | 0 |
| 58 | MG | 2a | 1825 | 1/1 | 0.86 | 0.14 | 62,62,62,62 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58 | MG | 2A | 3742 | 1/1 | 0.86 | 0.12 | 32,32,32,32 | 0 |
| 58 | MG | 2A | 3745 | 1/1 | 0.86 | 0.11 | 39,39,39,39 | 0 |
| 58 | MG | 1h | 201 | 1/1 | 0.86 | 0.09 | 55,55,55,55 | 0 |
| 58 | MG | 2A | 3113 | 1/1 | 0.86 | 0.16 | 44,44,44,44 | 0 |
| 58 | MG | 2g | 201 | 1/1 | 0.86 | 0.14 | 63,63,63,63 | 0 |
| 58 | MG | 2A | 3357 | 1/1 | 0.86 | 0.16 | 52,52,52,52 | 0 |
| 58 | MG | 2A | 3763 | 1/1 | 0.86 | 0.12 | 47,47,47,47 | 0 |
| 58 | MG | 1s | 101 | 1/1 | 0.86 | 0.17 | 54,54,54,54 | 0 |
| 58 | MG | 2A | 3363 | 1/1 | 0.86 | 0.11 | 51,51,51,51 | 0 |
| 58 | MG | 1A | 3362 | 1/1 | 0.86 | 0.11 | 56,56,56,56 | 0 |
| 58 | MG | 1v | 101 | 1/1 | 0.86 | 0.23 | 65,65,65,65 | 0 |
| 58 | MG | 2A | 3385 | 1/1 | 0.86 | 0.12 | 61,61,61,61 | 0 |
| 58 | MG | 2A | 3777 | 1/1 | 0.86 | 0.14 | 60,60,60,60 | 0 |
| 58 | MG | 1A | 3359 | 1/1 | 0.86 | 0.19 | 64,64,64,64 | 0 |
| 58 | MG | 2A | 3797 | 1/1 | 0.86 | 0.12 | 56,56,56,56 | 0 |
| 58 | MG | 2y | 105 | 1/1 | 0.86 | 0.23 | 68,68,68,68 | 0 |
| 58 | MG | 1A | 3540 | 1/1 | 0.87 | 0.21 | 46,46,46,46 | 0 |
| 58 | MG | 1a | 1802 | 1/1 | 0.87 | 0.08 | 46,46,46,46 | 0 |
| 58 | MG | 2A | 3882 | 1/1 | 0.87 | 0.14 | 59,59,59,59 | 0 |
| 58 | MG | 2A | 3244 | 1/1 | 0.87 | 0.14 | 56,56,56,56 | 0 |
| 58 | MG | 2A | 3250 | 1/1 | 0.87 | 0.12 | 57,57,57,57 | 0 |
| 58 | MG | 2B | 211 | 1/1 | 0.87 | 0.16 | 64,64,64,64 | 0 |
| 58 | MG | 1a | 1809 | 1/1 | 0.87 | 0.11 | 63,63,63,63 | 0 |
| 58 | MG | 2A | 3256 | 1/1 | 0.87 | 0.23 | 49,49,49,49 | 0 |
| 58 | MG | 1A | 3985 | 1/1 | 0.87 | 0.15 | 58,58,58,58 | 0 |
| 58 | MG | 1a | 1602 | 1/1 | 0.87 | 0.17 | 57,57,57,57 | 0 |
| 58 | MG | 1l | 201 | 1/1 | 0.87 | 0.15 | 64,64,64,64 | 0 |
| 58 | MG | 2W | 201 | 1/1 | 0.87 | 0.22 | 67,67,67,67 | 0 |
| 58 | MG | 25 | 104 | 1/1 | 0.87 | 0.10 | 55,55,55,55 | 0 |
| 58 | MG | 1A | 3543 | 1/1 | 0.87 | 0.21 | 46,46,46,46 | 0 |
| 58 | MG | 1a | 1607 | 1/1 | 0.87 | 0.08 | 50,50,50,50 | 0 |
| 58 | MG | 1A | 3266 | 1/1 | 0.87 | 0.19 | 60,60,60,60 | 0 |
| 58 | MG | 2a | 1606 | 1/1 | 0.87 | 0.17 | 49,49,49,49 | 0 |
| 58 | MG | 2A | 3647 | 1/1 | 0.87 | 0.16 | 53,53,53,53 | 0 |
| 58 | MG | 2A | 3278 | 1/1 | 0.87 | 0.12 | 51,51,51,51 | 0 |
| 58 | MG | 1a | 1635 | 1/1 | 0.87 | 0.14 | 48,48,48,48 | 0 |
| 58 | MG | 2a | 1620 | 1/1 | 0.87 | 0.16 | 80,80,80,80 | 0 |
| 58 | MG | 1x | 106 | 1/1 | 0.87 | 0.27 | 51,51,51,51 | 0 |
| 58 | MG | 1A | 3191 | 1/1 | 0.87 | 0.10 | 43,43,43,43 | 0 |
| 58 | MG | 2a | 1629 | 1/1 | 0.87 | 0.12 | 59,59,59,59 | 0 |
| 58 | MG | 2A | 3039 | 1/1 | 0.87 | 0.11 | 50,50,50,50 | 0 |
| 58 | MG | 2A | 3051 | 1/1 | 0.87 | 0.09 | 35,35,35,35 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58 | MG | 2A | 3058 | 1/1 | 0.87 | 0.12 | 60,60,60,60 | 0 |
| 58 | MG | 2A | 3298 | 1/1 | 0.87 | 0.13 | 61,61,61,61 | 0 |
| 58 | MG | 1A | 3669 | 1/1 | 0.87 | 0.09 | 25,25,25,25 | 0 |
| 58 | MG | 2A | 3073 | 1/1 | 0.87 | 0.11 | 46,46,46,46 | 0 |
| 58 | MG | 1A | 3405 | 1/1 | 0.87 | 0.18 | 38,38,38,38 | 0 |
| 58 | MG | 2A | 3702 | 1/1 | 0.87 | 0.11 | 43,43,43,43 | 0 |
| 58 | MG | 2A | 3704 | 1/1 | 0.87 | 0.09 | 65,65,65,65 | 0 |
| 58 | MG | 2A | 3310 | 1/1 | 0.87 | 0.24 | 53,53,53,53 | 0 |
| 58 | MG | 2a | 1700 | 1/1 | 0.87 | 0.12 | 62,62,62,62 | 0 |
| 58 | MG | 2A | 3316 | 1/1 | 0.87 | 0.22 | 67,67,67,67 | 0 |
| 58 | MG | 1a | 1670 | 1/1 | 0.87 | 0.26 | 60,60,60,60 | 0 |
| 58 | MG | 2A | 3090 | 1/1 | 0.87 | 0.11 | 65,65,65,65 | 0 |
| 58 | MG | 2a | 1733 | 1/1 | 0.87 | 0.14 | 62,62,62,62 | 0 |
| 58 | MG | 2A | 3336 | 1/1 | 0.87 | 0.30 | 52,52,52,52 | 0 |
| 58 | MG | 1A | 3852 | 1/1 | 0.87 | 0.16 | 53,53,53,53 | 0 |
| 58 | MG | 1a | 1676 | 1/1 | 0.87 | 0.09 | 54,54,54,54 | 0 |
| 58 | MG | 2a | 1752 | 1/1 | 0.87 | 0.13 | 61,61,61,61 | 0 |
| 58 | MG | 1B | 234 | 1/1 | 0.87 | 0.12 | 63,63,63,63 | 0 |
| 58 | MG | 2A | 3105 | 1/1 | 0.87 | 0.15 | 51,51,51,51 | 0 |
| 58 | MG | 1A | 4035 | 1/1 | 0.87 | 0.10 | 35,35,35,35 | 0 |
| 58 | MG | 2A | 3358 | 1/1 | 0.87 | 0.20 | 54,54,54,54 | 0 |
| 58 | MG | 2A | 3114 | 1/1 | 0.87 | 0.17 | 57,57,57,57 | 0 |
| 58 | MG | 1O | 201 | 1/1 | 0.87 | 0.15 | 62,62,62,62 | 0 |
| 58 | MG | 2A | 3364 | 1/1 | 0.87 | 0.10 | 46,46,46,46 | 0 |
| 58 | MG | 2A | 3759 | 1/1 | 0.87 | 0.14 | 47,47,47,47 | 0 |
| 58 | MG | 2A | 3127 | 1/1 | 0.87 | 0.08 | 55,55,55,55 | 0 |
| 58 | MG | 2A | 3154 | 1/1 | 0.87 | 0.13 | 61,61,61,61 | 0 |
| 58 | MG | 2a | 1799 | 1/1 | 0.87 | 0.14 | 51,51,51,51 | 0 |
| 58 | MG | 1A | 3407 | 1/1 | 0.87 | 0.19 | 56,56,56,56 | 0 |
| 58 | MG | 1S | 201 | 1/1 | 0.87 | 0.45 | 43,43,43,43 | 0 |
| 58 | MG | 1A | 3861 | 1/1 | 0.87 | 0.13 | 53,53,53,53 | 0 |
| 58 | MG | 2A | 3192 | 1/1 | 0.87 | 0.19 | 62,62,62,62 | 0 |
| 58 | MG | 1U | 210 | 1/1 | 0.87 | 0.16 | 43,43,43,43 | 0 |
| 58 | MG | 2A | 3202 | 1/1 | 0.87 | 0.19 | 50,50,50,50 | 0 |
| 58 | MG | 1A | 3872 | 1/1 | 0.87 | 0.15 | 34,34,34,34 | 0 |
| 58 | MG | 2a | 1824 | 1/1 | 0.87 | 0.12 | 59,59,59,59 | 0 |
| 58 | MG | 2A | 3781 | 1/1 | 0.87 | 0.12 | 61,61,61,61 | 0 |
| 58 | MG | 2A | 3406 | 1/1 | 0.87 | 0.12 | 52,52,52,52 | 0 |
| 58 | MG | 2A | 3206 | 1/1 | 0.87 | 0.11 | 45,45,45,45 | 0 |
| 58 | MG | 2A | 3809 | 1/1 | 0.87 | 0.12 | 63,63,63,63 | 0 |
| 58 | MG | 2A | 3432 | 1/1 | 0.87 | 0.27 | 60,60,60,60 | 0 |
| 58 | MG | 2A | 3207 | 1/1 | 0.87 | 0.20 | 65,65,65,65 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58 | MG | 2A | 3819 | 1/1 | 0.87 | 0.10 | 74,74,74,74 | 0 |
| 58 | MG | 2A | 3445 | 1/1 | 0.87 | 0.14 | 44,44,44,44 | 0 |
| 58 | MG | 2I | 205 | 1/1 | 0.87 | 0.14 | 52,52,52,52 | 0 |
| 58 | MG | 1A | 4056 | 1/1 | 0.87 | 0.11 | 46,46,46,46 | 0 |
| 58 | MG | 2v | 102 | 1/1 | 0.87 | 0.11 | 42,42,42,42 | 0 |
| 58 | MG | 1a | 1758 | 1/1 | 0.87 | 0.11 | 40,40,40,40 | 0 |
| 58 | MG | 1A | 3511 | 1/1 | 0.87 | 0.10 | 59,59,59,59 | 0 |
| 58 | MG | 1A | 3830 | 1/1 | 0.87 | 0.12 | 40,40,40,40 | 0 |
| 58 | MG | 2A | 3224 | 1/1 | 0.87 | 0.12 | 56,56,56,56 | 0 |
| 58 | MG | 1A | 3074 | 1/1 | 0.87 | 0.23 | 54,54,54,54 | 0 |
| 58 | MG | 1A | 3955 | 1/1 | 0.87 | 0.11 | 53,53,53,53 | 0 |
| 58 | MG | 2A | 3498 | 1/1 | 0.87 | 0.19 | 42,42,42,42 | 0 |
| 58 | MG | 1A | 3726 | 1/1 | 0.87 | 0.09 | 33,33,33,33 | 0 |
| 58 | MG | 2A | 3351 | 1/1 | 0.88 | 0.19 | 52,52,52,52 | 0 |
| 58 | MG | 1B | 214 | 1/1 | 0.88 | 0.25 | 56,56,56,56 | 0 |
| 58 | MG | 1A | 3611 | 1/1 | 0.88 | 0.10 | 43,43,43,43 | 0 |
| 58 | MG | 2A | 3214 | 1/1 | 0.88 | 0.21 | 60,60,60,60 | 0 |
| 58 | MG | 2A | 3215 | 1/1 | 0.88 | 0.15 | 56,56,56,56 | 0 |
| 58 | MG | 2a | 1621 | 1/1 | 0.88 | 0.15 | 52,52,52,52 | 0 |
| 58 | MG | 2A | 3216 | 1/1 | 0.88 | 0.12 | 52,52,52,52 | 0 |
| 58 | MG | 1A | 3850 | 1/1 | 0.88 | 0.09 | 49,49,49,49 | 0 |
| 58 | MG | 1x | 101 | 1/1 | 0.88 | 0.21 | 48,48,48,48 | 0 |
| 58 | MG | 2A | 3384 | 1/1 | 0.88 | 0.11 | 50,50,50,50 | 0 |
| 58 | MG | 2A | 3222 | 1/1 | 0.88 | 0.25 | 55,55,55,55 | 0 |
| 58 | MG | 1A | 3612 | 1/1 | 0.88 | 0.10 | 19,19,19,19 | 0 |
| 58 | MG | 2a | 1640 | 1/1 | 0.88 | 0.18 | 53,53,53,53 | 0 |
| 58 | MG | 2A | 3391 | 1/1 | 0.88 | 0.12 | 53,53,53,53 | 0 |
| 58 | MG | 1A | 4027 | 1/1 | 0.88 | 0.10 | 53,53,53,53 | 0 |
| 58 | MG | 1B | 232 | 1/1 | 0.88 | 0.36 | 58,58,58,58 | 0 |
| 58 | MG | 1A | 4032 | 1/1 | 0.88 | 0.11 | 42,42,42,42 | 0 |
| 58 | MG | 2A | 3744 | 1/1 | 0.88 | 0.21 | 56,56,56,56 | 0 |
| 58 | MG | 1B | 235 | 1/1 | 0.88 | 0.20 | 56,56,56,56 | 0 |
| 58 | MG | 2A | 3750 | 1/1 | 0.88 | 0.12 | 67,67,67,67 | 0 |
| 58 | MG | 2A | 3054 | 1/1 | 0.88 | 0.27 | 53,53,53,53 | 0 |
| 58 | MG | 2a | 1701 | 1/1 | 0.88 | 0.28 | 66,66,66,66 | 0 |
| 58 | MG | 1A | 3619 | 1/1 | 0.88 | 0.09 | 5,5,5,5 | 0 |
| 58 | MG | 2A | 3409 | 1/1 | 0.88 | 0.12 | 54,54,54,54 | 0 |
| 58 | MG | 2a | 1722 | 1/1 | 0.88 | 0.26 | 66,66,66,66 | 0 |
| 58 | MG | 2A | 3064 | 1/1 | 0.88 | 0.08 | 56,56,56,56 | 0 |
| 58 | MG | 2A | 3420 | 1/1 | 0.88 | 0.18 | 45,45,45,45 | 0 |
| 58 | MG | 2A | 3251 | 1/1 | 0.88 | 0.14 | 57,57,57,57 | 0 |
| 58 | MG | 2A | 3252 | 1/1 | 0.88 | 0.18 | 62,62,62,62 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58 | MG | 1G | 204 | 1/1 | 0.88 | 0.12 | 47,47,47,47 | 0 |
| 58 | MG | 1A | 3658 | 1/1 | 0.88 | 0.08 | 36,36,36,36 | 0 |
| 58 | MG | 1a | 1710 | 1/1 | 0.88 | 0.15 | 49,49,49,49 | 0 |
| 58 | MG | 1A | 3865 | 1/1 | 0.88 | 0.10 | 51,51,51,51 | 0 |
| 58 | MG | 1A | 4042 | 1/1 | 0.88 | 0.10 | 35,35,35,35 | 0 |
| 58 | MG | 1A | 3470 | 1/1 | 0.88 | 0.14 | 53,53,53,53 | 0 |
| 58 | MG | 1a | 1738 | 1/1 | 0.88 | 0.15 | 47,47,47,47 | 0 |
| 58 | MG | 2A | 3100 | 1/1 | 0.88 | 0.16 | 62,62,62,62 | 0 |
| 58 | MG | 1A | 3895 | 1/1 | 0.88 | 0.11 | 24,24,24,24 | 0 |
| 58 | MG | 1A | 4051 | 1/1 | 0.88 | 0.08 | 26,26,26,26 | 0 |
| 58 | MG | 1A | 3906 | 1/1 | 0.88 | 0.12 | 49,49,49,49 | 0 |
| 58 | MG | 2A | 3524 | 1/1 | 0.88 | 0.13 | 52,52,52,52 | 0 |
| 58 | MG | 2A | 3526 | 1/1 | 0.88 | 0.10 | 51,51,51,51 | 0 |
| 58 | MG | 2A | 3825 | 1/1 | 0.88 | 0.10 | 42,42,42,42 | 0 |
| 58 | MG | 1A | 3416 | 1/1 | 0.88 | 0.10 | 46,46,46,46 | 0 |
| 58 | MG | 2A | 3116 | 1/1 | 0.88 | 0.13 | 48,48,48,48 | 0 |
| 58 | MG | 1A | 3381 | 1/1 | 0.88 | 0.22 | 45,45,45,45 | 0 |
| 58 | MG | 2A | 3122 | 1/1 | 0.88 | 0.18 | 70,70,70,70 | 0 |
| 58 | MG | 1A | 3026 | 1/1 | 0.88 | 0.12 | 45,45,45,45 | 0 |
| 58 | MG | 2A | 3593 | 1/1 | 0.88 | 0.08 | 46,46,46,46 | 0 |
| 58 | MG | 2A | 3300 | 1/1 | 0.88 | 0.09 | 44,44,44,44 | 0 |
| 58 | MG | 1A | 3537 | 1/1 | 0.88 | 0.15 | 51,51,51,51 | 0 |
| 58 | MG | 2A | 3163 | 1/1 | 0.88 | 0.18 | 45,45,45,45 | 0 |
| 58 | MG | 2A | 3170 | 1/1 | 0.88 | 0.10 | 60,60,60,60 | 0 |
| 58 | MG | 2A | 3627 | 1/1 | 0.88 | 0.14 | 42,42,42,42 | 0 |
| 58 | MG | 1a | 1782 | 1/1 | 0.88 | 0.12 | 49,49,49,49 | 0 |
| 58 | MG | 2A | 3636 | 1/1 | 0.88 | 0.14 | 31,31,31,31 | 0 |
| 58 | MG | 2A | 3314 | 1/1 | 0.88 | 0.14 | 49,49,49,49 | 0 |
| 58 | MG | 1A | 3438 | 1/1 | 0.88 | 0.09 | 40,40,40,40 | 0 |
| 58 | MG | 1l | 105 | 1/1 | 0.88 | 0.08 | 59,59,59,59 | 0 |
| 58 | MG | 2A | 3322 | 1/1 | 0.88 | 0.13 | 56,56,56,56 | 0 |
| 58 | MG | 2t | 201 | 1/1 | 0.88 | 0.09 | 52,52,52,52 | 0 |
| 58 | MG | 2A | 3326 | 1/1 | 0.88 | 0.11 | 58,58,58,58 | 0 |
| 58 | MG | 1A | 3480 | 1/1 | 0.88 | 0.11 | 50,50,50,50 | 0 |
| 58 | MG | 2A | 3674 | 1/1 | 0.88 | 0.14 | 38,38,38,38 | 0 |
| 58 | MG | 1A | 3412 | 1/1 | 0.88 | 0.14 | 53,53,53,53 | 0 |
| 58 | MG | 2w | 112 | 1/1 | 0.88 | 0.12 | 56,56,56,56 | 0 |
| 58 | MG | 2l | 101 | 1/1 | 0.88 | 0.11 | 59,59,59,59 | 0 |
| 58 | MG | 1A | 3603 | 1/1 | 0.88 | 0.09 | 31,31,31,31 | 0 |
| 58 | MG | 1B | 209 | 1/1 | 0.88 | 0.10 | 54,54,54,54 | 0 |
| 58 | MG | 1A | 3752 | 1/1 | 0.88 | 0.07 | 27,27,27,27 | 0 |
| 58 | MG | 1a | 1612 | 1/1 | 0.88 | 0.11 | 58,58,58,58 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58 | MG | 1a | 1702 | 1/1 | 0.89 | 0.15 | 52,52,52,52 | 0 |
| 58 | MG | 1G | 203 | 1/1 | 0.89 | 0.10 | 51,51,51,51 | 0 |
| 58 | MG | 2A | 3534 | 1/1 | 0.89 | 0.09 | 24,24,24,24 | 0 |
| 58 | MG | 2A | 3292 | 1/1 | 0.89 | 0.30 | 63,63,63,63 | 0 |
| 58 | MG | 1A | 3167 | 1/1 | 0.89 | 0.12 | 39,39,39,39 | 0 |
| 58 | MG | 1A | 3413 | 1/1 | 0.89 | 0.33 | 46,46,46,46 | 0 |
| 58 | MG | 1A | 3876 | 1/1 | 0.89 | 0.18 | 22,22,22,22 | 0 |
| 58 | MG | 2B | 204 | 1/1 | 0.89 | 0.15 | 62,62,62,62 | 0 |
| 58 | MG | 1A | 3881 | 1/1 | 0.89 | 0.16 | 24,24,24,24 | 0 |
| 58 | MG | 2A | 3589 | 1/1 | 0.89 | 0.08 | 25,25,25,25 | 0 |
| 58 | MG | 1a | 1734 | 1/1 | 0.89 | 0.10 | 53,53,53,53 | 0 |
| 58 | MG | 2E | 303 | 1/1 | 0.89 | 0.08 | 46,46,46,46 | 0 |
| 58 | MG | 1A | 3251 | 1/1 | 0.89 | 0.12 | 51,51,51,51 | 0 |
| 58 | MG | 2G | 201 | 1/1 | 0.89 | 0.18 | 59,59,59,59 | 0 |
| 58 | MG | 2Q | 202 | 1/1 | 0.89 | 0.13 | 38,38,38,38 | 0 |
| 58 | MG | 2Q | 203 | 1/1 | 0.89 | 0.33 | 56,56,56,56 | 0 |
| 58 | MG | 2A | 3600 | 1/1 | 0.89 | 0.13 | 42,42,42,42 | 0 |
| 58 | MG | 2A | 3306 | 1/1 | 0.89 | 0.09 | 47,47,47,47 | 0 |
| 58 | MG | 2V | 202 | 1/1 | 0.89 | 0.08 | 54,54,54,54 | 0 |
| 58 | MG | 1A | 3901 | 1/1 | 0.89 | 0.15 | 26,26,26,26 | 0 |
| 58 | MG | 2A | 3622 | 1/1 | 0.89 | 0.10 | 34,34,34,34 | 0 |
| 58 | MG | 1A | 3904 | 1/1 | 0.89 | 0.10 | 37,37,37,37 | 0 |
| 58 | MG | 1A | 3378 | 1/1 | 0.89 | 0.14 | 41,41,41,41 | 0 |
| 58 | MG | 1A | 4063 | 1/1 | 0.89 | 0.18 | 30,30,30,30 | 0 |
| 58 | MG | 1A | 3811 | 1/1 | 0.89 | 0.09 | 37,37,37,37 | 0 |
| 58 | MG | 2a | 1604 | 1/1 | 0.89 | 0.15 | 56,56,56,56 | 0 |
| 58 | MG | 2A | 3179 | 1/1 | 0.89 | 0.22 | 41,41,41,41 | 0 |
| 58 | MG | 2a | 1607 | 1/1 | 0.89 | 0.25 | 63,63,63,63 | 0 |
| 58 | MG | 2A | 3324 | 1/1 | 0.89 | 0.16 | 59,59,59,59 | 0 |
| 58 | MG | 1A | 3933 | 1/1 | 0.89 | 0.07 | 25,25,25,25 | 0 |
| 58 | MG | 2a | 1612 | 1/1 | 0.89 | 0.22 | 58,58,58,58 | 0 |
| 58 | MG | 2A | 3656 | 1/1 | 0.89 | 0.12 | 42,42,42,42 | 0 |
| 58 | MG | 1Z | 3700 | 1/1 | 0.89 | 0.08 | 44,44,44,44 | 0 |
| 58 | MG | 10 | 106 | 1/1 | 0.89 | 0.10 | 48,48,48,48 | 0 |
| 58 | MG | 2A | 3337 | 1/1 | 0.89 | 0.16 | 60,60,60,60 | 0 |
| 58 | MG | 2A | 3671 | 1/1 | 0.89 | 0.11 | 65,65,65,65 | 0 |
| 58 | MG | 1A | 3666 | 1/1 | 0.89 | 0.13 | 36,36,36,36 | 0 |
| 58 | MG | 2A | 3203 | 1/1 | 0.89 | 0.13 | 39,39,39,39 | 0 |
| 58 | MG | 2A | 3679 | 1/1 | 0.89 | 0.11 | 49,49,49,49 | 0 |
| 58 | MG | 10 | 108 | 1/1 | 0.89 | 0.12 | 51,51,51,51 | 0 |
| 58 | MG | 1A | 3552 | 1/1 | 0.89 | 0.18 | 45,45,45,45 | 0 |
| 58 | MG | 2a | 1646 | 1/1 | 0.89 | 0.26 | 56,56,56,56 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58 | MG | 1A | 3172 | 1/1 | 0.89 | 0.15 | 48,48,48,48 | 0 |
| 58 | MG | 2A | 3355 | 1/1 | 0.89 | 0.11 | 56,56,56,56 | 0 |
| 58 | MG | 2A | 3691 | 1/1 | 0.89 | 0.12 | 49,49,49,49 | 0 |
| 58 | MG | 2A | 3694 | 1/1 | 0.89 | 0.15 | 25,25,25,25 | 0 |
| 58 | MG | 2A | 3356 | 1/1 | 0.89 | 0.09 | 51,51,51,51 | 0 |
| 58 | MG | 2a | 1679 | 1/1 | 0.89 | 0.16 | 43,43,43,43 | 0 |
| 58 | MG | 2a | 1684 | 1/1 | 0.89 | 0.12 | 43,43,43,43 | 0 |
| 58 | MG | 2A | 3208 | 1/1 | 0.89 | 0.09 | 53,53,53,53 | 0 |
| 58 | MG | 1l | 106 | 1/1 | 0.89 | 0.10 | 45,45,45,45 | 0 |
| 58 | MG | 2A | 3703 | 1/1 | 0.89 | 0.12 | 59,59,59,59 | 0 |
| 58 | MG | 1A | 3388 | 1/1 | 0.89 | 0.09 | 55,55,55,55 | 0 |
| 58 | MG | 1A | 3455 | 1/1 | 0.89 | 0.22 | 51,51,51,51 | 0 |
| 58 | MG | 2a | 1706 | 1/1 | 0.89 | 0.10 | 60,60,60,60 | 0 |
| 58 | MG | 1A | 3714 | 1/1 | 0.89 | 0.12 | 40,40,40,40 | 0 |
| 58 | MG | 2A | 3365 | 1/1 | 0.89 | 0.09 | 57,57,57,57 | 0 |
| 58 | MG | 2A | 3366 | 1/1 | 0.89 | 0.10 | 51,51,51,51 | 0 |
| 58 | MG | 2a | 1730 | 1/1 | 0.89 | 0.32 | 60,60,60,60 | 0 |
| 58 | MG | 2A | 3719 | 1/1 | 0.89 | 0.07 | 38,38,38,38 | 0 |
| 58 | MG | 2a | 1734 | 1/1 | 0.89 | 0.12 | 57,57,57,57 | 0 |
| 58 | MG | 1A | 3987 | 1/1 | 0.89 | 0.21 | 58,58,58,58 | 0 |
| 58 | MG | 1A | 3508 | 1/1 | 0.89 | 0.12 | 58,58,58,58 | 0 |
| 58 | MG | 2A | 3723 | 1/1 | 0.89 | 0.09 | 46,46,46,46 | 0 |
| 58 | MG | 1A | 3457 | 1/1 | 0.89 | 0.28 | 41,41,41,41 | 0 |
| 58 | MG | 1w | 107 | 1/1 | 0.89 | 0.14 | 51,51,51,51 | 0 |
| 58 | MG | 2A | 3388 | 1/1 | 0.89 | 0.30 | 56,56,56,56 | 0 |
| 58 | MG | 1A | 3998 | 1/1 | 0.89 | 0.22 | 53,53,53,53 | 0 |
| 58 | MG | 2a | 1764 | 1/1 | 0.89 | 0.13 | 67,67,67,67 | 0 |
| 58 | MG | 2A | 3225 | 1/1 | 0.89 | 0.10 | 47,47,47,47 | 0 |
| 58 | MG | 1A | 3735 | 1/1 | 0.89 | 0.15 | 63,63,63,63 | 0 |
| 58 | MG | 2A | 3400 | 1/1 | 0.89 | 0.09 | 59,59,59,59 | 0 |
| 58 | MG | 2A | 3746 | 1/1 | 0.89 | 0.10 | 62,62,62,62 | 0 |
| 58 | MG | 1a | 1638 | 1/1 | 0.89 | 0.12 | 61,61,61,61 | 0 |
| 58 | MG | 1B | 223 | 1/1 | 0.89 | 0.10 | 40,40,40,40 | 0 |
| 58 | MG | 2A | 3036 | 1/1 | 0.89 | 0.14 | 51,51,51,51 | 0 |
| 58 | MG | 2A | 3241 | 1/1 | 0.89 | 0.14 | 50,50,50,50 | 0 |
| 58 | MG | 2a | 1800 | 1/1 | 0.89 | 0.10 | 59,59,59,59 | 0 |
| 58 | MG | 1B | 226 | 1/1 | 0.89 | 0.10 | 49,49,49,49 | 0 |
| 58 | MG | 2a | 1805 | 1/1 | 0.89 | 0.14 | 63,63,63,63 | 0 |
| 58 | MG | 1A | 3736 | 1/1 | 0.89 | 0.08 | 40,40,40,40 | 0 |
| 58 | MG | 1a | 1651 | 1/1 | 0.89 | 0.15 | 55,55,55,55 | 0 |
| 58 | MG | 1A | 3029 | 1/1 | 0.89 | 0.08 | 30,30,30,30 | 0 |
| 58 | MG | 2A | 3421 | 1/1 | 0.89 | 0.23 | 38,38,38,38 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58 | MG | 1A | 3598 | 1/1 | 0.89 | 0.22 | 53,53,53,53 | 0 |
| 58 | MG | 2A | 3434 | 1/1 | 0.89 | 0.17 | 58,58,58,58 | 0 |
| 58 | MG | 2A | 3065 | 1/1 | 0.89 | 0.13 | 44,44,44,44 | 0 |
| 58 | MG | 1A | 3272 | 1/1 | 0.89 | 0.18 | 52,52,52,52 | 0 |
| 58 | MG | 2A | 3449 | 1/1 | 0.89 | 0.15 | 52,52,52,52 | 0 |
| 58 | MG | 2A | 3792 | 1/1 | 0.89 | 0.11 | 46,46,46,46 | 0 |
| 58 | MG | 2a | 1841 | 1/1 | 0.89 | 0.20 | 60,60,60,60 | 0 |
| 58 | MG | 1a | 1679 | 1/1 | 0.89 | 0.22 | 48,48,48,48 | 0 |
| 58 | MG | 1a | 1685 | 1/1 | 0.89 | 0.10 | 47,47,47,47 | 0 |
| 58 | MG | 2A | 3079 | 1/1 | 0.89 | 0.10 | 37,37,37,37 | 0 |
| 58 | MG | 2A | 3082 | 1/1 | 0.89 | 0.12 | 50,50,50,50 | 0 |
| 58 | MG | 2A | 3484 | 1/1 | 0.89 | 0.12 | 51,51,51,51 | 0 |
| 58 | MG | 2A | 3487 | 1/1 | 0.89 | 0.10 | 51,51,51,51 | 0 |
| 58 | MG | 1A | 3102 | 1/1 | 0.89 | 0.15 | 50,50,50,50 | 0 |
| 58 | MG | 2A | 3490 | 1/1 | 0.89 | 0.07 | 44,44,44,44 | 0 |
| 58 | MG | 2A | 3837 | 1/1 | 0.89 | 0.10 | 47,47,47,47 | 0 |
| 58 | MG | 1E | 309 | 1/1 | 0.89 | 0.12 | 48,48,48,48 | 0 |
| 58 | MG | 2A | 3277 | 1/1 | 0.89 | 0.16 | 58,58,58,58 | 0 |
| 58 | MG | 1a | 1689 | 1/1 | 0.89 | 0.08 | 50,50,50,50 | 0 |
| 58 | MG | 2w | 107 | 1/1 | 0.89 | 0.21 | 60,60,60,60 | 0 |
| 58 | MG | 2w | 109 | 1/1 | 0.89 | 0.31 | 66,66,66,66 | 0 |
| 58 | MG | 2A | 3849 | 1/1 | 0.89 | 0.09 | 22,22,22,22 | 0 |
| 58 | MG | 2x | 102 | 1/1 | 0.89 | 0.23 | 40,40,40,40 | 0 |
| 58 | MG | 1a | 1692 | 1/1 | 0.89 | 0.34 | 61,61,61,61 | 0 |
| 58 | MG | 2A | 3516 | 1/1 | 0.89 | 0.16 | 49,49,49,49 | 0 |
| 58 | MG | 1a | 1695 | 1/1 | 0.89 | 0.30 | 48,48,48,48 | 0 |
| 58 | MG | 2A | 3520 | 1/1 | 0.89 | 0.12 | 52,52,52,52 | 0 |
| 58 | MG | 2A | 3870 | 1/1 | 0.89 | 0.09 | 52,52,52,52 | 0 |
| 58 | MG | 1A | 3599 | 1/1 | 0.90 | 0.16 | 61,61,61,61 | 0 |
| 58 | MG | 2B | 207 | 1/1 | 0.90 | 0.11 | 53,53,53,53 | 0 |
| 58 | MG | 2B | 210 | 1/1 | 0.90 | 0.06 | 56,56,56,56 | 0 |
| 58 | MG | 1A | 4024 | 1/1 | 0.90 | 0.11 | 51,51,51,51 | 0 |
| 58 | MG | 2A | 3309 | 1/1 | 0.90 | 0.33 | 39,39,39,39 | 0 |
| 58 | MG | 1E | 312 | 1/1 | 0.90 | 0.15 | 44,44,44,44 | 0 |
| 58 | MG | 1F | 312 | 1/1 | 0.90 | 0.13 | 39,39,39,39 | 0 |
| 58 | MG | 2E | 306 | 1/1 | 0.90 | 0.14 | 46,46,46,46 | 0 |
| 58 | MG | 2E | 309 | 1/1 | 0.90 | 0.09 | 38,38,38,38 | 0 |
| 58 | MG | 1A | 3541 | 1/1 | 0.90 | 0.13 | 32,32,32,32 | 0 |
| 58 | MG | 2F | 301 | 1/1 | 0.90 | 0.12 | 37,37,37,37 | 0 |
| 58 | MG | 2A | 3621 | 1/1 | 0.90 | 0.14 | 60,60,60,60 | 0 |
| 58 | MG | 2N | 201 | 1/1 | 0.90 | 0.19 | 55,55,55,55 | 0 |
| 58 | MG | 1A | 3433 | 1/1 | 0.90 | 0.14 | 35,35,35,35 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58 | MG | 1A | 3867 | 1/1 | 0.90 | 0.11 | 43,43,43,43 | 0 |
| 58 | MG | 2A | 3137 | 1/1 | 0.90 | 0.11 | 49,49,49,49 | 0 |
| 58 | MG | 2A | 3147 | 1/1 | 0.90 | 0.15 | 47,47,47,47 | 0 |
| 58 | MG | 2V | 201 | 1/1 | 0.90 | 0.36 | 44,44,44,44 | 0 |
| 58 | MG | 2A | 3332 | 1/1 | 0.90 | 0.32 | 59,59,59,59 | 0 |
| 58 | MG | 2A | 3642 | 1/1 | 0.90 | 0.12 | 55,55,55,55 | 0 |
| 58 | MG | 1O | 204 | 1/1 | 0.90 | 0.16 | 49,49,49,49 | 0 |
| 58 | MG | 1A | 3757 | 1/1 | 0.90 | 0.08 | 18,18,18,18 | 0 |
| 58 | MG | 1A | 3259 | 1/1 | 0.90 | 0.12 | 55,55,55,55 | 0 |
| 58 | MG | 1A | 3298 | 1/1 | 0.90 | 0.19 | 57,57,57,57 | 0 |
| 58 | MG | 2A | 3657 | 1/1 | 0.90 | 0.16 | 58,58,58,58 | 0 |
| 58 | MG | 2A | 3174 | 1/1 | 0.90 | 0.16 | 63,63,63,63 | 0 |
| 58 | MG | 2A | 3659 | 1/1 | 0.90 | 0.07 | 53,53,53,53 | 0 |
| 58 | MG | 1A | 3888 | 1/1 | 0.90 | 0.06 | 15,15,15,15 | 0 |
| 58 | MG | 2A | 3664 | 1/1 | 0.90 | 0.13 | 55,55,55,55 | 0 |
| 58 | MG | 1A | 4045 | 1/1 | 0.90 | 0.21 | 45,45,45,45 | 0 |
| 58 | MG | 2A | 3347 | 1/1 | 0.90 | 0.11 | 58,58,58,58 | 0 |
| 58 | MG | 2a | 1614 | 1/1 | 0.90 | 0.18 | 53,53,53,53 | 0 |
| 58 | MG | 2a | 1615 | 1/1 | 0.90 | 0.20 | 62,62,62,62 | 0 |
| 58 | MG | 2A | 3350 | 1/1 | 0.90 | 0.13 | 53,53,53,53 | 0 |
| 58 | MG | 2A | 3182 | 1/1 | 0.90 | 0.16 | 38,38,38,38 | 0 |
| 58 | MG | 2A | 3353 | 1/1 | 0.90 | 0.10 | 47,47,47,47 | 0 |
| 58 | MG | 2a | 1624 | 1/1 | 0.90 | 0.12 | 56,56,56,56 | 0 |
| 58 | MG | 1a | 1742 | 1/1 | 0.90 | 0.12 | 45,45,45,45 | 0 |
| 58 | MG | 1A | 3639 | 1/1 | 0.90 | 0.08 | 43,43,43,43 | 0 |
| 58 | MG | 1a | 1750 | 1/1 | 0.90 | 0.12 | 45,45,45,45 | 0 |
| 58 | MG | 2A | 3201 | 1/1 | 0.90 | 0.16 | 47,47,47,47 | 0 |
| 58 | MG | 1A | 3644 | 1/1 | 0.90 | 0.13 | 53,53,53,53 | 0 |
| 58 | MG | 1A | 3494 | 1/1 | 0.90 | 0.09 | 45,45,45,45 | 0 |
| 58 | MG | 2a | 1639 | 1/1 | 0.90 | 0.14 | 48,48,48,48 | 0 |
| 58 | MG | 1a | 1759 | 1/1 | 0.90 | 0.14 | 55,55,55,55 | 0 |
| 58 | MG | 2A | 3699 | 1/1 | 0.90 | 0.16 | 44,44,44,44 | 0 |
| 58 | MG | 2A | 3700 | 1/1 | 0.90 | 0.14 | 52,52,52,52 | 0 |
| 58 | MG | 1A | 3659 | 1/1 | 0.90 | 0.12 | 45,45,45,45 | 0 |
| 58 | MG | 1A | 3913 | 1/1 | 0.90 | 0.17 | 48,48,48,48 | 0 |
| 58 | MG | 2A | 3372 | 1/1 | 0.90 | 0.17 | 46,46,46,46 | 0 |
| 58 | MG | 2a | 1662 | 1/1 | 0.90 | 0.22 | 56,56,56,56 | 0 |
| 58 | MG | 1A | 3816 | 1/1 | 0.90 | 0.13 | 54,54,54,54 | 0 |
| 58 | MG | 2a | 1670 | 1/1 | 0.90 | 0.18 | 51,51,51,51 | 0 |
| 58 | MG | 2a | 1678 | 1/1 | 0.90 | 0.17 | 50,50,50,50 | 0 |
| 58 | MG | 2A | 3375 | 1/1 | 0.90 | 0.30 | 62,62,62,62 | 0 |
| 58 | MG | 1A | 4075 | 1/1 | 0.90 | 0.10 | 13,13,13,13 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58 | MG | 2A | 3210 | 1/1 | 0.90 | 0.11 | 64,64,64,64 | 0 |
| 58 | MG | 1A | 4085 | 1/1 | 0.90 | 0.09 | 23,23,23,23 | 0 |
| 58 | MG | 10 | 109 | 1/1 | 0.90 | 0.08 | 42,42,42,42 | 0 |
| 58 | MG | 1A | 3932 | 1/1 | 0.90 | 0.10 | 40,40,40,40 | 0 |
| 58 | MG | 1A | 3817 | 1/1 | 0.90 | 0.12 | 52,52,52,52 | 0 |
| 58 | MG | 1A | 3551 | 1/1 | 0.90 | 0.15 | 46,46,46,46 | 0 |
| 58 | MG | 2A | 3395 | 1/1 | 0.90 | 0.12 | 45,45,45,45 | 0 |
| 58 | MG | 2a | 1717 | 1/1 | 0.90 | 0.13 | 56,56,56,56 | 0 |
| 58 | MG | 2a | 1718 | 1/1 | 0.90 | 0.11 | 51,51,51,51 | 0 |
| 58 | MG | 1A | 4095 | 1/1 | 0.90 | 0.13 | 50,50,50,50 | 0 |
| 58 | MG | 2a | 1725 | 1/1 | 0.90 | 0.11 | 54,54,54,54 | 0 |
| 58 | MG | 1b | 301 | 1/1 | 0.90 | 0.09 | 53,53,53,53 | 0 |
| 58 | MG | 2A | 3402 | 1/1 | 0.90 | 0.09 | 63,63,63,63 | 0 |
| 58 | MG | 17 | 103 | 1/1 | 0.90 | 0.08 | 49,49,49,49 | 0 |
| 58 | MG | 1A | 4099 | 1/1 | 0.90 | 0.09 | 41,41,41,41 | 0 |
| 58 | MG | 2a | 1741 | 1/1 | 0.90 | 0.22 | 34,34,34,34 | 0 |
| 58 | MG | 2A | 3228 | 1/1 | 0.90 | 0.12 | 52,52,52,52 | 0 |
| 58 | MG | 1A | 3115 | 1/1 | 0.90 | 0.19 | 32,32,32,32 | 0 |
| 58 | MG | 1a | 1604 | 1/1 | 0.90 | 0.08 | 48,48,48,48 | 0 |
| 58 | MG | 1A | 3458 | 1/1 | 0.90 | 0.10 | 56,56,56,56 | 0 |
| 58 | MG | 1A | 3364 | 1/1 | 0.90 | 0.15 | 56,56,56,56 | 0 |
| 58 | MG | 1w | 108 | 1/1 | 0.90 | 0.13 | 60,60,60,60 | 0 |
| 58 | MG | 2A | 3760 | 1/1 | 0.90 | 0.19 | 40,40,40,40 | 0 |
| 58 | MG | 1A | 3966 | 1/1 | 0.90 | 0.13 | 38,38,38,38 | 0 |
| 58 | MG | 1a | 1617 | 1/1 | 0.90 | 0.11 | 53,53,53,53 | 0 |
| 58 | MG | 2A | 3437 | 1/1 | 0.90 | 0.20 | 42,42,42,42 | 0 |
| 58 | MG | 1A | 3235 | 1/1 | 0.90 | 0.14 | 43,43,43,43 | 0 |
| 58 | MG | 2a | 1788 | 1/1 | 0.90 | 0.10 | 37,37,37,37 | 0 |
| 58 | MG | 1a | 1627 | 1/1 | 0.90 | 0.15 | 42,42,42,42 | 0 |
| 58 | MG | 1A | 3973 | 1/1 | 0.90 | 0.11 | 34,34,34,34 | 0 |
| 58 | MG | 2A | 3451 | 1/1 | 0.90 | 0.22 | 47,47,47,47 | 0 |
| 58 | MG | 2A | 3776 | 1/1 | 0.90 | 0.18 | 63,63,63,63 | 0 |
| 58 | MG | 2A | 3452 | 1/1 | 0.90 | 0.27 | 50,50,50,50 | 0 |
| 58 | MG | 2A | 3455 | 1/1 | 0.90 | 0.22 | 58,58,58,58 | 0 |
| 58 | MG | 1A | 3979 | 1/1 | 0.90 | 0.11 | 62,62,62,62 | 0 |
| 58 | MG | 2A | 3788 | 1/1 | 0.90 | 0.15 | 60,60,60,60 | 0 |
| 58 | MG | 1B | 218 | 1/1 | 0.90 | 0.09 | 43,43,43,43 | 0 |
| 58 | MG | 1A | 3567 | 1/1 | 0.90 | 0.11 | 45,45,45,45 | 0 |
| 58 | MG | 2A | 3799 | 1/1 | 0.90 | 0.11 | 71,71,71,71 | 0 |
| 58 | MG | 2A | 3057 | 1/1 | 0.90 | 0.12 | 43,43,43,43 | 0 |
| 58 | MG | 2A | 3482 | 1/1 | 0.90 | 0.13 | 38,38,38,38 | 0 |
| 58 | MG | 1A | 3267 | 1/1 | 0.90 | 0.16 | 49,49,49,49 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58 | MG | 2A | 3811 | 1/1 | 0.90 | 0.09 | 63,63,63,63 | 0 |
| 58 | MG | 2A | 3812 | 1/1 | 0.90 | 0.10 | 60,60,60,60 | 0 |
| 58 | MG | 2A | 3485 | 1/1 | 0.90 | 0.14 | 44,44,44,44 | 0 |
| 58 | MG | 2a | 1829 | 1/1 | 0.90 | 0.14 | 50,50,50,50 | 0 |
| 58 | MG | 2a | 1834 | 1/1 | 0.90 | 0.19 | 68,68,68,68 | 0 |
| 58 | MG | 1A | 3582 | 1/1 | 0.90 | 0.08 | 28,28,28,28 | 0 |
| 58 | MG | 1a | 1656 | 1/1 | 0.90 | 0.16 | 52,52,52,52 | 0 |
| 58 | MG | 2A | 3273 | 1/1 | 0.90 | 0.17 | 54,54,54,54 | 0 |
| 58 | MG | 2A | 3826 | 1/1 | 0.90 | 0.08 | 31,31,31,31 | 0 |
| 58 | MG | 2A | 3067 | 1/1 | 0.90 | 0.12 | 52,52,52,52 | 0 |
| 58 | MG | 1a | 1663 | 1/1 | 0.90 | 0.12 | 53,53,53,53 | 0 |
| 58 | MG | 1a | 1665 | 1/1 | 0.90 | 0.09 | 56,56,56,56 | 0 |
| 58 | MG | 1a | 1666 | 1/1 | 0.90 | 0.12 | 45,45,45,45 | 0 |
| 58 | MG | 2A | 3077 | 1/1 | 0.90 | 0.15 | 43,43,43,43 | 0 |
| 58 | MG | 1A | 3531 | 1/1 | 0.90 | 0.34 | 50,50,50,50 | 0 |
| 58 | MG | 2A | 3289 | 1/1 | 0.90 | 0.18 | 57,57,57,57 | 0 |
| 58 | MG | 1B | 229 | 1/1 | 0.90 | 0.10 | 44,44,44,44 | 0 |
| 58 | MG | 2A | 3868 | 1/1 | 0.90 | 0.11 | 39,39,39,39 | 0 |
| 58 | MG | 1a | 1675 | 1/1 | 0.90 | 0.24 | 56,56,56,56 | 0 |
| 58 | MG | 1A | 3728 | 1/1 | 0.90 | 0.10 | 47,47,47,47 | 0 |
| 58 | MG | 2A | 3091 | 1/1 | 0.90 | 0.15 | 54,54,54,54 | 0 |
| 58 | MG | 2w | 110 | 1/1 | 0.90 | 0.10 | 58,58,58,58 | 0 |
| 58 | MG | 2A | 3552 | 1/1 | 0.90 | 0.08 | 33,33,33,33 | 0 |
| 58 | MG | 1a | 1678 | 1/1 | 0.90 | 0.19 | 51,51,51,51 | 0 |
| 58 | MG | 1A | 4003 | 1/1 | 0.90 | 0.12 | 23,23,23,23 | 0 |
| 58 | MG | 1A | 3342 | 1/1 | 0.90 | 0.07 | 40,40,40,40 | 0 |
| 58 | MG | 2A | 3581 | 1/1 | 0.90 | 0.09 | 48,48,48,48 | 0 |
| 58 | MG | 2B | 201 | 1/1 | 0.90 | 0.13 | 56,56,56,56 | 0 |
| 58 | MG | 1A | 3211 | 1/1 | 0.90 | 0.09 | 39,39,39,39 | 0 |
| 58 | MG | 2y | 106 | 1/1 | 0.90 | 0.17 | 66,66,66,66 | 0 |
| 58 | MG | 1a | 1693 | 1/1 | 0.91 | 0.20 | 41,41,41,41 | 0 |
| 58 | MG | 1A | 3103 | 1/1 | 0.91 | 0.07 | 46,46,46,46 | 0 |
| 58 | MG | 1T | 203 | 1/1 | 0.91 | 0.20 | 44,44,44,44 | 0 |
| 58 | MG | 2E | 308 | 1/1 | 0.91 | 0.07 | 54,54,54,54 | 0 |
| 58 | MG | 1a | 1704 | 1/1 | 0.91 | 0.12 | 41,41,41,41 | 0 |
| 58 | MG | 2A | 3610 | 1/1 | 0.91 | 0.08 | 26,26,26,26 | 0 |
| 58 | MG | 1U | 202 | 1/1 | 0.91 | 0.15 | 47,47,47,47 | 0 |
| 58 | MG | 2F | 306 | 1/1 | 0.91 | 0.09 | 44,44,44,44 | 0 |
| 58 | MG | 1a | 1707 | 1/1 | 0.91 | 0.14 | 48,48,48,48 | 0 |
| 58 | MG | 2A | 3312 | 1/1 | 0.91 | 0.09 | 55,55,55,55 | 0 |
| 58 | MG | 2A | 3624 | 1/1 | 0.91 | 0.06 | 23,23,23,23 | 0 |
| 58 | MG | 2A | 3111 | 1/1 | 0.91 | 0.09 | 46,46,46,46 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58 | MG | 2S | 201 | 1/1 | 0.91 | 0.20 | 64,64,64,64 | 0 |
| 58 | MG | 1A | 3878 | 1/1 | 0.91 | 0.23 | 27,27,27,27 | 0 |
| 58 | MG | 2A | 3318 | 1/1 | 0.91 | 0.12 | 49,49,49,49 | 0 |
| 58 | MG | 2A | 3630 | 1/1 | 0.91 | 0.11 | 26,26,26,26 | 0 |
| 58 | MG | 1A | 3335 | 1/1 | 0.91 | 0.09 | 47,47,47,47 | 0 |
| 58 | MG | 1V | 207 | 1/1 | 0.91 | 0.11 | 43,43,43,43 | 0 |
| 58 | MG | 2W | 202 | 1/1 | 0.91 | 0.11 | 61,61,61,61 | 0 |
| 58 | MG | 1a | 1715 | 1/1 | 0.91 | 0.16 | 37,37,37,37 | 0 |
| 58 | MG | 1a | 1716 | 1/1 | 0.91 | 0.26 | 48,48,48,48 | 0 |
| 58 | MG | 26 | 101 | 1/1 | 0.91 | 0.12 | 45,45,45,45 | 0 |
| 58 | MG | 2A | 3328 | 1/1 | 0.91 | 0.15 | 46,46,46,46 | 0 |
| 58 | MG | 28 | 104 | 1/1 | 0.91 | 0.14 | 44,44,44,44 | 0 |
| 58 | MG | 2A | 3330 | 1/1 | 0.91 | 0.11 | 55,55,55,55 | 0 |
| 58 | MG | 1a | 1720 | 1/1 | 0.91 | 0.09 | 48,48,48,48 | 0 |
| 58 | MG | 2A | 3333 | 1/1 | 0.91 | 0.12 | 57,57,57,57 | 0 |
| 58 | MG | 1a | 1722 | 1/1 | 0.91 | 0.26 | 52,52,52,52 | 0 |
| 58 | MG | 2A | 3144 | 1/1 | 0.91 | 0.14 | 29,29,29,29 | 0 |
| 58 | MG | 2A | 3146 | 1/1 | 0.91 | 0.22 | 60,60,60,60 | 0 |
| 58 | MG | 1a | 1726 | 1/1 | 0.91 | 0.25 | 56,56,56,56 | 0 |
| 58 | MG | 1a | 1729 | 1/1 | 0.91 | 0.10 | 53,53,53,53 | 0 |
| 58 | MG | 2a | 1613 | 1/1 | 0.91 | 0.24 | 61,61,61,61 | 0 |
| 58 | MG | 1A | 3885 | 1/1 | 0.91 | 0.09 | 33,33,33,33 | 0 |
| 58 | MG | 1A | 4052 | 1/1 | 0.91 | 0.06 | 40,40,40,40 | 0 |
| 58 | MG | 1A | 3574 | 1/1 | 0.91 | 0.14 | 46,46,46,46 | 0 |
| 58 | MG | 2a | 1617 | 1/1 | 0.91 | 0.08 | 57,57,57,57 | 0 |
| 58 | MG | 1A | 3889 | 1/1 | 0.91 | 0.07 | 20,20,20,20 | 0 |
| 58 | MG | 1A | 3409 | 1/1 | 0.91 | 0.13 | 39,39,39,39 | 0 |
| 58 | MG | 1A | 3069 | 1/1 | 0.91 | 0.08 | 36,36,36,36 | 0 |
| 58 | MG | 2A | 3181 | 1/1 | 0.91 | 0.21 | 58,58,58,58 | 0 |
| 58 | MG | 1A | 3346 | 1/1 | 0.91 | 0.08 | 37,37,37,37 | 0 |
| 58 | MG | 2A | 3692 | 1/1 | 0.91 | 0.08 | 43,43,43,43 | 0 |
| 58 | MG | 2A | 3186 | 1/1 | 0.91 | 0.11 | 49,49,49,49 | 0 |
| 58 | MG | 2A | 3190 | 1/1 | 0.91 | 0.13 | 58,58,58,58 | 0 |
| 58 | MG | 2A | 3359 | 1/1 | 0.91 | 0.23 | 56,56,56,56 | 0 |
| 58 | MG | 1A | 4076 | 1/1 | 0.91 | 0.10 | 55,55,55,55 | 0 |
| 58 | MG | 1a | 1757 | 1/1 | 0.91 | 0.08 | 47,47,47,47 | 0 |
| 58 | MG | 2a | 1641 | 1/1 | 0.91 | 0.23 | 53,53,53,53 | 0 |
| 58 | MG | 2a | 1644 | 1/1 | 0.91 | 0.10 | 54,54,54,54 | 0 |
| 58 | MG | 1A | 3594 | 1/1 | 0.91 | 0.13 | 30,30,30,30 | 0 |
| 58 | MG | 2a | 1647 | 1/1 | 0.91 | 0.13 | 50,50,50,50 | 0 |
| 58 | MG | 2A | 3199 | 1/1 | 0.91 | 0.21 | 51,51,51,51 | 0 |
| 58 | MG | 1A | 3911 | 1/1 | 0.91 | 0.09 | 41,41,41,41 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58 | MG | 2A | 3369 | 1/1 | 0.91 | 0.08 | 52,52,52,52 | 0 |
| 58 | MG | 1A | 3349 | 1/1 | 0.91 | 0.25 | 65,65,65,65 | 0 |
| 58 | MG | 1A | 3268 | 1/1 | 0.91 | 0.06 | 37,37,37,37 | 0 |
| 58 | MG | 2A | 3711 | 1/1 | 0.91 | 0.18 | 53,53,53,53 | 0 |
| 58 | MG | 1a | 1773 | 1/1 | 0.91 | 0.09 | 57,57,57,57 | 0 |
| 58 | MG | 1A | 3927 | 1/1 | 0.91 | 0.10 | 46,46,46,46 | 0 |
| 58 | MG | 1A | 4096 | 1/1 | 0.91 | 0.11 | 45,45,45,45 | 0 |
| 58 | MG | 1A | 3795 | 1/1 | 0.91 | 0.12 | 38,38,38,38 | 0 |
| 58 | MG | 1A | 3424 | 1/1 | 0.91 | 0.08 | 39,39,39,39 | 0 |
| 58 | MG | 1A | 3804 | 1/1 | 0.91 | 0.09 | 27,27,27,27 | 0 |
| 58 | MG | 1A | 3604 | 1/1 | 0.91 | 0.10 | 28,28,28,28 | 0 |
| 58 | MG | 2A | 3213 | 1/1 | 0.91 | 0.23 | 53,53,53,53 | 0 |
| 58 | MG | 2a | 1702 | 1/1 | 0.91 | 0.26 | 51,51,51,51 | 0 |
| 58 | MG | 2A | 3394 | 1/1 | 0.91 | 0.25 | 64,64,64,64 | 0 |
| 58 | MG | 1A | 3516 | 1/1 | 0.91 | 0.16 | 47,47,47,47 | 0 |
| 58 | MG | 1a | 1810 | 1/1 | 0.91 | 0.14 | 48,48,48,48 | 0 |
| 58 | MG | 2a | 1715 | 1/1 | 0.91 | 0.14 | 53,53,53,53 | 0 |
| 58 | MG | 1a | 1811 | 1/1 | 0.91 | 0.10 | 53,53,53,53 | 0 |
| 58 | MG | 1A | 3523 | 1/1 | 0.91 | 0.13 | 55,55,55,55 | 0 |
| 58 | MG | 1a | 1615 | 1/1 | 0.91 | 0.09 | 61,61,61,61 | 0 |
| 58 | MG | 1A | 3357 | 1/1 | 0.91 | 0.09 | 44,44,44,44 | 0 |
| 58 | MG | 2A | 3223 | 1/1 | 0.91 | 0.35 | 52,52,52,52 | 0 |
| 58 | MG | 1A | 3429 | 1/1 | 0.91 | 0.16 | 41,41,41,41 | 0 |
| 58 | MG | 1A | 3641 | 1/1 | 0.91 | 0.14 | 42,42,42,42 | 0 |
| 58 | MG | 1a | 1630 | 1/1 | 0.91 | 0.23 | 39,39,39,39 | 0 |
| 58 | MG | 2a | 1739 | 1/1 | 0.91 | 0.12 | 66,66,66,66 | 0 |
| 58 | MG | 2A | 3416 | 1/1 | 0.91 | 0.23 | 44,44,44,44 | 0 |
| 58 | MG | 2A | 3766 | 1/1 | 0.91 | 0.10 | 46,46,46,46 | 0 |
| 58 | MG | 2A | 3230 | 1/1 | 0.91 | 0.16 | 40,40,40,40 | 0 |
| 58 | MG | 1A | 3533 | 1/1 | 0.91 | 0.07 | 41,41,41,41 | 0 |
| 58 | MG | 2A | 3431 | 1/1 | 0.91 | 0.10 | 43,43,43,43 | 0 |
| 58 | MG | 2a | 1753 | 1/1 | 0.91 | 0.12 | 77,77,77,77 | 0 |
| 58 | MG | 1A | 3981 | 1/1 | 0.91 | 0.09 | 35,35,35,35 | 0 |
| 58 | MG | 1A | 3834 | 1/1 | 0.91 | 0.10 | 55,55,55,55 | 0 |
| 58 | MG | 1A | 3001 | 1/1 | 0.91 | 0.07 | 29,29,29,29 | 0 |
| 58 | MG | 2A | 3442 | 1/1 | 0.91 | 0.17 | 49,49,49,49 | 0 |
| 58 | MG | 1x | 103 | 1/1 | 0.91 | 0.12 | 46,46,46,46 | 0 |
| 58 | MG | 2A | 3780 | 1/1 | 0.91 | 0.08 | 39,39,39,39 | 0 |
| 58 | MG | 1A | 3002 | 1/1 | 0.91 | 0.10 | 41,41,41,41 | 0 |
| 58 | MG | 1A | 3448 | 1/1 | 0.91 | 0.12 | 35,35,35,35 | 0 |
| 58 | MG | 1a | 1652 | 1/1 | 0.91 | 0.20 | 53,53,53,53 | 0 |
| 58 | MG | 2A | 3794 | 1/1 | 0.91 | 0.16 | 73,73,73,73 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58 | MG | 2A | 3007 | 1/1 | 0.91 | 0.09 | 44,44,44,44 | 0 |
| 58 | MG | 2A | 3024 | 1/1 | 0.91 | 0.10 | 36,36,36,36 | 0 |
| 58 | MG | 2A | 3464 | 1/1 | 0.91 | 0.12 | 43,43,43,43 | 0 |
| 58 | MG | 2A | 3802 | 1/1 | 0.91 | 0.10 | 34,34,34,34 | 0 |
| 58 | MG | 1A | 3454 | 1/1 | 0.91 | 0.12 | 31,31,31,31 | 0 |
| 58 | MG | 2A | 3255 | 1/1 | 0.91 | 0.16 | 61,61,61,61 | 0 |
| 58 | MG | 1A | 3100 | 1/1 | 0.91 | 0.10 | 44,44,44,44 | 0 |
| 58 | MG | 2A | 3474 | 1/1 | 0.91 | 0.24 | 45,45,45,45 | 0 |
| 58 | MG | 2A | 3813 | 1/1 | 0.91 | 0.08 | 35,35,35,35 | 0 |
| 58 | MG | 2a | 1813 | 1/1 | 0.91 | 0.21 | 50,50,50,50 | 0 |
| 58 | MG | 2a | 1815 | 1/1 | 0.91 | 0.10 | 43,43,43,43 | 0 |
| 58 | MG | 2A | 3045 | 1/1 | 0.91 | 0.08 | 55,55,55,55 | 0 |
| 58 | MG | 2A | 3481 | 1/1 | 0.91 | 0.24 | 51,51,51,51 | 0 |
| 58 | MG | 2A | 3261 | 1/1 | 0.91 | 0.22 | 55,55,55,55 | 0 |
| 58 | MG | 2a | 1822 | 1/1 | 0.91 | 0.20 | 55,55,55,55 | 0 |
| 58 | MG | 2A | 3047 | 1/1 | 0.91 | 0.14 | 53,53,53,53 | 0 |
| 58 | MG | 2A | 3267 | 1/1 | 0.91 | 0.14 | 53,53,53,53 | 0 |
| 58 | MG | 1A | 3363 | 1/1 | 0.91 | 0.11 | 49,49,49,49 | 0 |
| 58 | MG | 2a | 1828 | 1/1 | 0.91 | 0.16 | 50,50,50,50 | 0 |
| 58 | MG | 1A | 3025 | 1/1 | 0.91 | 0.26 | 35,35,35,35 | 0 |
| 58 | MG | 2A | 3840 | 1/1 | 0.91 | 0.07 | 31,31,31,31 | 0 |
| 58 | MG | 1E | 306 | 1/1 | 0.91 | 0.10 | 38,38,38,38 | 0 |
| 58 | MG | 2a | 1839 | 1/1 | 0.91 | 0.17 | 50,50,50,50 | 0 |
| 58 | MG | 1a | 1671 | 1/1 | 0.91 | 0.13 | 50,50,50,50 | 0 |
| 58 | MG | 1A | 3702 | 1/1 | 0.91 | 0.10 | 47,47,47,47 | 0 |
| 58 | MG | 2A | 3276 | 1/1 | 0.91 | 0.14 | 54,54,54,54 | 0 |
| 58 | MG | 1E | 311 | 1/1 | 0.91 | 0.07 | 16,16,16,16 | 0 |
| 58 | MG | 1A | 3313 | 1/1 | 0.91 | 0.17 | 61,61,61,61 | 0 |
| 58 | MG | 2A | 3867 | 1/1 | 0.91 | 0.09 | 49,49,49,49 | 0 |
| 58 | MG | 2l | 204 | 1/1 | 0.91 | 0.09 | 52,52,52,52 | 0 |
| 58 | MG | 2A | 3280 | 1/1 | 0.91 | 0.14 | 59,59,59,59 | 0 |
| 58 | MG | 2A | 3068 | 1/1 | 0.91 | 0.07 | 36,36,36,36 | 0 |
| 58 | MG | 1A | 3314 | 1/1 | 0.91 | 0.09 | 47,47,47,47 | 0 |
| 58 | MG | 2v | 101 | 1/1 | 0.91 | 0.20 | 56,56,56,56 | 0 |
| 58 | MG | 2A | 3071 | 1/1 | 0.91 | 0.13 | 46,46,46,46 | 0 |
| 58 | MG | 1A | 4031 | 1/1 | 0.91 | 0.10 | 56,56,56,56 | 0 |
| 58 | MG | 2A | 3290 | 1/1 | 0.91 | 0.21 | 53,53,53,53 | 0 |
| 58 | MG | 1a | 1680 | 1/1 | 0.91 | 0.13 | 47,47,47,47 | 0 |
| 58 | MG | 2w | 106 | 1/1 | 0.91 | 0.11 | 36,36,36,36 | 0 |
| 58 | MG | 1A | 3859 | 1/1 | 0.91 | 0.12 | 19,19,19,19 | 0 |
| 58 | MG | 1A | 3715 | 1/1 | 0.91 | 0.10 | 49,49,49,49 | 0 |
| 58 | MG | 1A | 3316 | 1/1 | 0.91 | 0.18 | 47,47,47,47 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58 | MG | 2w | 111 | 1/1 | 0.91 | 0.13 | 60,60,60,60 | 0 |
| 58 | MG | 1A | 3321 | 1/1 | 0.91 | 0.18 | 49,49,49,49 | 0 |
| 58 | MG | 1A | 3265 | 1/1 | 0.91 | 0.11 | 50,50,50,50 | 0 |
| 58 | MG | 2x | 104 | 1/1 | 0.91 | 0.13 | 49,49,49,49 | 0 |
| 58 | MG | 2A | 3584 | 1/1 | 0.91 | 0.10 | 48,48,48,48 | 0 |
| 58 | MG | 2A | 3586 | 1/1 | 0.91 | 0.10 | 43,43,43,43 | 0 |
| 58 | MG | 2A | 3301 | 1/1 | 0.91 | 0.20 | 40,40,40,40 | 0 |
| 58 | MG | 2B | 212 | 1/1 | 0.91 | 0.20 | 56,56,56,56 | 0 |
| 58 | MG | 2A | 3592 | 1/1 | 0.91 | 0.09 | 58,58,58,58 | 0 |
| 58 | MG | 2D | 307 | 1/1 | 0.91 | 0.22 | 44,44,44,44 | 0 |
| 58 | MG | 2A | 3327 | 1/1 | 0.92 | 0.23 | 44,44,44,44 | 0 |
| 58 | MG | 1A | 3385 | 1/1 | 0.92 | 0.12 | 43,43,43,43 | 0 |
| 58 | MG | 1A | 3327 | 1/1 | 0.92 | 0.10 | 47,47,47,47 | 0 |
| 58 | MG | 2A | 3161 | 1/1 | 0.92 | 0.11 | 44,44,44,44 | 0 |
| 58 | MG | 1A | 3682 | 1/1 | 0.92 | 0.10 | 47,47,47,47 | 0 |
| 58 | MG | 2A | 3166 | 1/1 | 0.92 | 0.25 | 65,65,65,65 | 0 |
| 58 | MG | 2A | 3168 | 1/1 | 0.92 | 0.14 | 35,35,35,35 | 0 |
| 58 | MG | 1A | 3396 | 1/1 | 0.92 | 0.40 | 41,41,41,41 | 0 |
| 58 | MG | 1A | 3846 | 1/1 | 0.92 | 0.10 | 62,62,62,62 | 0 |
| 58 | MG | 2Z | 301 | 1/1 | 0.92 | 0.10 | 58,58,58,58 | 0 |
| 58 | MG | 2A | 3637 | 1/1 | 0.92 | 0.12 | 37,37,37,37 | 0 |
| 58 | MG | 1A | 3473 | 1/1 | 0.92 | 0.17 | 47,47,47,47 | 0 |
| 58 | MG | 2A | 3341 | 1/1 | 0.92 | 0.34 | 72,72,72,72 | 0 |
| 58 | MG | 1A | 3195 | 1/1 | 0.92 | 0.08 | 43,43,43,43 | 0 |
| 58 | MG | 2A | 3343 | 1/1 | 0.92 | 0.20 | 55,55,55,55 | 0 |
| 58 | MG | 1A | 3095 | 1/1 | 0.92 | 0.16 | 47,47,47,47 | 0 |
| 58 | MG | 1A | 4040 | 1/1 | 0.92 | 0.06 | 26,26,26,26 | 0 |
| 58 | MG | 1A | 3713 | 1/1 | 0.92 | 0.08 | 45,45,45,45 | 0 |
| 58 | MG | 1A | 3140 | 1/1 | 0.92 | 0.22 | 36,36,36,36 | 0 |
| 58 | MG | 2A | 3352 | 1/1 | 0.92 | 0.13 | 51,51,51,51 | 0 |
| 58 | MG | 2A | 3663 | 1/1 | 0.92 | 0.07 | 55,55,55,55 | 0 |
| 58 | MG | 1A | 3269 | 1/1 | 0.92 | 0.11 | 45,45,45,45 | 0 |
| 58 | MG | 2A | 3354 | 1/1 | 0.92 | 0.14 | 56,56,56,56 | 0 |
| 58 | MG | 1a | 1760 | 1/1 | 0.92 | 0.10 | 47,47,47,47 | 0 |
| 58 | MG | 1A | 3716 | 1/1 | 0.92 | 0.19 | 44,44,44,44 | 0 |
| 58 | MG | 1A | 3719 | 1/1 | 0.92 | 0.10 | 26,26,26,26 | 0 |
| 58 | MG | 2A | 3198 | 1/1 | 0.92 | 0.15 | 60,60,60,60 | 0 |
| 58 | MG | 1A | 3868 | 1/1 | 0.92 | 0.16 | 65,65,65,65 | 0 |
| 58 | MG | 15 | 103 | 1/1 | 0.92 | 0.29 | 37,37,37,37 | 0 |
| 58 | MG | 2A | 3683 | 1/1 | 0.92 | 0.17 | 59,59,59,59 | 0 |
| 58 | MG | 15 | 109 | 1/1 | 0.92 | 0.10 | 42,42,42,42 | 0 |
| 58 | MG | 2A | 3687 | 1/1 | 0.92 | 0.11 | 39,39,39,39 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58 | MG | 1A | 3870 | 1/1 | 0.92 | 0.14 | 34,34,34,34 | 0 |
| 58 | MG | 2a | 1628 | 1/1 | 0.92 | 0.09 | 53,53,53,53 | 0 |
| 58 | MG | 1A | 3871 | 1/1 | 0.92 | 0.08 | 34,34,34,34 | 0 |
| 58 | MG | 2a | 1630 | 1/1 | 0.92 | 0.17 | 43,43,43,43 | 0 |
| 58 | MG | 1A | 4062 | 1/1 | 0.92 | 0.09 | 49,49,49,49 | 0 |
| 58 | MG | 1A | 3723 | 1/1 | 0.92 | 0.11 | 28,28,28,28 | 0 |
| 58 | MG | 1a | 1804 | 1/1 | 0.92 | 0.08 | 62,62,62,62 | 0 |
| 58 | MG | 1A | 4067 | 1/1 | 0.92 | 0.08 | 35,35,35,35 | 0 |
| 58 | MG | 1A | 3271 | 1/1 | 0.92 | 0.17 | 33,33,33,33 | 0 |
| 58 | MG | 1A | 3483 | 1/1 | 0.92 | 0.06 | 32,32,32,32 | 0 |
| 58 | MG | 1a | 1608 | 1/1 | 0.92 | 0.23 | 44,44,44,44 | 0 |
| 58 | MG | 1A | 3488 | 1/1 | 0.92 | 0.19 | 24,24,24,24 | 0 |
| 58 | MG | 1a | 1614 | 1/1 | 0.92 | 0.08 | 48,48,48,48 | 0 |
| 58 | MG | 2a | 1648 | 1/1 | 0.92 | 0.13 | 56,56,56,56 | 0 |
| 58 | MG | 1A | 4083 | 1/1 | 0.92 | 0.07 | 37,37,37,37 | 0 |
| 58 | MG | 2a | 1650 | 1/1 | 0.92 | 0.08 | 51,51,51,51 | 0 |
| 58 | MG | 1l | 202 | 1/1 | 0.92 | 0.08 | 49,49,49,49 | 0 |
| 58 | MG | 2a | 1654 | 1/1 | 0.92 | 0.15 | 47,47,47,47 | 0 |
| 58 | MG | 1A | 3146 | 1/1 | 0.92 | 0.13 | 34,34,34,34 | 0 |
| 58 | MG | 2a | 1658 | 1/1 | 0.92 | 0.11 | 55,55,55,55 | 0 |
| 58 | MG | 1A | 3051 | 1/1 | 0.92 | 0.13 | 20,20,20,20 | 0 |
| 58 | MG | 1A | 3737 | 1/1 | 0.92 | 0.08 | 58,58,58,58 | 0 |
| 58 | MG | 2A | 3397 | 1/1 | 0.92 | 0.15 | 53,53,53,53 | 0 |
| 58 | MG | 2A | 3399 | 1/1 | 0.92 | 0.08 | 52,52,52,52 | 0 |
| 58 | MG | 1w | 101 | 1/1 | 0.92 | 0.10 | 43,43,43,43 | 0 |
| 58 | MG | 1A | 3890 | 1/1 | 0.92 | 0.12 | 27,27,27,27 | 0 |
| 58 | MG | 2a | 1682 | 1/1 | 0.92 | 0.11 | 51,51,51,51 | 0 |
| 58 | MG | 1a | 1632 | 1/1 | 0.92 | 0.13 | 53,53,53,53 | 0 |
| 58 | MG | 2a | 1686 | 1/1 | 0.92 | 0.15 | 42,42,42,42 | 0 |
| 58 | MG | 2A | 3727 | 1/1 | 0.92 | 0.14 | 52,52,52,52 | 0 |
| 58 | MG | 1A | 3496 | 1/1 | 0.92 | 0.07 | 39,39,39,39 | 0 |
| 58 | MG | 1A | 3900 | 1/1 | 0.92 | 0.07 | 20,20,20,20 | 0 |
| 58 | MG | 1x | 104 | 1/1 | 0.92 | 0.24 | 45,45,45,45 | 0 |
| 58 | MG | 1a | 1640 | 1/1 | 0.92 | 0.08 | 51,51,51,51 | 0 |
| 58 | MG | 1A | 3744 | 1/1 | 0.92 | 0.06 | 11,11,11,11 | 0 |
| 58 | MG | 2A | 3240 | 1/1 | 0.92 | 0.12 | 34,34,34,34 | 0 |
| 58 | MG | 2a | 1707 | 1/1 | 0.92 | 0.13 | 45,45,45,45 | 0 |
| 58 | MG | 1x | 108 | 1/1 | 0.92 | 0.10 | 18,18,18,18 | 0 |
| 58 | MG | 2a | 1713 | 1/1 | 0.92 | 0.16 | 59,59,59,59 | 0 |
| 58 | MG | 1A | 3275 | 1/1 | 0.92 | 0.10 | 35,35,35,35 | 0 |
| 58 | MG | 2A | 3005 | 1/1 | 0.92 | 0.25 | 55,55,55,55 | 0 |
| 58 | MG | 2A | 3426 | 1/1 | 0.92 | 0.13 | 46,46,46,46 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58 | MG | 2A | 3427 | 1/1 | 0.92 | 0.17 | 45,45,45,45 | 0 |
| 58 | MG | 1A | 4103 | 1/1 | 0.92 | 0.09 | 40,40,40,40 | 0 |
| 58 | MG | 2A | 3017 | 1/1 | 0.92 | 0.13 | 28,28,28,28 | 0 |
| 58 | MG | 2A | 3433 | 1/1 | 0.92 | 0.22 | 50,50,50,50 | 0 |
| 58 | MG | 2A | 3023 | 1/1 | 0.92 | 0.08 | 51,51,51,51 | 0 |
| 58 | MG | 1a | 1647 | 1/1 | 0.92 | 0.26 | 60,60,60,60 | 0 |
| 58 | MG | 2a | 1737 | 1/1 | 0.92 | 0.20 | 40,40,40,40 | 0 |
| 58 | MG | 2A | 3438 | 1/1 | 0.92 | 0.19 | 47,47,47,47 | 0 |
| 58 | MG | 2A | 3441 | 1/1 | 0.92 | 0.15 | 43,43,43,43 | 0 |
| 58 | MG | 2a | 1743 | 1/1 | 0.92 | 0.16 | 52,52,52,52 | 0 |
| 58 | MG | 2A | 3032 | 1/1 | 0.92 | 0.10 | 30,30,30,30 | 0 |
| 58 | MG | 2a | 1747 | 1/1 | 0.92 | 0.18 | 51,51,51,51 | 0 |
| 58 | MG | 1A | 3236 | 1/1 | 0.92 | 0.24 | 42,42,42,42 | 0 |
| 58 | MG | 1A | 3908 | 1/1 | 0.92 | 0.08 | 24,24,24,24 | 0 |
| 58 | MG | 1A | 3425 | 1/1 | 0.92 | 0.14 | 34,34,34,34 | 0 |
| 58 | MG | 2A | 3265 | 1/1 | 0.92 | 0.12 | 47,47,47,47 | 0 |
| 58 | MG | 1A | 3760 | 1/1 | 0.92 | 0.08 | 32,32,32,32 | 0 |
| 58 | MG | 2A | 3454 | 1/1 | 0.92 | 0.16 | 48,48,48,48 | 0 |
| 58 | MG | 1A | 3920 | 1/1 | 0.92 | 0.07 | 18,18,18,18 | 0 |
| 58 | MG | 2A | 3790 | 1/1 | 0.92 | 0.10 | 52,52,52,52 | 0 |
| 58 | MG | 1A | 3921 | 1/1 | 0.92 | 0.11 | 32,32,32,32 | 0 |
| 58 | MG | 2A | 3270 | 1/1 | 0.92 | 0.11 | 56,56,56,56 | 0 |
| 58 | MG | 2A | 3468 | 1/1 | 0.92 | 0.12 | 63,63,63,63 | 0 |
| 58 | MG | 1B | 216 | 1/1 | 0.92 | 0.07 | 38,38,38,38 | 0 |
| 58 | MG | 1A | 3764 | 1/1 | 0.92 | 0.07 | 13,13,13,13 | 0 |
| 58 | MG | 1A | 3250 | 1/1 | 0.92 | 0.25 | 45,45,45,45 | 0 |
| 58 | MG | 2A | 3806 | 1/1 | 0.92 | 0.08 | 48,48,48,48 | 0 |
| 58 | MG | 2A | 3475 | 1/1 | 0.92 | 0.15 | 53,53,53,53 | 0 |
| 58 | MG | 2a | 1798 | 1/1 | 0.92 | 0.11 | 36,36,36,36 | 0 |
| 58 | MG | 1A | 3929 | 1/1 | 0.92 | 0.11 | 18,18,18,18 | 0 |
| 58 | MG | 2A | 3479 | 1/1 | 0.92 | 0.11 | 54,54,54,54 | 0 |
| 58 | MG | 2a | 1802 | 1/1 | 0.92 | 0.08 | 49,49,49,49 | 0 |
| 58 | MG | 2a | 1803 | 1/1 | 0.92 | 0.22 | 53,53,53,53 | 0 |
| 58 | MG | 1A | 3428 | 1/1 | 0.92 | 0.28 | 41,41,41,41 | 0 |
| 58 | MG | 1A | 3307 | 1/1 | 0.92 | 0.14 | 36,36,36,36 | 0 |
| 58 | MG | 1A | 3312 | 1/1 | 0.92 | 0.15 | 39,39,39,39 | 0 |
| 58 | MG | 1A | 3945 | 1/1 | 0.92 | 0.08 | 19,19,19,19 | 0 |
| 58 | MG | 1a | 1683 | 1/1 | 0.92 | 0.17 | 54,54,54,54 | 0 |
| 58 | MG | 1A | 3615 | 1/1 | 0.92 | 0.09 | 40,40,40,40 | 0 |
| 58 | MG | 1A | 3530 | 1/1 | 0.92 | 0.26 | 55,55,55,55 | 0 |
| 58 | MG | 2a | 1816 | 1/1 | 0.92 | 0.20 | 54,54,54,54 | 0 |
| 58 | MG | 2A | 3835 | 1/1 | 0.92 | 0.06 | 43,43,43,43 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58 | MG | 1A | 3628 | 1/1 | 0.92 | 0.08 | 31,31,31,31 | 0 |
| 58 | MG | 1A | 3171 | 1/1 | 0.92 | 0.21 | 27,27,27,27 | 0 |
| 58 | MG | 1A | 3968 | 1/1 | 0.92 | 0.06 | 31,31,31,31 | 0 |
| 58 | MG | 2A | 3841 | 1/1 | 0.92 | 0.09 | 41,41,41,41 | 0 |
| 58 | MG | 2A | 3500 | 1/1 | 0.92 | 0.10 | 39,39,39,39 | 0 |
| 58 | MG | 1A | 3020 | 1/1 | 0.92 | 0.08 | 37,37,37,37 | 0 |
| 58 | MG | 2A | 3509 | 1/1 | 0.92 | 0.11 | 38,38,38,38 | 0 |
| 58 | MG | 1A | 3453 | 1/1 | 0.92 | 0.14 | 49,49,49,49 | 0 |
| 58 | MG | 2a | 1830 | 1/1 | 0.92 | 0.11 | 52,52,52,52 | 0 |
| 58 | MG | 1a | 1696 | 1/1 | 0.92 | 0.20 | 38,38,38,38 | 0 |
| 58 | MG | 1A | 3822 | 1/1 | 0.92 | 0.09 | 31,31,31,31 | 0 |
| 58 | MG | 1F | 310 | 1/1 | 0.92 | 0.10 | 51,51,51,51 | 0 |
| 58 | MG | 2A | 3525 | 1/1 | 0.92 | 0.08 | 34,34,34,34 | 0 |
| 58 | MG | 2a | 1842 | 1/1 | 0.92 | 0.10 | 64,64,64,64 | 0 |
| 58 | MG | 1A | 3823 | 1/1 | 0.92 | 0.08 | 22,22,22,22 | 0 |
| 58 | MG | 2A | 3102 | 1/1 | 0.92 | 0.21 | 50,50,50,50 | 0 |
| 58 | MG | 2A | 3535 | 1/1 | 0.92 | 0.12 | 45,45,45,45 | 0 |
| 58 | MG | 2A | 3538 | 1/1 | 0.92 | 0.09 | 45,45,45,45 | 0 |
| 58 | MG | 2A | 3540 | 1/1 | 0.92 | 0.13 | 36,36,36,36 | 0 |
| 58 | MG | 1a | 1706 | 1/1 | 0.92 | 0.19 | 61,61,61,61 | 0 |
| 58 | MG | 1A | 3645 | 1/1 | 0.92 | 0.09 | 69,69,69,69 | 0 |
| 58 | MG | 1a | 1709 | 1/1 | 0.92 | 0.17 | 56,56,56,56 | 0 |
| 58 | MG | 2A | 3559 | 1/1 | 0.92 | 0.15 | 25,25,25,25 | 0 |
| 58 | MG | 2A | 3562 | 1/1 | 0.92 | 0.10 | 42,42,42,42 | 0 |
| 58 | MG | 2A | 3572 | 1/1 | 0.92 | 0.15 | 46,46,46,46 | 0 |
| 58 | MG | 2w | 101 | 1/1 | 0.92 | 0.10 | 49,49,49,49 | 0 |
| 58 | MG | 1A | 3648 | 1/1 | 0.92 | 0.08 | 27,27,27,27 | 0 |
| 58 | MG | 1A | 3654 | 1/1 | 0.92 | 0.09 | 34,34,34,34 | 0 |
| 58 | MG | 2w | 104 | 1/1 | 0.92 | 0.09 | 65,65,65,65 | 0 |
| 58 | MG | 2A | 3311 | 1/1 | 0.92 | 0.13 | 60,60,60,60 | 0 |
| 58 | MG | 1A | 3833 | 1/1 | 0.92 | 0.10 | 44,44,44,44 | 0 |
| 58 | MG | 2A | 3313 | 1/1 | 0.92 | 0.12 | 49,49,49,49 | 0 |
| 58 | MG | 1A | 3997 | 1/1 | 0.92 | 0.15 | 40,40,40,40 | 0 |
| 58 | MG | 1A | 3185 | 1/1 | 0.92 | 0.11 | 53,53,53,53 | 0 |
| 58 | MG | 2A | 3133 | 1/1 | 0.92 | 0.09 | 53,53,53,53 | 0 |
| 58 | MG | 1A | 3835 | 1/1 | 0.92 | 0.07 | 39,39,39,39 | 0 |
| 58 | MG | 1A | 3379 | 1/1 | 0.92 | 0.09 | 41,41,41,41 | 0 |
| 58 | MG | 2x | 103 | 1/1 | 0.92 | 0.33 | 65,65,65,65 | 0 |
| 58 | MG | 2A | 3145 | 1/1 | 0.92 | 0.13 | 37,37,37,37 | 0 |
| 58 | MG | 2A | 3601 | 1/1 | 0.92 | 0.14 | 44,44,44,44 | 0 |
| 58 | MG | 2A | 3607 | 1/1 | 0.92 | 0.11 | 41,41,41,41 | 0 |
| 58 | MG | 2y | 102 | 1/1 | 0.92 | 0.12 | 62,62,62,62 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58 | MG | 2A | 3325 | 1/1 | 0.92 | 0.08 | 60,60,60,60 | 0 |
| 58 | MG | 2F | 309 | 1/1 | 0.92 | 0.10 | 47,47,47,47 | 0 |
| 58 | MG | 2A | 3609 | 1/1 | 0.92 | 0.08 | 43,43,43,43 | 0 |
| 58 | MG | 1A | 3066 | 1/1 | 0.92 | 0.12 | 36,36,36,36 | 0 |
| 58 | MG | 2B | 203 | 1/1 | 0.93 | 0.11 | 57,57,57,57 | 0 |
| 58 | MG | 1A | 3829 | 1/1 | 0.93 | 0.14 | 27,27,27,27 | 0 |
| 58 | MG | 2B | 206 | 1/1 | 0.93 | 0.16 | 53,53,53,53 | 0 |
| 58 | MG | 1A | 3386 | 1/1 | 0.93 | 0.14 | 37,37,37,37 | 0 |
| 58 | MG | 2B | 209 | 1/1 | 0.93 | 0.10 | 43,43,43,43 | 0 |
| 58 | MG | 1A | 3961 | 1/1 | 0.93 | 0.06 | 34,34,34,34 | 0 |
| 58 | MG | 2A | 3008 | 1/1 | 0.93 | 0.17 | 44,44,44,44 | 0 |
| 58 | MG | 2A | 3010 | 1/1 | 0.93 | 0.13 | 41,41,41,41 | 0 |
| 58 | MG | 1A | 3964 | 1/1 | 0.93 | 0.07 | 12,12,12,12 | 0 |
| 58 | MG | 2D | 304 | 1/1 | 0.93 | 0.06 | 39,39,39,39 | 0 |
| 58 | MG | 1a | 1658 | 1/1 | 0.93 | 0.17 | 41,41,41,41 | 0 |
| 58 | MG | 1a | 1662 | 1/1 | 0.93 | 0.22 | 44,44,44,44 | 0 |
| 58 | MG | 2A | 3029 | 1/1 | 0.93 | 0.17 | 49,49,49,49 | 0 |
| 58 | MG | 2A | 3031 | 1/1 | 0.93 | 0.11 | 38,38,38,38 | 0 |
| 58 | MG | 1A | 3535 | 1/1 | 0.93 | 0.29 | 28,28,28,28 | 0 |
| 58 | MG | 2A | 3549 | 1/1 | 0.93 | 0.10 | 35,35,35,35 | 0 |
| 58 | MG | 1a | 1664 | 1/1 | 0.93 | 0.14 | 46,46,46,46 | 0 |
| 58 | MG | 1A | 3254 | 1/1 | 0.93 | 0.08 | 45,45,45,45 | 0 |
| 58 | MG | 2A | 3557 | 1/1 | 0.93 | 0.06 | 27,27,27,27 | 0 |
| 58 | MG | 2A | 3042 | 1/1 | 0.93 | 0.12 | 38,38,38,38 | 0 |
| 58 | MG | 1B | 225 | 1/1 | 0.93 | 0.08 | 40,40,40,40 | 0 |
| 58 | MG | 2A | 3563 | 1/1 | 0.93 | 0.13 | 48,48,48,48 | 0 |
| 58 | MG | 1a | 1669 | 1/1 | 0.93 | 0.15 | 42,42,42,42 | 0 |
| 58 | MG | 2A | 3048 | 1/1 | 0.93 | 0.14 | 39,39,39,39 | 0 |
| 58 | MG | 2R | 201 | 1/1 | 0.93 | 0.11 | 57,57,57,57 | 0 |
| 58 | MG | 2R | 203 | 1/1 | 0.93 | 0.12 | 42,42,42,42 | 0 |
| 58 | MG | 1A | 3169 | 1/1 | 0.93 | 0.19 | 30,30,30,30 | 0 |
| 58 | MG | 1A | 3353 | 1/1 | 0.93 | 0.08 | 34,34,34,34 | 0 |
| 58 | MG | 1a | 1673 | 1/1 | 0.93 | 0.10 | 49,49,49,49 | 0 |
| 58 | MG | 2A | 3297 | 1/1 | 0.93 | 0.28 | 52,52,52,52 | 0 |
| 58 | MG | 1A | 3202 | 1/1 | 0.93 | 0.10 | 25,25,25,25 | 0 |
| 58 | MG | 2A | 3299 | 1/1 | 0.93 | 0.13 | 64,64,64,64 | 0 |
| 58 | MG | 2A | 3061 | 1/1 | 0.93 | 0.11 | 37,37,37,37 | 0 |
| 58 | MG | 2A | 3063 | 1/1 | 0.93 | 0.08 | 69,69,69,69 | 0 |
| 58 | MG | 2A | 3594 | 1/1 | 0.93 | 0.12 | 43,43,43,43 | 0 |
| 58 | MG | 1A | 3980 | 1/1 | 0.93 | 0.10 | 62,62,62,62 | 0 |
| 58 | MG | 1B | 233 | 1/1 | 0.93 | 0.09 | 43,43,43,43 | 0 |
| 58 | MG | 2A | 3304 | 1/1 | 0.93 | 0.10 | 46,46,46,46 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58 | MG | 2A | 3604 | 1/1 | 0.93 | 0.09 | 54,54,54,54 | 0 |
| 58 | MG | 1a | 1677 | 1/1 | 0.93 | 0.09 | 52,52,52,52 | 0 |
| 58 | MG | 1A | 3464 | 1/1 | 0.93 | 0.13 | 37,37,37,37 | 0 |
| 58 | MG | 1A | 3983 | 1/1 | 0.93 | 0.22 | 62,62,62,62 | 0 |
| 58 | MG | 2a | 1605 | 1/1 | 0.93 | 0.13 | 52,52,52,52 | 0 |
| 58 | MG | 1A | 3693 | 1/1 | 0.93 | 0.08 | 15,15,15,15 | 0 |
| 58 | MG | 1a | 1682 | 1/1 | 0.93 | 0.10 | 63,63,63,63 | 0 |
| 58 | MG | 1A | 3986 | 1/1 | 0.93 | 0.09 | 48,48,48,48 | 0 |
| 58 | MG | 2A | 3075 | 1/1 | 0.93 | 0.15 | 40,40,40,40 | 0 |
| 58 | MG | 2A | 3623 | 1/1 | 0.93 | 0.13 | 53,53,53,53 | 0 |
| 58 | MG | 1E | 307 | 1/1 | 0.93 | 0.06 | 24,24,24,24 | 0 |
| 58 | MG | 1a | 1686 | 1/1 | 0.93 | 0.25 | 46,46,46,46 | 0 |
| 58 | MG | 1A | 3695 | 1/1 | 0.93 | 0.06 | 56,56,56,56 | 0 |
| 58 | MG | 2A | 3319 | 1/1 | 0.93 | 0.27 | 64,64,64,64 | 0 |
| 58 | MG | 1E | 310 | 1/1 | 0.93 | 0.07 | 21,21,21,21 | 0 |
| 58 | MG | 1A | 3468 | 1/1 | 0.93 | 0.12 | 45,45,45,45 | 0 |
| 58 | MG | 1a | 1690 | 1/1 | 0.93 | 0.21 | 39,39,39,39 | 0 |
| 58 | MG | 1A | 3053 | 1/1 | 0.93 | 0.26 | 48,48,48,48 | 0 |
| 58 | MG | 2A | 3644 | 1/1 | 0.93 | 0.11 | 36,36,36,36 | 0 |
| 58 | MG | 1A | 3996 | 1/1 | 0.93 | 0.09 | 41,41,41,41 | 0 |
| 58 | MG | 2A | 3646 | 1/1 | 0.93 | 0.09 | 28,28,28,28 | 0 |
| 58 | MG | 1A | 3117 | 1/1 | 0.93 | 0.17 | 28,28,28,28 | 0 |
| 58 | MG | 2A | 3649 | 1/1 | 0.93 | 0.10 | 43,43,43,43 | 0 |
| 58 | MG | 1A | 3410 | 1/1 | 0.93 | 0.09 | 37,37,37,37 | 0 |
| 58 | MG | 1a | 1698 | 1/1 | 0.93 | 0.11 | 56,56,56,56 | 0 |
| 58 | MG | 1A | 4000 | 1/1 | 0.93 | 0.11 | 38,38,38,38 | 0 |
| 58 | MG | 2a | 1635 | 1/1 | 0.93 | 0.18 | 40,40,40,40 | 0 |
| 58 | MG | 2a | 1636 | 1/1 | 0.93 | 0.22 | 44,44,44,44 | 0 |
| 58 | MG | 2a | 1637 | 1/1 | 0.93 | 0.14 | 52,52,52,52 | 0 |
| 58 | MG | 2A | 3106 | 1/1 | 0.93 | 0.21 | 57,57,57,57 | 0 |
| 58 | MG | 2A | 3110 | 1/1 | 0.93 | 0.07 | 58,58,58,58 | 0 |
| 58 | MG | 2A | 3335 | 1/1 | 0.93 | 0.15 | 45,45,45,45 | 0 |
| 58 | MG | 2a | 1642 | 1/1 | 0.93 | 0.37 | 58,58,58,58 | 0 |
| 58 | MG | 2A | 3662 | 1/1 | 0.93 | 0.12 | 43,43,43,43 | 0 |
| 58 | MG | 2a | 1645 | 1/1 | 0.93 | 0.08 | 52,52,52,52 | 0 |
| 58 | MG | 1N | 203 | 1/1 | 0.93 | 0.13 | 40,40,40,40 | 0 |
| 58 | MG | 1A | 3228 | 1/1 | 0.93 | 0.08 | 34,34,34,34 | 0 |
| 58 | MG | 2A | 3669 | 1/1 | 0.93 | 0.10 | 47,47,47,47 | 0 |
| 58 | MG | 1A | 4008 | 1/1 | 0.93 | 0.08 | 51,51,51,51 | 0 |
| 58 | MG | 1A | 3175 | 1/1 | 0.93 | 0.13 | 30,30,30,30 | 0 |
| 58 | MG | 1A | 3557 | 1/1 | 0.93 | 0.18 | 48,48,48,48 | 0 |
| 58 | MG | 2a | 1653 | 1/1 | 0.93 | 0.30 | 54,54,54,54 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58 | MG | 1A | 4021 | 1/1 | 0.93 | 0.09 | 30,30,30,30 | 0 |
| 58 | MG | 2A | 3123 | 1/1 | 0.93 | 0.07 | 43,43,43,43 | 0 |
| 58 | MG | 1T | 201 | 1/1 | 0.93 | 0.16 | 46,46,46,46 | 0 |
| 58 | MG | 2A | 3128 | 1/1 | 0.93 | 0.10 | 54,54,54,54 | 0 |
| 58 | MG | 1T | 202 | 1/1 | 0.93 | 0.13 | 47,47,47,47 | 0 |
| 58 | MG | 2a | 1664 | 1/1 | 0.93 | 0.10 | 55,55,55,55 | 0 |
| 58 | MG | 1A | 3720 | 1/1 | 0.93 | 0.12 | 47,47,47,47 | 0 |
| 58 | MG | 2A | 3143 | 1/1 | 0.93 | 0.09 | 38,38,38,38 | 0 |
| 58 | MG | 2a | 1671 | 1/1 | 0.93 | 0.21 | 46,46,46,46 | 0 |
| 58 | MG | 2a | 1677 | 1/1 | 0.93 | 0.15 | 50,50,50,50 | 0 |
| 58 | MG | 2A | 3688 | 1/1 | 0.93 | 0.14 | 51,51,51,51 | 0 |
| 58 | MG | 1A | 3860 | 1/1 | 0.93 | 0.06 | 24,24,24,24 | 0 |
| 58 | MG | 1A | 4025 | 1/1 | 0.93 | 0.16 | 44,44,44,44 | 0 |
| 58 | MG | 1A | 3477 | 1/1 | 0.93 | 0.22 | 43,43,43,43 | 0 |
| 58 | MG | 1A | 3101 | 1/1 | 0.93 | 0.14 | 48,48,48,48 | 0 |
| 58 | MG | 2a | 1687 | 1/1 | 0.93 | 0.11 | 38,38,38,38 | 0 |
| 58 | MG | 2a | 1688 | 1/1 | 0.93 | 0.07 | 42,42,42,42 | 0 |
| 58 | MG | 2a | 1691 | 1/1 | 0.93 | 0.24 | 49,49,49,49 | 0 |
| 58 | MG | 2a | 1692 | 1/1 | 0.93 | 0.15 | 48,48,48,48 | 0 |
| 58 | MG | 2a | 1695 | 1/1 | 0.93 | 0.09 | 56,56,56,56 | 0 |
| 58 | MG | 2A | 3151 | 1/1 | 0.93 | 0.14 | 34,34,34,34 | 0 |
| 58 | MG | 2A | 3152 | 1/1 | 0.93 | 0.14 | 49,49,49,49 | 0 |
| 58 | MG | 2a | 1699 | 1/1 | 0.93 | 0.24 | 57,57,57,57 | 0 |
| 58 | MG | 1A | 3479 | 1/1 | 0.93 | 0.12 | 47,47,47,47 | 0 |
| 58 | MG | 2A | 3155 | 1/1 | 0.93 | 0.10 | 43,43,43,43 | 0 |
| 58 | MG | 1A | 3727 | 1/1 | 0.93 | 0.08 | 42,42,42,42 | 0 |
| 58 | MG | 1A | 3249 | 1/1 | 0.93 | 0.13 | 41,41,41,41 | 0 |
| 58 | MG | 2A | 3165 | 1/1 | 0.93 | 0.12 | 40,40,40,40 | 0 |
| 58 | MG | 1A | 3423 | 1/1 | 0.93 | 0.08 | 38,38,38,38 | 0 |
| 58 | MG | 2A | 3167 | 1/1 | 0.93 | 0.12 | 44,44,44,44 | 0 |
| 58 | MG | 2A | 3371 | 1/1 | 0.93 | 0.11 | 48,48,48,48 | 0 |
| 58 | MG | 2a | 1714 | 1/1 | 0.93 | 0.17 | 58,58,58,58 | 0 |
| 58 | MG | 1Y | 203 | 1/1 | 0.93 | 0.21 | 47,47,47,47 | 0 |
| 58 | MG | 2A | 3717 | 1/1 | 0.93 | 0.17 | 57,57,57,57 | 0 |
| 58 | MG | 1A | 3367 | 1/1 | 0.93 | 0.09 | 46,46,46,46 | 0 |
| 58 | MG | 2a | 1719 | 1/1 | 0.93 | 0.11 | 62,62,62,62 | 0 |
| 58 | MG | 2a | 1720 | 1/1 | 0.93 | 0.20 | 34,34,34,34 | 0 |
| 58 | MG | 1a | 1743 | 1/1 | 0.93 | 0.10 | 51,51,51,51 | 0 |
| 58 | MG | 1a | 1746 | 1/1 | 0.93 | 0.08 | 37,37,37,37 | 0 |
| 58 | MG | 1Z | 3701 | 1/1 | 0.93 | 0.07 | 45,45,45,45 | 0 |
| 58 | MG | 2a | 1728 | 1/1 | 0.93 | 0.21 | 52,52,52,52 | 0 |
| 58 | MG | 10 | 105 | 1/1 | 0.93 | 0.10 | 41,41,41,41 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58 | MG | 2a | 1731 | 1/1 | 0.93 | 0.26 | 48,48,48,48 | 0 |
| 58 | MG | 2A | 3180 | 1/1 | 0.93 | 0.16 | 50,50,50,50 | 0 |
| 58 | MG | 1A | 3873 | 1/1 | 0.93 | 0.10 | 25,25,25,25 | 0 |
| 58 | MG | 2A | 3730 | 1/1 | 0.93 | 0.08 | 40,40,40,40 | 0 |
| 58 | MG | 1a | 1752 | 1/1 | 0.93 | 0.12 | 53,53,53,53 | 0 |
| 58 | MG | 2a | 1740 | 1/1 | 0.93 | 0.15 | 51,51,51,51 | 0 |
| 58 | MG | 2A | 3183 | 1/1 | 0.93 | 0.09 | 44,44,44,44 | 0 |
| 58 | MG | 1A | 3328 | 1/1 | 0.93 | 0.09 | 29,29,29,29 | 0 |
| 58 | MG | 2A | 3741 | 1/1 | 0.93 | 0.07 | 42,42,42,42 | 0 |
| 58 | MG | 2a | 1746 | 1/1 | 0.93 | 0.30 | 50,50,50,50 | 0 |
| 58 | MG | 2A | 3188 | 1/1 | 0.93 | 0.12 | 54,54,54,54 | 0 |
| 58 | MG | 1A | 3490 | 1/1 | 0.93 | 0.09 | 44,44,44,44 | 0 |
| 58 | MG | 2A | 3398 | 1/1 | 0.93 | 0.13 | 54,54,54,54 | 0 |
| 58 | MG | 1A | 3491 | 1/1 | 0.93 | 0.08 | 33,33,33,33 | 0 |
| 58 | MG | 1A | 4049 | 1/1 | 0.93 | 0.08 | 25,25,25,25 | 0 |
| 58 | MG | 2a | 1754 | 1/1 | 0.93 | 0.11 | 50,50,50,50 | 0 |
| 58 | MG | 2A | 3194 | 1/1 | 0.93 | 0.19 | 55,55,55,55 | 0 |
| 58 | MG | 2a | 1756 | 1/1 | 0.93 | 0.12 | 64,64,64,64 | 0 |
| 58 | MG | 2A | 3753 | 1/1 | 0.93 | 0.10 | 47,47,47,47 | 0 |
| 58 | MG | 2a | 1759 | 1/1 | 0.93 | 0.10 | 52,52,52,52 | 0 |
| 58 | MG | 2A | 3754 | 1/1 | 0.93 | 0.12 | 49,49,49,49 | 0 |
| 58 | MG | 1A | 3747 | 1/1 | 0.93 | 0.05 | 12,12,12,12 | 0 |
| 58 | MG | 2a | 1772 | 1/1 | 0.93 | 0.09 | 54,54,54,54 | 0 |
| 58 | MG | 2a | 1777 | 1/1 | 0.93 | 0.08 | 59,59,59,59 | 0 |
| 58 | MG | 1a | 1766 | 1/1 | 0.93 | 0.17 | 45,45,45,45 | 0 |
| 58 | MG | 1a | 1768 | 1/1 | 0.93 | 0.10 | 54,54,54,54 | 0 |
| 58 | MG | 2A | 3200 | 1/1 | 0.93 | 0.15 | 46,46,46,46 | 0 |
| 58 | MG | 1A | 3369 | 1/1 | 0.93 | 0.08 | 42,42,42,42 | 0 |
| 58 | MG | 2A | 3407 | 1/1 | 0.93 | 0.10 | 44,44,44,44 | 0 |
| 58 | MG | 1A | 3751 | 1/1 | 0.93 | 0.12 | 31,31,31,31 | 0 |
| 58 | MG | 1A | 3495 | 1/1 | 0.93 | 0.16 | 55,55,55,55 | 0 |
| 58 | MG | 2A | 3413 | 1/1 | 0.93 | 0.17 | 41,41,41,41 | 0 |
| 58 | MG | 2A | 3770 | 1/1 | 0.93 | 0.08 | 41,41,41,41 | 0 |
| 58 | MG | 1a | 1781 | 1/1 | 0.93 | 0.09 | 48,48,48,48 | 0 |
| 58 | MG | 1A | 4061 | 1/1 | 0.93 | 0.12 | 34,34,34,34 | 0 |
| 58 | MG | 1a | 1787 | 1/1 | 0.93 | 0.14 | 49,49,49,49 | 0 |
| 58 | MG | 1a | 1788 | 1/1 | 0.93 | 0.10 | 51,51,51,51 | 0 |
| 58 | MG | 1A | 3891 | 1/1 | 0.93 | 0.08 | 28,28,28,28 | 0 |
| 58 | MG | 2A | 3429 | 1/1 | 0.93 | 0.22 | 53,53,53,53 | 0 |
| 58 | MG | 1A | 3077 | 1/1 | 0.93 | 0.19 | 30,30,30,30 | 0 |
| 58 | MG | 2A | 3787 | 1/1 | 0.93 | 0.08 | 49,49,49,49 | 0 |
| 58 | MG | 2A | 3211 | 1/1 | 0.93 | 0.09 | 44,44,44,44 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58 | MG | 2A | 3789 | 1/1 | 0.93 | 0.06 | 55,55,55,55 | 0 |
| 58 | MG | 1A | 3607 | 1/1 | 0.93 | 0.09 | 39,39,39,39 | 0 |
| 58 | MG | 1A | 3096 | 1/1 | 0.93 | 0.10 | 41,41,41,41 | 0 |
| 58 | MG | 1A | 3380 | 1/1 | 0.93 | 0.07 | 36,36,36,36 | 0 |
| 58 | MG | 1a | 1807 | 1/1 | 0.93 | 0.15 | 38,38,38,38 | 0 |
| 58 | MG | 1A | 3435 | 1/1 | 0.93 | 0.20 | 57,57,57,57 | 0 |
| 58 | MG | 1A | 3786 | 1/1 | 0.93 | 0.08 | 47,47,47,47 | 0 |
| 58 | MG | 2A | 3801 | 1/1 | 0.93 | 0.09 | 38,38,38,38 | 0 |
| 58 | MG | 1A | 3509 | 1/1 | 0.93 | 0.12 | 38,38,38,38 | 0 |
| 58 | MG | 2A | 3803 | 1/1 | 0.93 | 0.14 | 45,45,45,45 | 0 |
| 58 | MG | 2A | 3805 | 1/1 | 0.93 | 0.09 | 56,56,56,56 | 0 |
| 58 | MG | 1A | 3252 | 1/1 | 0.93 | 0.08 | 37,37,37,37 | 0 |
| 58 | MG | 2A | 3447 | 1/1 | 0.93 | 0.14 | 49,49,49,49 | 0 |
| 58 | MG | 1a | 1817 | 1/1 | 0.93 | 0.10 | 47,47,47,47 | 0 |
| 58 | MG | 1A | 3442 | 1/1 | 0.93 | 0.29 | 51,51,51,51 | 0 |
| 58 | MG | 2a | 1837 | 1/1 | 0.93 | 0.17 | 42,42,42,42 | 0 |
| 58 | MG | 1e | 201 | 1/1 | 0.93 | 0.10 | 54,54,54,54 | 0 |
| 58 | MG | 1A | 3520 | 1/1 | 0.93 | 0.38 | 34,34,34,34 | 0 |
| 58 | MG | 1a | 1619 | 1/1 | 0.93 | 0.10 | 36,36,36,36 | 0 |
| 58 | MG | 2A | 3462 | 1/1 | 0.93 | 0.09 | 54,54,54,54 | 0 |
| 58 | MG | 1a | 1622 | 1/1 | 0.93 | 0.09 | 41,41,41,41 | 0 |
| 58 | MG | 1A | 3642 | 1/1 | 0.93 | 0.07 | 8,8,8,8 | 0 |
| 58 | MG | 1A | 3445 | 1/1 | 0.93 | 0.13 | 39,39,39,39 | 0 |
| 58 | MG | 1A | 3928 | 1/1 | 0.93 | 0.08 | 37,37,37,37 | 0 |
| 58 | MG | 2l | 202 | 1/1 | 0.93 | 0.10 | 48,48,48,48 | 0 |
| 58 | MG | 2A | 3239 | 1/1 | 0.93 | 0.08 | 41,41,41,41 | 0 |
| 58 | MG | 1A | 3815 | 1/1 | 0.93 | 0.07 | 42,42,42,42 | 0 |
| 58 | MG | 2p | 101 | 1/1 | 0.93 | 0.23 | 57,57,57,57 | 0 |
| 58 | MG | 2A | 3839 | 1/1 | 0.93 | 0.07 | 47,47,47,47 | 0 |
| 58 | MG | 1w | 103 | 1/1 | 0.93 | 0.27 | 50,50,50,50 | 0 |
| 58 | MG | 1w | 106 | 1/1 | 0.93 | 0.12 | 44,44,44,44 | 0 |
| 58 | MG | 2A | 3844 | 1/1 | 0.93 | 0.12 | 61,61,61,61 | 0 |
| 58 | MG | 1a | 1634 | 1/1 | 0.93 | 0.18 | 53,53,53,53 | 0 |
| 58 | MG | 2A | 3246 | 1/1 | 0.93 | 0.07 | 45,45,45,45 | 0 |
| 58 | MG | 1A | 3931 | 1/1 | 0.93 | 0.08 | 36,36,36,36 | 0 |
| 58 | MG | 2A | 3483 | 1/1 | 0.93 | 0.09 | 50,50,50,50 | 0 |
| 58 | MG | 1A | 3382 | 1/1 | 0.93 | 0.07 | 40,40,40,40 | 0 |
| 58 | MG | 2A | 3855 | 1/1 | 0.93 | 0.10 | 35,35,35,35 | 0 |
| 58 | MG | 1x | 102 | 1/1 | 0.93 | 0.22 | 51,51,51,51 | 0 |
| 58 | MG | 2A | 3863 | 1/1 | 0.93 | 0.08 | 36,36,36,36 | 0 |
| 58 | MG | 1A | 3529 | 1/1 | 0.93 | 0.07 | 37,37,37,37 | 0 |
| 58 | MG | 1A | 3651 | 1/1 | 0.93 | 0.09 | 41,41,41,41 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58 | MG | 1a | 1642 | 1/1 | 0.93 | 0.24 | 54,54,54,54 | 0 |
| 58 | MG | 1A | 3449 | 1/1 | 0.93 | 0.15 | 34,34,34,34 | 0 |
| 58 | MG | 2A | 3258 | 1/1 | 0.93 | 0.14 | 44,44,44,44 | 0 |
| 58 | MG | 2A | 3494 | 1/1 | 0.93 | 0.12 | 50,50,50,50 | 0 |
| 58 | MG | 2A | 3260 | 1/1 | 0.93 | 0.11 | 47,47,47,47 | 0 |
| 58 | MG | 2A | 3878 | 1/1 | 0.93 | 0.12 | 52,52,52,52 | 0 |
| 58 | MG | 1x | 107 | 1/1 | 0.93 | 0.19 | 49,49,49,49 | 0 |
| 58 | MG | 2A | 3502 | 1/1 | 0.93 | 0.15 | 37,37,37,37 | 0 |
| 58 | MG | 1A | 3297 | 1/1 | 0.93 | 0.20 | 37,37,37,37 | 0 |
| 58 | MG | 2A | 3508 | 1/1 | 0.93 | 0.09 | 39,39,39,39 | 0 |
| 58 | MG | 1x | 109 | 1/1 | 0.93 | 0.08 | 43,43,43,43 | 0 |
| 60 | ZN | 24 | 501 | 1/1 | 0.93 | 0.10 | 113,113,113,113 | 0 |
| 58 | MG | 2B | 214 | 1/1 | 0.94 | 0.09 | 43,43,43,43 | 0 |
| 58 | MG | 2A | 3043 | 1/1 | 0.94 | 0.11 | 52,52,52,52 | 0 |
| 58 | MG | 2A | 3279 | 1/1 | 0.94 | 0.20 | 56,56,56,56 | 0 |
| 58 | MG | 2A | 3544 | 1/1 | 0.94 | 0.08 | 28,28,28,28 | 0 |
| 58 | MG | 1a | 1661 | 1/1 | 0.94 | 0.12 | 46,46,46,46 | 0 |
| 58 | MG | 2E | 302 | 1/1 | 0.94 | 0.12 | 47,47,47,47 | 0 |
| 58 | MG | 2A | 3046 | 1/1 | 0.94 | 0.07 | 38,38,38,38 | 0 |
| 58 | MG | 1A | 3722 | 1/1 | 0.94 | 0.08 | 35,35,35,35 | 0 |
| 58 | MG | 1A | 4101 | 1/1 | 0.94 | 0.07 | 41,41,41,41 | 0 |
| 58 | MG | 2A | 3050 | 1/1 | 0.94 | 0.25 | 53,53,53,53 | 0 |
| 58 | MG | 2A | 3560 | 1/1 | 0.94 | 0.08 | 42,42,42,42 | 0 |
| 58 | MG | 2A | 3561 | 1/1 | 0.94 | 0.06 | 24,24,24,24 | 0 |
| 58 | MG | 2F | 303 | 1/1 | 0.94 | 0.10 | 59,59,59,59 | 0 |
| 58 | MG | 2F | 304 | 1/1 | 0.94 | 0.23 | 48,48,48,48 | 0 |
| 58 | MG | 2F | 305 | 1/1 | 0.94 | 0.11 | 40,40,40,40 | 0 |
| 58 | MG | 1A | 4102 | 1/1 | 0.94 | 0.11 | 39,39,39,39 | 0 |
| 58 | MG | 2A | 3052 | 1/1 | 0.94 | 0.07 | 44,44,44,44 | 0 |
| 58 | MG | 2A | 3569 | 1/1 | 0.94 | 0.14 | 22,22,22,22 | 0 |
| 58 | MG | 2A | 3571 | 1/1 | 0.94 | 0.06 | 28,28,28,28 | 0 |
| 58 | MG | 2O | 201 | 1/1 | 0.94 | 0.19 | 43,43,43,43 | 0 |
| 58 | MG | 1A | 3899 | 1/1 | 0.94 | 0.14 | 55,55,55,55 | 0 |
| 58 | MG | 1A | 3443 | 1/1 | 0.94 | 0.14 | 52,52,52,52 | 0 |
| 58 | MG | 2A | 3294 | 1/1 | 0.94 | 0.14 | 49,49,49,49 | 0 |
| 58 | MG | 1A | 3444 | 1/1 | 0.94 | 0.24 | 55,55,55,55 | 0 |
| 58 | MG | 1A | 3050 | 1/1 | 0.94 | 0.08 | 40,40,40,40 | 0 |
| 58 | MG | 1A | 3203 | 1/1 | 0.94 | 0.16 | 18,18,18,18 | 0 |
| 58 | MG | 2U | 201 | 1/1 | 0.94 | 0.28 | 41,41,41,41 | 0 |
| 58 | MG | 1B | 213 | 1/1 | 0.94 | 0.18 | 43,43,43,43 | 0 |
| 58 | MG | 1A | 3209 | 1/1 | 0.94 | 0.12 | 33,33,33,33 | 0 |
| 58 | MG | 2A | 3066 | 1/1 | 0.94 | 0.18 | 49,49,49,49 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58 | MG | 1A | 3909 | 1/1 | 0.94 | 0.28 | 15,15,15,15 | 0 |
| 58 | MG | 1A | 3550 | 1/1 | 0.94 | 0.18 | 48,48,48,48 | 0 |
| 58 | MG | 1A | 3452 | 1/1 | 0.94 | 0.10 | 32,32,32,32 | 0 |
| 58 | MG | 2A | 3598 | 1/1 | 0.94 | 0.13 | 49,49,49,49 | 0 |
| 58 | MG | 1A | 3919 | 1/1 | 0.94 | 0.06 | 15,15,15,15 | 0 |
| 58 | MG | 1A | 3088 | 1/1 | 0.94 | 0.21 | 29,29,29,29 | 0 |
| 58 | MG | 2A | 3308 | 1/1 | 0.94 | 0.08 | 47,47,47,47 | 0 |
| 58 | MG | 1A | 3280 | 1/1 | 0.94 | 0.07 | 40,40,40,40 | 0 |
| 58 | MG | 1A | 3741 | 1/1 | 0.94 | 0.09 | 40,40,40,40 | 0 |
| 58 | MG | 2a | 1601 | 1/1 | 0.94 | 0.10 | 54,54,54,54 | 0 |
| 58 | MG | 1A | 3925 | 1/1 | 0.94 | 0.10 | 39,39,39,39 | 0 |
| 58 | MG | 1a | 1684 | 1/1 | 0.94 | 0.06 | 47,47,47,47 | 0 |
| 58 | MG | 2A | 3611 | 1/1 | 0.94 | 0.08 | 45,45,45,45 | 0 |
| 58 | MG | 2A | 3615 | 1/1 | 0.94 | 0.10 | 24,24,24,24 | 0 |
| 58 | MG | 1A | 3371 | 1/1 | 0.94 | 0.21 | 38,38,38,38 | 0 |
| 58 | MG | 2a | 1608 | 1/1 | 0.94 | 0.18 | 47,47,47,47 | 0 |
| 58 | MG | 1A | 3374 | 1/1 | 0.94 | 0.08 | 39,39,39,39 | 0 |
| 58 | MG | 2A | 3089 | 1/1 | 0.94 | 0.10 | 44,44,44,44 | 0 |
| 58 | MG | 2A | 3317 | 1/1 | 0.94 | 0.06 | 37,37,37,37 | 0 |
| 58 | MG | 1A | 3748 | 1/1 | 0.94 | 0.11 | 39,39,39,39 | 0 |
| 58 | MG | 1A | 3563 | 1/1 | 0.94 | 0.17 | 34,34,34,34 | 0 |
| 58 | MG | 1A | 3377 | 1/1 | 0.94 | 0.13 | 43,43,43,43 | 0 |
| 58 | MG | 1A | 3126 | 1/1 | 0.94 | 0.08 | 43,43,43,43 | 0 |
| 58 | MG | 1A | 3462 | 1/1 | 0.94 | 0.09 | 53,53,53,53 | 0 |
| 58 | MG | 1A | 3759 | 1/1 | 0.94 | 0.09 | 33,33,33,33 | 0 |
| 58 | MG | 1A | 3946 | 1/1 | 0.94 | 0.08 | 17,17,17,17 | 0 |
| 58 | MG | 2A | 3641 | 1/1 | 0.94 | 0.08 | 37,37,37,37 | 0 |
| 58 | MG | 2A | 3104 | 1/1 | 0.94 | 0.07 | 39,39,39,39 | 0 |
| 58 | MG | 1A | 3948 | 1/1 | 0.94 | 0.14 | 54,54,54,54 | 0 |
| 58 | MG | 2A | 3329 | 1/1 | 0.94 | 0.23 | 46,46,46,46 | 0 |
| 58 | MG | 1a | 1697 | 1/1 | 0.94 | 0.13 | 45,45,45,45 | 0 |
| 58 | MG | 2A | 3108 | 1/1 | 0.94 | 0.24 | 40,40,40,40 | 0 |
| 58 | MG | 1A | 3024 | 1/1 | 0.94 | 0.09 | 39,39,39,39 | 0 |
| 58 | MG | 1a | 1701 | 1/1 | 0.94 | 0.15 | 44,44,44,44 | 0 |
| 58 | MG | 2A | 3112 | 1/1 | 0.94 | 0.14 | 28,28,28,28 | 0 |
| 58 | MG | 1A | 3580 | 1/1 | 0.94 | 0.25 | 32,32,32,32 | 0 |
| 58 | MG | 1A | 3300 | 1/1 | 0.94 | 0.07 | 39,39,39,39 | 0 |
| 58 | MG | 1E | 314 | 1/1 | 0.94 | 0.18 | 45,45,45,45 | 0 |
| 58 | MG | 2A | 3339 | 1/1 | 0.94 | 0.08 | 52,52,52,52 | 0 |
| 58 | MG | 1F | 307 | 1/1 | 0.94 | 0.09 | 19,19,19,19 | 0 |
| 58 | MG | 1A | 3960 | 1/1 | 0.94 | 0.09 | 46,46,46,46 | 0 |
| 58 | MG | 1A | 3302 | 1/1 | 0.94 | 0.10 | 36,36,36,36 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58 | MG | 2a | 1643 | 1/1 | 0.94 | 0.18 | 54,54,54,54 | 0 |
| 58 | MG | 2A | 3668 | 1/1 | 0.94 | 0.05 | 37,37,37,37 | 0 |
| 58 | MG | 2A | 3125 | 1/1 | 0.94 | 0.09 | 37,37,37,37 | 0 |
| 58 | MG | 1A | 3784 | 1/1 | 0.94 | 0.14 | 42,42,42,42 | 0 |
| 58 | MG | 1A | 3230 | 1/1 | 0.94 | 0.15 | 51,51,51,51 | 0 |
| 58 | MG | 2A | 3349 | 1/1 | 0.94 | 0.20 | 52,52,52,52 | 0 |
| 58 | MG | 2A | 3131 | 1/1 | 0.94 | 0.10 | 39,39,39,39 | 0 |
| 58 | MG | 2A | 3676 | 1/1 | 0.94 | 0.17 | 53,53,53,53 | 0 |
| 58 | MG | 2A | 3677 | 1/1 | 0.94 | 0.14 | 26,26,26,26 | 0 |
| 58 | MG | 1A | 3787 | 1/1 | 0.94 | 0.11 | 33,33,33,33 | 0 |
| 58 | MG | 1N | 206 | 1/1 | 0.94 | 0.24 | 38,38,38,38 | 0 |
| 58 | MG | 1A | 3234 | 1/1 | 0.94 | 0.12 | 34,34,34,34 | 0 |
| 58 | MG | 2a | 1657 | 1/1 | 0.94 | 0.07 | 46,46,46,46 | 0 |
| 58 | MG | 1O | 203 | 1/1 | 0.94 | 0.11 | 34,34,34,34 | 0 |
| 58 | MG | 1A | 3972 | 1/1 | 0.94 | 0.09 | 42,42,42,42 | 0 |
| 58 | MG | 1A | 3595 | 1/1 | 0.94 | 0.06 | 31,31,31,31 | 0 |
| 58 | MG | 1a | 1728 | 1/1 | 0.94 | 0.09 | 49,49,49,49 | 0 |
| 58 | MG | 2A | 3148 | 1/1 | 0.94 | 0.15 | 34,34,34,34 | 0 |
| 58 | MG | 2a | 1668 | 1/1 | 0.94 | 0.10 | 48,48,48,48 | 0 |
| 58 | MG | 1P | 201 | 1/1 | 0.94 | 0.35 | 30,30,30,30 | 0 |
| 58 | MG | 2A | 3360 | 1/1 | 0.94 | 0.09 | 53,53,53,53 | 0 |
| 58 | MG | 1Q | 207 | 1/1 | 0.94 | 0.09 | 30,30,30,30 | 0 |
| 58 | MG | 2A | 3362 | 1/1 | 0.94 | 0.18 | 56,56,56,56 | 0 |
| 58 | MG | 1R | 201 | 1/1 | 0.94 | 0.06 | 38,38,38,38 | 0 |
| 58 | MG | 1a | 1737 | 1/1 | 0.94 | 0.15 | 53,53,53,53 | 0 |
| 58 | MG | 2A | 3157 | 1/1 | 0.94 | 0.14 | 38,38,38,38 | 0 |
| 58 | MG | 2A | 3158 | 1/1 | 0.94 | 0.13 | 32,32,32,32 | 0 |
| 58 | MG | 1A | 3976 | 1/1 | 0.94 | 0.10 | 44,44,44,44 | 0 |
| 58 | MG | 2A | 3162 | 1/1 | 0.94 | 0.28 | 56,56,56,56 | 0 |
| 58 | MG | 2a | 1689 | 1/1 | 0.94 | 0.12 | 47,47,47,47 | 0 |
| 58 | MG | 2a | 1690 | 1/1 | 0.94 | 0.19 | 33,33,33,33 | 0 |
| 58 | MG | 2A | 3705 | 1/1 | 0.94 | 0.12 | 54,54,54,54 | 0 |
| 58 | MG | 2A | 3707 | 1/1 | 0.94 | 0.08 | 55,55,55,55 | 0 |
| 58 | MG | 1S | 202 | 1/1 | 0.94 | 0.11 | 39,39,39,39 | 0 |
| 58 | MG | 1A | 3977 | 1/1 | 0.94 | 0.12 | 55,55,55,55 | 0 |
| 58 | MG | 1A | 3091 | 1/1 | 0.94 | 0.10 | 44,44,44,44 | 0 |
| 58 | MG | 2A | 3380 | 1/1 | 0.94 | 0.07 | 51,51,51,51 | 0 |
| 58 | MG | 2A | 3712 | 1/1 | 0.94 | 0.11 | 40,40,40,40 | 0 |
| 58 | MG | 2A | 3382 | 1/1 | 0.94 | 0.27 | 42,42,42,42 | 0 |
| 58 | MG | 1A | 3153 | 1/1 | 0.94 | 0.17 | 31,31,31,31 | 0 |
| 58 | MG | 1A | 3601 | 1/1 | 0.94 | 0.14 | 36,36,36,36 | 0 |
| 58 | MG | 2A | 3169 | 1/1 | 0.94 | 0.08 | 43,43,43,43 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58 | MG | 1A | 3391 | 1/1 | 0.94 | 0.06 | 39,39,39,39 | 0 |
| 58 | MG | 2A | 3171 | 1/1 | 0.94 | 0.06 | 50,50,50,50 | 0 |
| 58 | MG | 1U | 204 | 1/1 | 0.94 | 0.12 | 27,27,27,27 | 0 |
| 58 | MG | 1A | 3395 | 1/1 | 0.94 | 0.10 | 48,48,48,48 | 0 |
| 58 | MG | 1a | 1753 | 1/1 | 0.94 | 0.09 | 59,59,59,59 | 0 |
| 58 | MG | 2a | 1716 | 1/1 | 0.94 | 0.18 | 49,49,49,49 | 0 |
| 58 | MG | 2A | 3177 | 1/1 | 0.94 | 0.12 | 52,52,52,52 | 0 |
| 58 | MG | 1a | 1756 | 1/1 | 0.94 | 0.13 | 41,41,41,41 | 0 |
| 58 | MG | 1A | 3247 | 1/1 | 0.94 | 0.17 | 38,38,38,38 | 0 |
| 58 | MG | 2A | 3737 | 1/1 | 0.94 | 0.11 | 53,53,53,53 | 0 |
| 58 | MG | 2a | 1721 | 1/1 | 0.94 | 0.15 | 43,43,43,43 | 0 |
| 58 | MG | 1V | 206 | 1/1 | 0.94 | 0.10 | 39,39,39,39 | 0 |
| 58 | MG | 2a | 1724 | 1/1 | 0.94 | 0.24 | 45,45,45,45 | 0 |
| 58 | MG | 1A | 3398 | 1/1 | 0.94 | 0.12 | 51,51,51,51 | 0 |
| 58 | MG | 1A | 3400 | 1/1 | 0.94 | 0.23 | 50,50,50,50 | 0 |
| 58 | MG | 1A | 3487 | 1/1 | 0.94 | 0.09 | 29,29,29,29 | 0 |
| 58 | MG | 1a | 1763 | 1/1 | 0.94 | 0.07 | 49,49,49,49 | 0 |
| 58 | MG | 1A | 3825 | 1/1 | 0.94 | 0.09 | 24,24,24,24 | 0 |
| 58 | MG | 1A | 3248 | 1/1 | 0.94 | 0.10 | 35,35,35,35 | 0 |
| 58 | MG | 1A | 3623 | 1/1 | 0.94 | 0.11 | 23,23,23,23 | 0 |
| 58 | MG | 2a | 1736 | 1/1 | 0.94 | 0.27 | 47,47,47,47 | 0 |
| 58 | MG | 1A | 3624 | 1/1 | 0.94 | 0.07 | 24,24,24,24 | 0 |
| 58 | MG | 2a | 1738 | 1/1 | 0.94 | 0.10 | 59,59,59,59 | 0 |
| 58 | MG | 1A | 3402 | 1/1 | 0.94 | 0.27 | 30,30,30,30 | 0 |
| 58 | MG | 2A | 3756 | 1/1 | 0.94 | 0.06 | 40,40,40,40 | 0 |
| 58 | MG | 2A | 3758 | 1/1 | 0.94 | 0.09 | 20,20,20,20 | 0 |
| 58 | MG | 1A | 4005 | 1/1 | 0.94 | 0.22 | 22,22,22,22 | 0 |
| 58 | MG | 1A | 3166 | 1/1 | 0.94 | 0.15 | 44,44,44,44 | 0 |
| 58 | MG | 1A | 3640 | 1/1 | 0.94 | 0.09 | 30,30,30,30 | 0 |
| 58 | MG | 2A | 3762 | 1/1 | 0.94 | 0.08 | 46,46,46,46 | 0 |
| 58 | MG | 2A | 3419 | 1/1 | 0.94 | 0.15 | 28,28,28,28 | 0 |
| 58 | MG | 1A | 3326 | 1/1 | 0.94 | 0.07 | 34,34,34,34 | 0 |
| 58 | MG | 1A | 3492 | 1/1 | 0.94 | 0.30 | 38,38,38,38 | 0 |
| 58 | MG | 1A | 3092 | 1/1 | 0.94 | 0.07 | 40,40,40,40 | 0 |
| 58 | MG | 1A | 3838 | 1/1 | 0.94 | 0.06 | 22,22,22,22 | 0 |
| 58 | MG | 1A | 3005 | 1/1 | 0.94 | 0.07 | 36,36,36,36 | 0 |
| 58 | MG | 2A | 3772 | 1/1 | 0.94 | 0.06 | 31,31,31,31 | 0 |
| 58 | MG | 1A | 4026 | 1/1 | 0.94 | 0.12 | 43,43,43,43 | 0 |
| 58 | MG | 15 | 106 | 1/1 | 0.94 | 0.16 | 37,37,37,37 | 0 |
| 58 | MG | 15 | 108 | 1/1 | 0.94 | 0.13 | 34,34,34,34 | 0 |
| 58 | MG | 1A | 3060 | 1/1 | 0.94 | 0.14 | 41,41,41,41 | 0 |
| 58 | MG | 2a | 1771 | 1/1 | 0.94 | 0.07 | 57,57,57,57 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58 | MG | 2A | 3436 | 1/1 | 0.94 | 0.20 | 39,39,39,39 | 0 |
| 58 | MG | 2a | 1776 | 1/1 | 0.94 | 0.17 | 43,43,43,43 | 0 |
| 58 | MG | 2A | 3779 | 1/1 | 0.94 | 0.07 | 46,46,46,46 | 0 |
| 58 | MG | 1A | 3502 | 1/1 | 0.94 | 0.21 | 25,25,25,25 | 0 |
| 58 | MG | 1a | 1812 | 1/1 | 0.94 | 0.14 | 42,42,42,42 | 0 |
| 58 | MG | 2a | 1782 | 1/1 | 0.94 | 0.11 | 57,57,57,57 | 0 |
| 58 | MG | 2A | 3440 | 1/1 | 0.94 | 0.08 | 50,50,50,50 | 0 |
| 58 | MG | 1A | 3332 | 1/1 | 0.94 | 0.07 | 41,41,41,41 | 0 |
| 58 | MG | 2a | 1789 | 1/1 | 0.94 | 0.13 | 52,52,52,52 | 0 |
| 58 | MG | 2a | 1790 | 1/1 | 0.94 | 0.22 | 54,54,54,54 | 0 |
| 58 | MG | 1A | 3844 | 1/1 | 0.94 | 0.12 | 42,42,42,42 | 0 |
| 58 | MG | 2A | 3443 | 1/1 | 0.94 | 0.15 | 42,42,42,42 | 0 |
| 58 | MG | 1A | 3019 | 1/1 | 0.94 | 0.09 | 30,30,30,30 | 0 |
| 58 | MG | 1A | 3847 | 1/1 | 0.94 | 0.06 | 50,50,50,50 | 0 |
| 58 | MG | 1f | 202 | 1/1 | 0.94 | 0.13 | 44,44,44,44 | 0 |
| 58 | MG | 2A | 3219 | 1/1 | 0.94 | 0.14 | 44,44,44,44 | 0 |
| 58 | MG | 1A | 3419 | 1/1 | 0.94 | 0.07 | 42,42,42,42 | 0 |
| 58 | MG | 1a | 1606 | 1/1 | 0.94 | 0.10 | 60,60,60,60 | 0 |
| 58 | MG | 2A | 3453 | 1/1 | 0.94 | 0.21 | 40,40,40,40 | 0 |
| 58 | MG | 1A | 3255 | 1/1 | 0.94 | 0.10 | 46,46,46,46 | 0 |
| 58 | MG | 2A | 3804 | 1/1 | 0.94 | 0.10 | 43,43,43,43 | 0 |
| 58 | MG | 2a | 1807 | 1/1 | 0.94 | 0.18 | 54,54,54,54 | 0 |
| 58 | MG | 1n | 101 | 1/1 | 0.94 | 0.07 | 34,34,34,34 | 0 |
| 58 | MG | 2A | 3456 | 1/1 | 0.94 | 0.22 | 49,49,49,49 | 0 |
| 58 | MG | 1A | 3337 | 1/1 | 0.94 | 0.22 | 53,53,53,53 | 0 |
| 58 | MG | 2a | 1811 | 1/1 | 0.94 | 0.13 | 48,48,48,48 | 0 |
| 58 | MG | 2a | 1812 | 1/1 | 0.94 | 0.07 | 45,45,45,45 | 0 |
| 58 | MG | 2A | 3463 | 1/1 | 0.94 | 0.14 | 57,57,57,57 | 0 |
| 58 | MG | 2A | 3227 | 1/1 | 0.94 | 0.09 | 52,52,52,52 | 0 |
| 58 | MG | 1A | 3668 | 1/1 | 0.94 | 0.06 | 17,17,17,17 | 0 |
| 58 | MG | 2A | 3467 | 1/1 | 0.94 | 0.12 | 49,49,49,49 | 0 |
| 58 | MG | 2A | 3815 | 1/1 | 0.94 | 0.08 | 57,57,57,57 | 0 |
| 58 | MG | 1A | 3858 | 1/1 | 0.94 | 0.09 | 13,13,13,13 | 0 |
| 58 | MG | 2A | 3470 | 1/1 | 0.94 | 0.09 | 34,34,34,34 | 0 |
| 58 | MG | 2A | 3820 | 1/1 | 0.94 | 0.09 | 32,32,32,32 | 0 |
| 58 | MG | 1A | 3256 | 1/1 | 0.94 | 0.08 | 49,49,49,49 | 0 |
| 58 | MG | 2a | 1826 | 1/1 | 0.94 | 0.11 | 55,55,55,55 | 0 |
| 58 | MG | 1A | 3672 | 1/1 | 0.94 | 0.06 | 20,20,20,20 | 0 |
| 58 | MG | 1a | 1618 | 1/1 | 0.94 | 0.08 | 43,43,43,43 | 0 |
| 58 | MG | 2A | 3827 | 1/1 | 0.94 | 0.09 | 36,36,36,36 | 0 |
| 58 | MG | 2A | 3832 | 1/1 | 0.94 | 0.07 | 56,56,56,56 | 0 |
| 58 | MG | 1A | 3517 | 1/1 | 0.94 | 0.07 | 54,54,54,54 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58 | MG | 1a | 1621 | 1/1 | 0.94 | 0.11 | 45,45,45,45 | 0 |
| 58 | MG | 2a | 1836 | 1/1 | 0.94 | 0.06 | 52,52,52,52 | 0 |
| 58 | MG | 1A | 3863 | 1/1 | 0.94 | 0.11 | 36,36,36,36 | 0 |
| 58 | MG | 1A | 3027 | 1/1 | 0.94 | 0.09 | 61,61,61,61 | 0 |
| 58 | MG | 2a | 1840 | 1/1 | 0.94 | 0.12 | 69,69,69,69 | 0 |
| 58 | MG | 1a | 1626 | 1/1 | 0.94 | 0.13 | 50,50,50,50 | 0 |
| 58 | MG | 1A | 3176 | 1/1 | 0.94 | 0.11 | 28,28,28,28 | 0 |
| 58 | MG | 2A | 3842 | 1/1 | 0.94 | 0.10 | 32,32,32,32 | 0 |
| 58 | MG | 1a | 1628 | 1/1 | 0.94 | 0.14 | 50,50,50,50 | 0 |
| 58 | MG | 2f | 202 | 1/1 | 0.94 | 0.08 | 51,51,51,51 | 0 |
| 58 | MG | 2A | 3845 | 1/1 | 0.94 | 0.07 | 52,52,52,52 | 0 |
| 58 | MG | 1A | 3524 | 1/1 | 0.94 | 0.07 | 47,47,47,47 | 0 |
| 58 | MG | 2A | 3486 | 1/1 | 0.94 | 0.07 | 32,32,32,32 | 0 |
| 58 | MG | 1A | 3526 | 1/1 | 0.94 | 0.26 | 54,54,54,54 | 0 |
| 58 | MG | 1A | 3699 | 1/1 | 0.94 | 0.08 | 20,20,20,20 | 0 |
| 58 | MG | 1A | 3263 | 1/1 | 0.94 | 0.08 | 29,29,29,29 | 0 |
| 58 | MG | 1A | 3709 | 1/1 | 0.94 | 0.10 | 39,39,39,39 | 0 |
| 58 | MG | 1A | 3875 | 1/1 | 0.94 | 0.04 | 27,27,27,27 | 0 |
| 58 | MG | 1A | 4079 | 1/1 | 0.94 | 0.07 | 37,37,37,37 | 0 |
| 58 | MG | 1A | 3004 | 1/1 | 0.94 | 0.11 | 18,18,18,18 | 0 |
| 58 | MG | 1A | 3431 | 1/1 | 0.94 | 0.10 | 24,24,24,24 | 0 |
| 58 | MG | 1A | 3189 | 1/1 | 0.94 | 0.09 | 24,24,24,24 | 0 |
| 58 | MG | 2A | 3262 | 1/1 | 0.94 | 0.11 | 52,52,52,52 | 0 |
| 58 | MG | 2A | 3505 | 1/1 | 0.94 | 0.06 | 40,40,40,40 | 0 |
| 58 | MG | 2A | 3018 | 1/1 | 0.94 | 0.15 | 48,48,48,48 | 0 |
| 58 | MG | 1A | 3049 | 1/1 | 0.94 | 0.06 | 8,8,8,8 | 0 |
| 58 | MG | 2A | 3511 | 1/1 | 0.94 | 0.12 | 42,42,42,42 | 0 |
| 58 | MG | 1a | 1650 | 1/1 | 0.94 | 0.12 | 45,45,45,45 | 0 |
| 58 | MG | 2w | 108 | 1/1 | 0.94 | 0.07 | 53,53,53,53 | 0 |
| 58 | MG | 2A | 3881 | 1/1 | 0.94 | 0.08 | 48,48,48,48 | 0 |
| 58 | MG | 2A | 3028 | 1/1 | 0.94 | 0.18 | 45,45,45,45 | 0 |
| 58 | MG | 1A | 3437 | 1/1 | 0.94 | 0.05 | 36,36,36,36 | 0 |
| 58 | MG | 2A | 3522 | 1/1 | 0.94 | 0.07 | 49,49,49,49 | 0 |
| 58 | MG | 1A | 3718 | 1/1 | 0.94 | 0.14 | 47,47,47,47 | 0 |
| 58 | MG | 1A | 3106 | 1/1 | 0.94 | 0.29 | 40,40,40,40 | 0 |
| 58 | MG | 2A | 3035 | 1/1 | 0.94 | 0.12 | 23,23,23,23 | 0 |
| 58 | MG | 2B | 205 | 1/1 | 0.94 | 0.14 | 51,51,51,51 | 0 |
| 58 | MG | 2x | 106 | 1/1 | 0.94 | 0.14 | 43,43,43,43 | 0 |
| 58 | MG | 1A | 3109 | 1/1 | 0.94 | 0.17 | 37,37,37,37 | 0 |
| 58 | MG | 1a | 1659 | 1/1 | 0.94 | 0.21 | 47,47,47,47 | 0 |
| 58 | MG | 2B | 208 | 1/1 | 0.94 | 0.24 | 50,50,50,50 | 0 |
| 58 | MG | 2A | 3536 | 1/1 | 0.94 | 0.15 | 48,48,48,48 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58 | MG | 2A | 3537 | 1/1 | 0.94 | 0.09 | 50,50,50,50 | 0 |
| 58 | MG | 1a | 1660 | 1/1 | 0.94 | 0.15 | 53,53,53,53 | 0 |
| 58 | MG | 2A | 3539 | 1/1 | 0.94 | 0.12 | 41,41,41,41 | 0 |
| 58 | MG | 2A | 3220 | 1/1 | 0.95 | 0.08 | 49,49,49,49 | 0 |
| 58 | MG | 2A | 3874 | 1/1 | 0.95 | 0.17 | 45,45,45,45 | 0 |
| 58 | MG | 2A | 3876 | 1/1 | 0.95 | 0.13 | 36,36,36,36 | 0 |
| 58 | MG | 1X | 101 | 1/1 | 0.95 | 0.12 | 28,28,28,28 | 0 |
| 58 | MG | 1A | 3991 | 1/1 | 0.95 | 0.05 | 23,23,23,23 | 0 |
| 58 | MG | 1A | 3993 | 1/1 | 0.95 | 0.05 | 11,11,11,11 | 0 |
| 58 | MG | 2A | 3880 | 1/1 | 0.95 | 0.08 | 53,53,53,53 | 0 |
| 58 | MG | 2A | 3489 | 1/1 | 0.95 | 0.07 | 39,39,39,39 | 0 |
| 58 | MG | 1A | 3819 | 1/1 | 0.95 | 0.06 | 46,46,46,46 | 0 |
| 58 | MG | 1A | 3820 | 1/1 | 0.95 | 0.32 | 26,26,26,26 | 0 |
| 58 | MG | 1A | 3340 | 1/1 | 0.95 | 0.15 | 41,41,41,41 | 0 |
| 58 | MG | 10 | 102 | 1/1 | 0.95 | 0.13 | 39,39,39,39 | 0 |
| 58 | MG | 2A | 3229 | 1/1 | 0.95 | 0.07 | 47,47,47,47 | 0 |
| 58 | MG | 2A | 3499 | 1/1 | 0.95 | 0.21 | 44,44,44,44 | 0 |
| 58 | MG | 1a | 1813 | 1/1 | 0.95 | 0.09 | 52,52,52,52 | 0 |
| 58 | MG | 2A | 3231 | 1/1 | 0.95 | 0.14 | 46,46,46,46 | 0 |
| 58 | MG | 2A | 3503 | 1/1 | 0.95 | 0.07 | 54,54,54,54 | 0 |
| 58 | MG | 1A | 3116 | 1/1 | 0.95 | 0.05 | 30,30,30,30 | 0 |
| 58 | MG | 1a | 1815 | 1/1 | 0.95 | 0.09 | 44,44,44,44 | 0 |
| 58 | MG | 1a | 1816 | 1/1 | 0.95 | 0.09 | 43,43,43,43 | 0 |
| 58 | MG | 1A | 3622 | 1/1 | 0.95 | 0.11 | 38,38,38,38 | 0 |
| 58 | MG | 1a | 1818 | 1/1 | 0.95 | 0.12 | 42,42,42,42 | 0 |
| 58 | MG | 2A | 3512 | 1/1 | 0.95 | 0.07 | 50,50,50,50 | 0 |
| 58 | MG | 2B | 217 | 1/1 | 0.95 | 0.07 | 47,47,47,47 | 0 |
| 58 | MG | 2B | 218 | 1/1 | 0.95 | 0.11 | 53,53,53,53 | 0 |
| 58 | MG | 2A | 3515 | 1/1 | 0.95 | 0.09 | 12,12,12,12 | 0 |
| 58 | MG | 2D | 301 | 1/1 | 0.95 | 0.10 | 35,35,35,35 | 0 |
| 58 | MG | 2D | 303 | 1/1 | 0.95 | 0.14 | 46,46,46,46 | 0 |
| 58 | MG | 1A | 3826 | 1/1 | 0.95 | 0.05 | 24,24,24,24 | 0 |
| 58 | MG | 1A | 3343 | 1/1 | 0.95 | 0.17 | 42,42,42,42 | 0 |
| 58 | MG | 2A | 3242 | 1/1 | 0.95 | 0.28 | 32,32,32,32 | 0 |
| 58 | MG | 1e | 202 | 1/1 | 0.95 | 0.18 | 55,55,55,55 | 0 |
| 58 | MG | 1A | 3222 | 1/1 | 0.95 | 0.08 | 31,31,31,31 | 0 |
| 58 | MG | 1A | 3348 | 1/1 | 0.95 | 0.11 | 43,43,43,43 | 0 |
| 58 | MG | 2A | 3249 | 1/1 | 0.95 | 0.09 | 54,54,54,54 | 0 |
| 58 | MG | 2A | 3529 | 1/1 | 0.95 | 0.07 | 28,28,28,28 | 0 |
| 58 | MG | 1A | 3227 | 1/1 | 0.95 | 0.11 | 31,31,31,31 | 0 |
| 58 | MG | 1A | 4012 | 1/1 | 0.95 | 0.05 | 23,23,23,23 | 0 |
| 58 | MG | 2F | 302 | 1/1 | 0.95 | 0.13 | 45,45,45,45 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58 | MG | 1m | 3001 | 1/1 | 0.95 | 0.07 | 38,38,38,38 | 0 |
| 58 | MG | 15 | 102 | 1/1 | 0.95 | 0.12 | 23,23,23,23 | 0 |
| 58 | MG | 1A | 4017 | 1/1 | 0.95 | 0.06 | 29,29,29,29 | 0 |
| 58 | MG | 1A | 4018 | 1/1 | 0.95 | 0.04 | 27,27,27,27 | 0 |
| 58 | MG | 1A | 3499 | 1/1 | 0.95 | 0.08 | 38,38,38,38 | 0 |
| 58 | MG | 1A | 4022 | 1/1 | 0.95 | 0.05 | 40,40,40,40 | 0 |
| 58 | MG | 2A | 3543 | 1/1 | 0.95 | 0.08 | 43,43,43,43 | 0 |
| 58 | MG | 1A | 3422 | 1/1 | 0.95 | 0.06 | 35,35,35,35 | 0 |
| 58 | MG | 2Q | 201 | 1/1 | 0.95 | 0.17 | 48,48,48,48 | 0 |
| 58 | MG | 1A | 3084 | 1/1 | 0.95 | 0.12 | 22,22,22,22 | 0 |
| 58 | MG | 2A | 3550 | 1/1 | 0.95 | 0.07 | 34,34,34,34 | 0 |
| 58 | MG | 18 | 101 | 1/1 | 0.95 | 0.36 | 49,49,49,49 | 0 |
| 58 | MG | 2R | 202 | 1/1 | 0.95 | 0.17 | 38,38,38,38 | 0 |
| 58 | MG | 2A | 3264 | 1/1 | 0.95 | 0.25 | 49,49,49,49 | 0 |
| 58 | MG | 1A | 3273 | 1/1 | 0.95 | 0.24 | 41,41,41,41 | 0 |
| 58 | MG | 2T | 201 | 1/1 | 0.95 | 0.10 | 52,52,52,52 | 0 |
| 58 | MG | 1a | 1601 | 1/1 | 0.95 | 0.27 | 48,48,48,48 | 0 |
| 58 | MG | 1A | 3507 | 1/1 | 0.95 | 0.07 | 53,53,53,53 | 0 |
| 58 | MG | 1A | 3121 | 1/1 | 0.95 | 0.14 | 35,35,35,35 | 0 |
| 58 | MG | 1A | 3174 | 1/1 | 0.95 | 0.16 | 41,41,41,41 | 0 |
| 58 | MG | 1A | 3122 | 1/1 | 0.95 | 0.11 | 28,28,28,28 | 0 |
| 58 | MG | 1A | 3657 | 1/1 | 0.95 | 0.06 | 28,28,28,28 | 0 |
| 58 | MG | 1A | 3512 | 1/1 | 0.95 | 0.08 | 46,46,46,46 | 0 |
| 58 | MG | 2X | 101 | 1/1 | 0.95 | 0.08 | 51,51,51,51 | 0 |
| 58 | MG | 1a | 1609 | 1/1 | 0.95 | 0.22 | 56,56,56,56 | 0 |
| 58 | MG | 1A | 3360 | 1/1 | 0.95 | 0.10 | 32,32,32,32 | 0 |
| 58 | MG | 23 | 101 | 1/1 | 0.95 | 0.17 | 47,47,47,47 | 0 |
| 58 | MG | 25 | 102 | 1/1 | 0.95 | 0.07 | 38,38,38,38 | 0 |
| 58 | MG | 25 | 103 | 1/1 | 0.95 | 0.05 | 34,34,34,34 | 0 |
| 58 | MG | 1x | 111 | 1/1 | 0.95 | 0.09 | 39,39,39,39 | 0 |
| 58 | MG | 2A | 3580 | 1/1 | 0.95 | 0.11 | 36,36,36,36 | 0 |
| 58 | MG | 27 | 102 | 1/1 | 0.95 | 0.15 | 41,41,41,41 | 0 |
| 58 | MG | 27 | 103 | 1/1 | 0.95 | 0.10 | 44,44,44,44 | 0 |
| 58 | MG | 1A | 3660 | 1/1 | 0.95 | 0.05 | 20,20,20,20 | 0 |
| 58 | MG | 28 | 103 | 1/1 | 0.95 | 0.06 | 39,39,39,39 | 0 |
| 58 | MG | 2A | 3001 | 1/1 | 0.95 | 0.16 | 37,37,37,37 | 0 |
| 58 | MG | 2A | 3003 | 1/1 | 0.95 | 0.14 | 44,44,44,44 | 0 |
| 58 | MG | 1A | 3664 | 1/1 | 0.95 | 0.04 | 12,12,12,12 | 0 |
| 58 | MG | 1a | 1616 | 1/1 | 0.95 | 0.15 | 41,41,41,41 | 0 |
| 58 | MG | 2a | 1603 | 1/1 | 0.95 | 0.07 | 56,56,56,56 | 0 |
| 58 | MG | 2A | 3284 | 1/1 | 0.95 | 0.07 | 40,40,40,40 | 0 |
| 58 | MG | 1A | 3430 | 1/1 | 0.95 | 0.12 | 32,32,32,32 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58 | MG | 2A | 3287 | 1/1 | 0.95 | 0.05 | 55,55,55,55 | 0 |
| 58 | MG | 1A | 4044 | 1/1 | 0.95 | 0.05 | 24,24,24,24 | 0 |
| 58 | MG | 2A | 3016 | 1/1 | 0.95 | 0.12 | 51,51,51,51 | 0 |
| 58 | MG | 1A | 3361 | 1/1 | 0.95 | 0.05 | 41,41,41,41 | 0 |
| 58 | MG | 1A | 3292 | 1/1 | 0.95 | 0.13 | 33,33,33,33 | 0 |
| 58 | MG | 2a | 1611 | 1/1 | 0.95 | 0.16 | 55,55,55,55 | 0 |
| 58 | MG | 2A | 3603 | 1/1 | 0.95 | 0.10 | 49,49,49,49 | 0 |
| 58 | MG | 2A | 3020 | 1/1 | 0.95 | 0.24 | 47,47,47,47 | 0 |
| 58 | MG | 2A | 3605 | 1/1 | 0.95 | 0.15 | 47,47,47,47 | 0 |
| 58 | MG | 2A | 3606 | 1/1 | 0.95 | 0.07 | 42,42,42,42 | 0 |
| 58 | MG | 2A | 3022 | 1/1 | 0.95 | 0.11 | 37,37,37,37 | 0 |
| 58 | MG | 1A | 4048 | 1/1 | 0.95 | 0.07 | 25,25,25,25 | 0 |
| 58 | MG | 2a | 1618 | 1/1 | 0.95 | 0.20 | 58,58,58,58 | 0 |
| 58 | MG | 2a | 1619 | 1/1 | 0.95 | 0.11 | 51,51,51,51 | 0 |
| 58 | MG | 1A | 3853 | 1/1 | 0.95 | 0.19 | 39,39,39,39 | 0 |
| 58 | MG | 1A | 4050 | 1/1 | 0.95 | 0.06 | 14,14,14,14 | 0 |
| 58 | MG | 2a | 1623 | 1/1 | 0.95 | 0.07 | 45,45,45,45 | 0 |
| 58 | MG | 1A | 3293 | 1/1 | 0.95 | 0.09 | 38,38,38,38 | 0 |
| 58 | MG | 2A | 3612 | 1/1 | 0.95 | 0.07 | 51,51,51,51 | 0 |
| 58 | MG | 2A | 3613 | 1/1 | 0.95 | 0.07 | 45,45,45,45 | 0 |
| 58 | MG | 1A | 3857 | 1/1 | 0.95 | 0.06 | 42,42,42,42 | 0 |
| 58 | MG | 1A | 3047 | 1/1 | 0.95 | 0.05 | 27,27,27,27 | 0 |
| 58 | MG | 2A | 3619 | 1/1 | 0.95 | 0.07 | 34,34,34,34 | 0 |
| 58 | MG | 2A | 3620 | 1/1 | 0.95 | 0.07 | 37,37,37,37 | 0 |
| 58 | MG | 1A | 3676 | 1/1 | 0.95 | 0.06 | 11,11,11,11 | 0 |
| 58 | MG | 1A | 4059 | 1/1 | 0.95 | 0.11 | 55,55,55,55 | 0 |
| 58 | MG | 2a | 1634 | 1/1 | 0.95 | 0.18 | 37,37,37,37 | 0 |
| 58 | MG | 1A | 3681 | 1/1 | 0.95 | 0.13 | 37,37,37,37 | 0 |
| 58 | MG | 2A | 3305 | 1/1 | 0.95 | 0.08 | 48,48,48,48 | 0 |
| 58 | MG | 2A | 3041 | 1/1 | 0.95 | 0.25 | 43,43,43,43 | 0 |
| 58 | MG | 1A | 3237 | 1/1 | 0.95 | 0.31 | 39,39,39,39 | 0 |
| 58 | MG | 1A | 3440 | 1/1 | 0.95 | 0.18 | 32,32,32,32 | 0 |
| 58 | MG | 1A | 4064 | 1/1 | 0.95 | 0.06 | 44,44,44,44 | 0 |
| 58 | MG | 2A | 3633 | 1/1 | 0.95 | 0.06 | 35,35,35,35 | 0 |
| 58 | MG | 2A | 3634 | 1/1 | 0.95 | 0.07 | 43,43,43,43 | 0 |
| 58 | MG | 1A | 3441 | 1/1 | 0.95 | 0.16 | 31,31,31,31 | 0 |
| 58 | MG | 1A | 3238 | 1/1 | 0.95 | 0.10 | 47,47,47,47 | 0 |
| 58 | MG | 1A | 4072 | 1/1 | 0.95 | 0.06 | 29,29,29,29 | 0 |
| 58 | MG | 1A | 3694 | 1/1 | 0.95 | 0.06 | 22,22,22,22 | 0 |
| 58 | MG | 1a | 1649 | 1/1 | 0.95 | 0.10 | 47,47,47,47 | 0 |
| 58 | MG | 2A | 3315 | 1/1 | 0.95 | 0.09 | 59,59,59,59 | 0 |
| 58 | MG | 1A | 3181 | 1/1 | 0.95 | 0.11 | 16,16,16,16 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58 | MG | 2A | 3053 | 1/1 | 0.95 | 0.12 | 49,49,49,49 | 0 |
| 58 | MG | 2a | 1652 | 1/1 | 0.95 | 0.06 | 57,57,57,57 | 0 |
| 58 | MG | 1A | 4077 | 1/1 | 0.95 | 0.07 | 34,34,34,34 | 0 |
| 58 | MG | 2A | 3650 | 1/1 | 0.95 | 0.13 | 46,46,46,46 | 0 |
| 58 | MG | 2A | 3654 | 1/1 | 0.95 | 0.16 | 49,49,49,49 | 0 |
| 58 | MG | 2a | 1656 | 1/1 | 0.95 | 0.07 | 64,64,64,64 | 0 |
| 58 | MG | 1A | 3534 | 1/1 | 0.95 | 0.23 | 31,31,31,31 | 0 |
| 58 | MG | 1A | 4082 | 1/1 | 0.95 | 0.08 | 36,36,36,36 | 0 |
| 58 | MG | 2A | 3321 | 1/1 | 0.95 | 0.06 | 45,45,45,45 | 0 |
| 58 | MG | 2A | 3060 | 1/1 | 0.95 | 0.17 | 44,44,44,44 | 0 |
| 58 | MG | 2a | 1663 | 1/1 | 0.95 | 0.08 | 55,55,55,55 | 0 |
| 58 | MG | 2A | 3323 | 1/1 | 0.95 | 0.06 | 35,35,35,35 | 0 |
| 58 | MG | 1A | 3370 | 1/1 | 0.95 | 0.17 | 39,39,39,39 | 0 |
| 58 | MG | 2a | 1667 | 1/1 | 0.95 | 0.15 | 28,28,28,28 | 0 |
| 58 | MG | 1A | 3536 | 1/1 | 0.95 | 0.15 | 25,25,25,25 | 0 |
| 58 | MG | 1A | 3874 | 1/1 | 0.95 | 0.14 | 23,23,23,23 | 0 |
| 58 | MG | 1A | 3710 | 1/1 | 0.95 | 0.09 | 28,28,28,28 | 0 |
| 58 | MG | 2a | 1672 | 1/1 | 0.95 | 0.15 | 45,45,45,45 | 0 |
| 58 | MG | 2A | 3665 | 1/1 | 0.95 | 0.09 | 44,44,44,44 | 0 |
| 58 | MG | 2A | 3666 | 1/1 | 0.95 | 0.10 | 47,47,47,47 | 0 |
| 58 | MG | 1A | 3184 | 1/1 | 0.95 | 0.14 | 37,37,37,37 | 0 |
| 58 | MG | 1A | 3712 | 1/1 | 0.95 | 0.06 | 34,34,34,34 | 0 |
| 58 | MG | 1A | 3539 | 1/1 | 0.95 | 0.17 | 41,41,41,41 | 0 |
| 58 | MG | 2a | 1685 | 1/1 | 0.95 | 0.08 | 47,47,47,47 | 0 |
| 58 | MG | 1A | 4097 | 1/1 | 0.95 | 0.09 | 53,53,53,53 | 0 |
| 58 | MG | 1A | 4098 | 1/1 | 0.95 | 0.13 | 44,44,44,44 | 0 |
| 58 | MG | 2A | 3072 | 1/1 | 0.95 | 0.05 | 42,42,42,42 | 0 |
| 58 | MG | 1a | 1668 | 1/1 | 0.95 | 0.09 | 44,44,44,44 | 0 |
| 58 | MG | 1A | 3883 | 1/1 | 0.95 | 0.10 | 57,57,57,57 | 0 |
| 58 | MG | 1A | 3447 | 1/1 | 0.95 | 0.14 | 43,43,43,43 | 0 |
| 58 | MG | 2A | 3680 | 1/1 | 0.95 | 0.13 | 50,50,50,50 | 0 |
| 58 | MG | 2a | 1693 | 1/1 | 0.95 | 0.14 | 37,37,37,37 | 0 |
| 58 | MG | 1A | 3131 | 1/1 | 0.95 | 0.11 | 52,52,52,52 | 0 |
| 58 | MG | 1A | 3308 | 1/1 | 0.95 | 0.15 | 36,36,36,36 | 0 |
| 58 | MG | 2a | 1697 | 1/1 | 0.95 | 0.18 | 30,30,30,30 | 0 |
| 58 | MG | 1A | 3311 | 1/1 | 0.95 | 0.12 | 48,48,48,48 | 0 |
| 58 | MG | 2A | 3084 | 1/1 | 0.95 | 0.09 | 42,42,42,42 | 0 |
| 58 | MG | 2A | 3086 | 1/1 | 0.95 | 0.11 | 40,40,40,40 | 0 |
| 58 | MG | 1A | 4104 | 1/1 | 0.95 | 0.27 | 44,44,44,44 | 0 |
| 58 | MG | 1A | 3547 | 1/1 | 0.95 | 0.14 | 34,34,34,34 | 0 |
| 58 | MG | 2A | 3346 | 1/1 | 0.95 | 0.08 | 54,54,54,54 | 0 |
| 58 | MG | 1B | 204 | 1/1 | 0.95 | 0.07 | 34,34,34,34 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58 | MG | 1A | 3187 | 1/1 | 0.95 | 0.11 | 49,49,49,49 | 0 |
| 58 | MG | 2A | 3695 | 1/1 | 0.95 | 0.08 | 51,51,51,51 | 0 |
| 58 | MG | 2a | 1710 | 1/1 | 0.95 | 0.05 | 38,38,38,38 | 0 |
| 58 | MG | 2a | 1712 | 1/1 | 0.95 | 0.07 | 49,49,49,49 | 0 |
| 58 | MG | 2A | 3095 | 1/1 | 0.95 | 0.08 | 31,31,31,31 | 0 |
| 58 | MG | 2A | 3698 | 1/1 | 0.95 | 0.06 | 48,48,48,48 | 0 |
| 58 | MG | 1A | 3896 | 1/1 | 0.95 | 0.07 | 16,16,16,16 | 0 |
| 58 | MG | 1A | 3897 | 1/1 | 0.95 | 0.05 | 12,12,12,12 | 0 |
| 58 | MG | 1a | 1681 | 1/1 | 0.95 | 0.09 | 55,55,55,55 | 0 |
| 58 | MG | 1A | 3188 | 1/1 | 0.95 | 0.05 | 28,28,28,28 | 0 |
| 58 | MG | 1A | 3137 | 1/1 | 0.95 | 0.14 | 26,26,26,26 | 0 |
| 58 | MG | 1A | 3456 | 1/1 | 0.95 | 0.06 | 40,40,40,40 | 0 |
| 58 | MG | 1A | 3315 | 1/1 | 0.95 | 0.10 | 32,32,32,32 | 0 |
| 58 | MG | 1A | 3553 | 1/1 | 0.95 | 0.10 | 38,38,38,38 | 0 |
| 58 | MG | 2A | 3107 | 1/1 | 0.95 | 0.04 | 35,35,35,35 | 0 |
| 58 | MG | 1A | 3384 | 1/1 | 0.95 | 0.06 | 34,34,34,34 | 0 |
| 58 | MG | 1A | 3138 | 1/1 | 0.95 | 0.08 | 41,41,41,41 | 0 |
| 58 | MG | 1A | 3461 | 1/1 | 0.95 | 0.07 | 51,51,51,51 | 0 |
| 58 | MG | 1A | 3560 | 1/1 | 0.95 | 0.10 | 41,41,41,41 | 0 |
| 58 | MG | 2A | 3716 | 1/1 | 0.95 | 0.07 | 34,34,34,34 | 0 |
| 58 | MG | 2a | 1732 | 1/1 | 0.95 | 0.10 | 42,42,42,42 | 0 |
| 58 | MG | 1a | 1691 | 1/1 | 0.95 | 0.18 | 33,33,33,33 | 0 |
| 58 | MG | 1A | 3319 | 1/1 | 0.95 | 0.06 | 28,28,28,28 | 0 |
| 58 | MG | 1A | 3015 | 1/1 | 0.95 | 0.08 | 23,23,23,23 | 0 |
| 58 | MG | 1a | 1694 | 1/1 | 0.95 | 0.17 | 30,30,30,30 | 0 |
| 58 | MG | 2A | 3370 | 1/1 | 0.95 | 0.08 | 57,57,57,57 | 0 |
| 58 | MG | 2A | 3119 | 1/1 | 0.95 | 0.17 | 53,53,53,53 | 0 |
| 58 | MG | 1A | 3466 | 1/1 | 0.95 | 0.06 | 43,43,43,43 | 0 |
| 58 | MG | 1A | 3923 | 1/1 | 0.95 | 0.06 | 17,17,17,17 | 0 |
| 58 | MG | 2a | 1742 | 1/1 | 0.95 | 0.16 | 53,53,53,53 | 0 |
| 58 | MG | 2A | 3374 | 1/1 | 0.95 | 0.22 | 67,67,67,67 | 0 |
| 58 | MG | 1A | 3389 | 1/1 | 0.95 | 0.06 | 32,32,32,32 | 0 |
| 58 | MG | 2A | 3376 | 1/1 | 0.95 | 0.10 | 38,38,38,38 | 0 |
| 58 | MG | 2A | 3735 | 1/1 | 0.95 | 0.09 | 49,49,49,49 | 0 |
| 58 | MG | 2A | 3378 | 1/1 | 0.95 | 0.19 | 48,48,48,48 | 0 |
| 58 | MG | 1A | 3570 | 1/1 | 0.95 | 0.07 | 30,30,30,30 | 0 |
| 58 | MG | 1a | 1700 | 1/1 | 0.95 | 0.11 | 48,48,48,48 | 0 |
| 58 | MG | 1A | 3322 | 1/1 | 0.95 | 0.23 | 25,25,25,25 | 0 |
| 58 | MG | 2A | 3743 | 1/1 | 0.95 | 0.09 | 47,47,47,47 | 0 |
| 58 | MG | 2A | 3132 | 1/1 | 0.95 | 0.08 | 42,42,42,42 | 0 |
| 58 | MG | 1D | 309 | 1/1 | 0.95 | 0.09 | 37,37,37,37 | 0 |
| 58 | MG | 2A | 3386 | 1/1 | 0.95 | 0.09 | 51,51,51,51 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58 | MG | 2A | 3748 | 1/1 | 0.95 | 0.06 | 47,47,47,47 | 0 |
| 58 | MG | 2a | 1761 | 1/1 | 0.95 | 0.08 | 71,71,71,71 | 0 |
| 58 | MG | 2A | 3749 | 1/1 | 0.95 | 0.24 | 41,41,41,41 | 0 |
| 58 | MG | 2a | 1763 | 1/1 | 0.95 | 0.09 | 59,59,59,59 | 0 |
| 58 | MG | 2A | 3387 | 1/1 | 0.95 | 0.08 | 58,58,58,58 | 0 |
| 58 | MG | 2A | 3134 | 1/1 | 0.95 | 0.10 | 45,45,45,45 | 0 |
| 58 | MG | 2A | 3135 | 1/1 | 0.95 | 0.18 | 37,37,37,37 | 0 |
| 58 | MG | 2a | 1773 | 1/1 | 0.95 | 0.06 | 66,66,66,66 | 0 |
| 58 | MG | 1a | 1703 | 1/1 | 0.95 | 0.11 | 36,36,36,36 | 0 |
| 58 | MG | 2A | 3392 | 1/1 | 0.95 | 0.15 | 39,39,39,39 | 0 |
| 58 | MG | 2A | 3140 | 1/1 | 0.95 | 0.07 | 54,54,54,54 | 0 |
| 58 | MG | 2A | 3757 | 1/1 | 0.95 | 0.08 | 43,43,43,43 | 0 |
| 58 | MG | 2a | 1781 | 1/1 | 0.95 | 0.07 | 54,54,54,54 | 0 |
| 58 | MG | 1A | 3575 | 1/1 | 0.95 | 0.19 | 34,34,34,34 | 0 |
| 58 | MG | 2a | 1784 | 1/1 | 0.95 | 0.07 | 59,59,59,59 | 0 |
| 58 | MG | 1D | 312 | 1/1 | 0.95 | 0.14 | 23,23,23,23 | 0 |
| 58 | MG | 2a | 1787 | 1/1 | 0.95 | 0.16 | 37,37,37,37 | 0 |
| 58 | MG | 1A | 3393 | 1/1 | 0.95 | 0.16 | 15,15,15,15 | 0 |
| 58 | MG | 1A | 3753 | 1/1 | 0.95 | 0.07 | 44,44,44,44 | 0 |
| 58 | MG | 1a | 1708 | 1/1 | 0.95 | 0.11 | 45,45,45,45 | 0 |
| 58 | MG | 1A | 3755 | 1/1 | 0.95 | 0.09 | 28,28,28,28 | 0 |
| 58 | MG | 1A | 3061 | 1/1 | 0.95 | 0.10 | 25,25,25,25 | 0 |
| 58 | MG | 1a | 1712 | 1/1 | 0.95 | 0.24 | 45,45,45,45 | 0 |
| 58 | MG | 1A | 3257 | 1/1 | 0.95 | 0.21 | 36,36,36,36 | 0 |
| 58 | MG | 1A | 3944 | 1/1 | 0.95 | 0.07 | 37,37,37,37 | 0 |
| 58 | MG | 1A | 3201 | 1/1 | 0.95 | 0.14 | 30,30,30,30 | 0 |
| 58 | MG | 1A | 3762 | 1/1 | 0.95 | 0.09 | 37,37,37,37 | 0 |
| 58 | MG | 2a | 1801 | 1/1 | 0.95 | 0.14 | 53,53,53,53 | 0 |
| 58 | MG | 1A | 3592 | 1/1 | 0.95 | 0.23 | 37,37,37,37 | 0 |
| 58 | MG | 2A | 3408 | 1/1 | 0.95 | 0.22 | 38,38,38,38 | 0 |
| 58 | MG | 1a | 1721 | 1/1 | 0.95 | 0.13 | 48,48,48,48 | 0 |
| 58 | MG | 2A | 3410 | 1/1 | 0.95 | 0.06 | 42,42,42,42 | 0 |
| 58 | MG | 1F | 311 | 1/1 | 0.95 | 0.16 | 20,20,20,20 | 0 |
| 58 | MG | 1A | 3765 | 1/1 | 0.95 | 0.06 | 19,19,19,19 | 0 |
| 58 | MG | 1F | 313 | 1/1 | 0.95 | 0.13 | 42,42,42,42 | 0 |
| 58 | MG | 2A | 3417 | 1/1 | 0.95 | 0.17 | 40,40,40,40 | 0 |
| 58 | MG | 2A | 3785 | 1/1 | 0.95 | 0.13 | 50,50,50,50 | 0 |
| 58 | MG | 1A | 3770 | 1/1 | 0.95 | 0.06 | 29,29,29,29 | 0 |
| 58 | MG | 1A | 3956 | 1/1 | 0.95 | 0.07 | 30,30,30,30 | 0 |
| 58 | MG | 1G | 205 | 1/1 | 0.95 | 0.09 | 44,44,44,44 | 0 |
| 58 | MG | 1a | 1735 | 1/1 | 0.95 | 0.05 | 38,38,38,38 | 0 |
| 58 | MG | 1N | 201 | 1/1 | 0.95 | 0.10 | 44,44,44,44 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58 | MG | 2A | 3793 | 1/1 | 0.95 | 0.11 | 58,58,58,58 | 0 |
| 58 | MG | 1A | 3399 | 1/1 | 0.95 | 0.08 | 52,52,52,52 | 0 |
| 58 | MG | 2A | 3430 | 1/1 | 0.95 | 0.12 | 40,40,40,40 | 0 |
| 58 | MG | 2A | 3798 | 1/1 | 0.95 | 0.06 | 38,38,38,38 | 0 |
| 58 | MG | 2A | 3173 | 1/1 | 0.95 | 0.07 | 41,41,41,41 | 0 |
| 58 | MG | 1a | 1739 | 1/1 | 0.95 | 0.05 | 22,22,22,22 | 0 |
| 58 | MG | 1A | 3959 | 1/1 | 0.95 | 0.07 | 36,36,36,36 | 0 |
| 58 | MG | 1A | 3329 | 1/1 | 0.95 | 0.11 | 35,35,35,35 | 0 |
| 58 | MG | 2A | 3435 | 1/1 | 0.95 | 0.27 | 55,55,55,55 | 0 |
| 58 | MG | 1A | 3776 | 1/1 | 0.95 | 0.05 | 14,14,14,14 | 0 |
| 58 | MG | 2a | 1831 | 1/1 | 0.95 | 0.10 | 49,49,49,49 | 0 |
| 58 | MG | 1A | 3962 | 1/1 | 0.95 | 0.07 | 36,36,36,36 | 0 |
| 58 | MG | 1A | 3151 | 1/1 | 0.95 | 0.31 | 32,32,32,32 | 0 |
| 58 | MG | 2A | 3439 | 1/1 | 0.95 | 0.18 | 52,52,52,52 | 0 |
| 58 | MG | 1a | 1748 | 1/1 | 0.95 | 0.17 | 38,38,38,38 | 0 |
| 58 | MG | 1A | 3076 | 1/1 | 0.95 | 0.06 | 25,25,25,25 | 0 |
| 58 | MG | 2A | 3184 | 1/1 | 0.95 | 0.09 | 39,39,39,39 | 0 |
| 58 | MG | 1Q | 205 | 1/1 | 0.95 | 0.09 | 40,40,40,40 | 0 |
| 58 | MG | 2A | 3814 | 1/1 | 0.95 | 0.07 | 42,42,42,42 | 0 |
| 58 | MG | 1A | 3481 | 1/1 | 0.95 | 0.14 | 32,32,32,32 | 0 |
| 58 | MG | 1A | 3602 | 1/1 | 0.95 | 0.12 | 48,48,48,48 | 0 |
| 58 | MG | 2A | 3446 | 1/1 | 0.95 | 0.06 | 33,33,33,33 | 0 |
| 58 | MG | 1R | 202 | 1/1 | 0.95 | 0.11 | 36,36,36,36 | 0 |
| 58 | MG | 1A | 3052 | 1/1 | 0.95 | 0.16 | 21,21,21,21 | 0 |
| 58 | MG | 1A | 3796 | 1/1 | 0.95 | 0.08 | 36,36,36,36 | 0 |
| 58 | MG | 1A | 3484 | 1/1 | 0.95 | 0.08 | 36,36,36,36 | 0 |
| 58 | MG | 1A | 3606 | 1/1 | 0.95 | 0.05 | 23,23,23,23 | 0 |
| 58 | MG | 1A | 3978 | 1/1 | 0.95 | 0.11 | 51,51,51,51 | 0 |
| 58 | MG | 1A | 3406 | 1/1 | 0.95 | 0.07 | 40,40,40,40 | 0 |
| 58 | MG | 2q | 202 | 1/1 | 0.95 | 0.10 | 49,49,49,49 | 0 |
| 58 | MG | 1A | 3807 | 1/1 | 0.95 | 0.06 | 10,10,10,10 | 0 |
| 58 | MG | 2A | 3457 | 1/1 | 0.95 | 0.21 | 50,50,50,50 | 0 |
| 58 | MG | 2A | 3458 | 1/1 | 0.95 | 0.18 | 50,50,50,50 | 0 |
| 58 | MG | 2A | 3461 | 1/1 | 0.95 | 0.21 | 32,32,32,32 | 0 |
| 58 | MG | 2v | 103 | 1/1 | 0.95 | 0.13 | 41,41,41,41 | 0 |
| 58 | MG | 1U | 203 | 1/1 | 0.95 | 0.12 | 21,21,21,21 | 0 |
| 58 | MG | 1A | 3610 | 1/1 | 0.95 | 0.06 | 23,23,23,23 | 0 |
| 58 | MG | 1U | 207 | 1/1 | 0.95 | 0.34 | 27,27,27,27 | 0 |
| 58 | MG | 2A | 3205 | 1/1 | 0.95 | 0.09 | 53,53,53,53 | 0 |
| 58 | MG | 1a | 1774 | 1/1 | 0.95 | 0.07 | 48,48,48,48 | 0 |
| 58 | MG | 2A | 3847 | 1/1 | 0.95 | 0.07 | 51,51,51,51 | 0 |
| 58 | MG | 1a | 1778 | 1/1 | 0.95 | 0.08 | 33,33,33,33 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58 | MG | 1A | 3982 | 1/1 | 0.95 | 0.05 | 45,45,45,45 | 0 |
| 58 | MG | 1A | 3812 | 1/1 | 0.95 | 0.09 | 35,35,35,35 | 0 |
| 58 | MG | 1A | 3813 | 1/1 | 0.95 | 0.05 | 34,34,34,34 | 0 |
| 58 | MG | 2A | 3854 | 1/1 | 0.95 | 0.06 | 34,34,34,34 | 0 |
| 58 | MG | 1A | 3210 | 1/1 | 0.95 | 0.07 | 29,29,29,29 | 0 |
| 58 | MG | 2A | 3857 | 1/1 | 0.95 | 0.07 | 30,30,30,30 | 0 |
| 58 | MG | 2A | 3859 | 1/1 | 0.95 | 0.04 | 46,46,46,46 | 0 |
| 58 | MG | 1A | 3083 | 1/1 | 0.95 | 0.13 | 34,34,34,34 | 0 |
| 58 | MG | 2A | 3861 | 1/1 | 0.95 | 0.14 | 60,60,60,60 | 0 |
| 58 | MG | 2A | 3862 | 1/1 | 0.95 | 0.12 | 47,47,47,47 | 0 |
| 58 | MG | 1W | 205 | 1/1 | 0.95 | 0.08 | 35,35,35,35 | 0 |
| 58 | MG | 2A | 3866 | 1/1 | 0.95 | 0.12 | 43,43,43,43 | 0 |
| 58 | MG | 1a | 1793 | 1/1 | 0.95 | 0.11 | 55,55,55,55 | 0 |
| 58 | MG | 1W | 207 | 1/1 | 0.95 | 0.14 | 14,14,14,14 | 0 |
| 58 | MG | 1A | 3613 | 1/1 | 0.95 | 0.09 | 41,41,41,41 | 0 |
| 58 | MG | 1a | 1799 | 1/1 | 0.95 | 0.07 | 62,62,62,62 | 0 |
| 58 | MG | 1a | 1801 | 1/1 | 0.95 | 0.09 | 62,62,62,62 | 0 |
| 58 | MG | 2A | 3583 | 1/1 | 0.96 | 0.07 | 20,20,20,20 | 0 |
| 58 | MG | 1A | 3079 | 1/1 | 0.96 | 0.05 | 18,18,18,18 | 0 |
| 58 | MG | 1a | 1646 | 1/1 | 0.96 | 0.10 | 60,60,60,60 | 0 |
| 58 | MG | 2A | 3587 | 1/1 | 0.96 | 0.14 | 40,40,40,40 | 0 |
| 58 | MG | 2A | 3588 | 1/1 | 0.96 | 0.12 | 49,49,49,49 | 0 |
| 58 | MG | 2A | 3040 | 1/1 | 0.96 | 0.07 | 42,42,42,42 | 0 |
| 58 | MG | 1A | 4088 | 1/1 | 0.96 | 0.10 | 34,34,34,34 | 0 |
| 58 | MG | 1A | 4089 | 1/1 | 0.96 | 0.07 | 33,33,33,33 | 0 |
| 58 | MG | 1A | 3469 | 1/1 | 0.96 | 0.15 | 27,27,27,27 | 0 |
| 58 | MG | 1A | 4091 | 1/1 | 0.96 | 0.06 | 30,30,30,30 | 0 |
| 58 | MG | 1A | 4092 | 1/1 | 0.96 | 0.07 | 31,31,31,31 | 0 |
| 58 | MG | 1A | 3320 | 1/1 | 0.96 | 0.07 | 42,42,42,42 | 0 |
| 58 | MG | 1A | 3081 | 1/1 | 0.96 | 0.09 | 23,23,23,23 | 0 |
| 58 | MG | 2A | 3602 | 1/1 | 0.96 | 0.07 | 26,26,26,26 | 0 |
| 58 | MG | 1A | 3893 | 1/1 | 0.96 | 0.07 | 32,32,32,32 | 0 |
| 58 | MG | 1A | 3733 | 1/1 | 0.96 | 0.06 | 16,16,16,16 | 0 |
| 58 | MG | 1A | 3139 | 1/1 | 0.96 | 0.15 | 22,22,22,22 | 0 |
| 58 | MG | 1A | 3011 | 1/1 | 0.96 | 0.06 | 31,31,31,31 | 0 |
| 58 | MG | 1A | 3142 | 1/1 | 0.96 | 0.19 | 38,38,38,38 | 0 |
| 58 | MG | 2A | 3055 | 1/1 | 0.96 | 0.05 | 38,38,38,38 | 0 |
| 58 | MG | 2T | 203 | 1/1 | 0.96 | 0.14 | 46,46,46,46 | 0 |
| 58 | MG | 2A | 3056 | 1/1 | 0.96 | 0.10 | 60,60,60,60 | 0 |
| 58 | MG | 1A | 3738 | 1/1 | 0.96 | 0.06 | 51,51,51,51 | 0 |
| 58 | MG | 1A | 3200 | 1/1 | 0.96 | 0.07 | 25,25,25,25 | 0 |
| 58 | MG | 1A | 3006 | 1/1 | 0.96 | 0.06 | 31,31,31,31 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58 | MG | 1a | 1667 | 1/1 | 0.96 | 0.11 | 38,38,38,38 | 0 |
| 58 | MG | 2A | 3614 | 1/1 | 0.96 | 0.06 | 18,18,18,18 | 0 |
| 58 | MG | 2A | 3062 | 1/1 | 0.96 | 0.20 | 52,52,52,52 | 0 |
| 58 | MG | 1A | 3905 | 1/1 | 0.96 | 0.10 | 33,33,33,33 | 0 |
| 58 | MG | 1A | 3262 | 1/1 | 0.96 | 0.05 | 33,33,33,33 | 0 |
| 58 | MG | 1A | 3745 | 1/1 | 0.96 | 0.12 | 24,24,24,24 | 0 |
| 58 | MG | 25 | 101 | 1/1 | 0.96 | 0.12 | 37,37,37,37 | 0 |
| 58 | MG | 1A | 3404 | 1/1 | 0.96 | 0.15 | 25,25,25,25 | 0 |
| 58 | MG | 1a | 1672 | 1/1 | 0.96 | 0.10 | 37,37,37,37 | 0 |
| 58 | MG | 1A | 3590 | 1/1 | 0.96 | 0.08 | 41,41,41,41 | 0 |
| 58 | MG | 1A | 3749 | 1/1 | 0.96 | 0.07 | 47,47,47,47 | 0 |
| 58 | MG | 27 | 101 | 1/1 | 0.96 | 0.13 | 28,28,28,28 | 0 |
| 58 | MG | 1A | 3147 | 1/1 | 0.96 | 0.12 | 37,37,37,37 | 0 |
| 58 | MG | 1A | 3593 | 1/1 | 0.96 | 0.24 | 27,27,27,27 | 0 |
| 58 | MG | 1A | 3482 | 1/1 | 0.96 | 0.08 | 40,40,40,40 | 0 |
| 58 | MG | 1A | 3264 | 1/1 | 0.96 | 0.10 | 36,36,36,36 | 0 |
| 58 | MG | 1A | 3597 | 1/1 | 0.96 | 0.11 | 38,38,38,38 | 0 |
| 58 | MG | 1A | 3016 | 1/1 | 0.96 | 0.07 | 34,34,34,34 | 0 |
| 58 | MG | 1A | 3926 | 1/1 | 0.96 | 0.09 | 36,36,36,36 | 0 |
| 58 | MG | 2A | 3080 | 1/1 | 0.96 | 0.09 | 41,41,41,41 | 0 |
| 58 | MG | 2A | 3081 | 1/1 | 0.96 | 0.14 | 35,35,35,35 | 0 |
| 58 | MG | 1A | 3758 | 1/1 | 0.96 | 0.09 | 51,51,51,51 | 0 |
| 58 | MG | 1A | 3336 | 1/1 | 0.96 | 0.17 | 38,38,38,38 | 0 |
| 58 | MG | 2A | 3085 | 1/1 | 0.96 | 0.16 | 40,40,40,40 | 0 |
| 58 | MG | 1A | 3206 | 1/1 | 0.96 | 0.09 | 42,42,42,42 | 0 |
| 58 | MG | 2A | 3087 | 1/1 | 0.96 | 0.05 | 36,36,36,36 | 0 |
| 58 | MG | 1A | 3930 | 1/1 | 0.96 | 0.06 | 35,35,35,35 | 0 |
| 58 | MG | 1A | 3411 | 1/1 | 0.96 | 0.11 | 49,49,49,49 | 0 |
| 58 | MG | 2A | 3651 | 1/1 | 0.96 | 0.22 | 37,37,37,37 | 0 |
| 58 | MG | 2A | 3652 | 1/1 | 0.96 | 0.07 | 32,32,32,32 | 0 |
| 58 | MG | 2A | 3653 | 1/1 | 0.96 | 0.10 | 44,44,44,44 | 0 |
| 58 | MG | 1A | 3338 | 1/1 | 0.96 | 0.19 | 42,42,42,42 | 0 |
| 58 | MG | 1B | 231 | 1/1 | 0.96 | 0.08 | 57,57,57,57 | 0 |
| 58 | MG | 2A | 3345 | 1/1 | 0.96 | 0.05 | 35,35,35,35 | 0 |
| 58 | MG | 2A | 3092 | 1/1 | 0.96 | 0.30 | 36,36,36,36 | 0 |
| 58 | MG | 1A | 3207 | 1/1 | 0.96 | 0.07 | 13,13,13,13 | 0 |
| 58 | MG | 1A | 3934 | 1/1 | 0.96 | 0.04 | 5,5,5,5 | 0 |
| 58 | MG | 1A | 3935 | 1/1 | 0.96 | 0.05 | 21,21,21,21 | 0 |
| 58 | MG | 2A | 3099 | 1/1 | 0.96 | 0.16 | 44,44,44,44 | 0 |
| 58 | MG | 1A | 3940 | 1/1 | 0.96 | 0.07 | 41,41,41,41 | 0 |
| 58 | MG | 1D | 307 | 1/1 | 0.96 | 0.08 | 23,23,23,23 | 0 |
| 58 | MG | 1A | 3766 | 1/1 | 0.96 | 0.05 | 22,22,22,22 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58 | MG | 1A | 3767 | 1/1 | 0.96 | 0.06 | 25,25,25,25 | 0 |
| 58 | MG | 2a | 1627 | 1/1 | 0.96 | 0.20 | 54,54,54,54 | 0 |
| 58 | MG | 1A | 3768 | 1/1 | 0.96 | 0.07 | 18,18,18,18 | 0 |
| 58 | MG | 1A | 3108 | 1/1 | 0.96 | 0.06 | 23,23,23,23 | 0 |
| 58 | MG | 1A | 3947 | 1/1 | 0.96 | 0.11 | 37,37,37,37 | 0 |
| 58 | MG | 1E | 308 | 1/1 | 0.96 | 0.09 | 43,43,43,43 | 0 |
| 58 | MG | 2A | 3109 | 1/1 | 0.96 | 0.10 | 32,32,32,32 | 0 |
| 58 | MG | 1A | 3159 | 1/1 | 0.96 | 0.33 | 31,31,31,31 | 0 |
| 58 | MG | 1A | 3161 | 1/1 | 0.96 | 0.04 | 43,43,43,43 | 0 |
| 58 | MG | 1A | 3952 | 1/1 | 0.96 | 0.05 | 53,53,53,53 | 0 |
| 58 | MG | 1A | 3775 | 1/1 | 0.96 | 0.06 | 23,23,23,23 | 0 |
| 58 | MG | 1A | 3347 | 1/1 | 0.96 | 0.12 | 26,26,26,26 | 0 |
| 58 | MG | 2a | 1638 | 1/1 | 0.96 | 0.13 | 53,53,53,53 | 0 |
| 58 | MG | 1A | 3782 | 1/1 | 0.96 | 0.07 | 22,22,22,22 | 0 |
| 58 | MG | 2A | 3367 | 1/1 | 0.96 | 0.15 | 41,41,41,41 | 0 |
| 58 | MG | 1A | 3498 | 1/1 | 0.96 | 0.11 | 37,37,37,37 | 0 |
| 58 | MG | 2A | 3685 | 1/1 | 0.96 | 0.10 | 36,36,36,36 | 0 |
| 58 | MG | 1A | 3162 | 1/1 | 0.96 | 0.16 | 20,20,20,20 | 0 |
| 58 | MG | 1A | 3500 | 1/1 | 0.96 | 0.08 | 31,31,31,31 | 0 |
| 58 | MG | 1A | 3791 | 1/1 | 0.96 | 0.05 | 35,35,35,35 | 0 |
| 58 | MG | 1G | 201 | 1/1 | 0.96 | 0.10 | 30,30,30,30 | 0 |
| 58 | MG | 1G | 202 | 1/1 | 0.96 | 0.15 | 43,43,43,43 | 0 |
| 58 | MG | 1A | 3963 | 1/1 | 0.96 | 0.06 | 39,39,39,39 | 0 |
| 58 | MG | 1A | 3616 | 1/1 | 0.96 | 0.16 | 37,37,37,37 | 0 |
| 58 | MG | 1A | 3618 | 1/1 | 0.96 | 0.05 | 26,26,26,26 | 0 |
| 58 | MG | 2A | 3379 | 1/1 | 0.96 | 0.06 | 38,38,38,38 | 0 |
| 58 | MG | 1I | 201 | 1/1 | 0.96 | 0.05 | 48,48,48,48 | 0 |
| 58 | MG | 1A | 3214 | 1/1 | 0.96 | 0.14 | 34,34,34,34 | 0 |
| 58 | MG | 1N | 202 | 1/1 | 0.96 | 0.12 | 31,31,31,31 | 0 |
| 58 | MG | 1a | 1725 | 1/1 | 0.96 | 0.11 | 54,54,54,54 | 0 |
| 58 | MG | 1A | 3800 | 1/1 | 0.96 | 0.06 | 11,11,11,11 | 0 |
| 58 | MG | 2A | 3142 | 1/1 | 0.96 | 0.12 | 40,40,40,40 | 0 |
| 58 | MG | 1A | 3802 | 1/1 | 0.96 | 0.11 | 30,30,30,30 | 0 |
| 58 | MG | 1N | 207 | 1/1 | 0.96 | 0.09 | 40,40,40,40 | 0 |
| 58 | MG | 2A | 3706 | 1/1 | 0.96 | 0.07 | 49,49,49,49 | 0 |
| 58 | MG | 2A | 3389 | 1/1 | 0.96 | 0.07 | 36,36,36,36 | 0 |
| 58 | MG | 1a | 1732 | 1/1 | 0.96 | 0.07 | 30,30,30,30 | 0 |
| 58 | MG | 1A | 3503 | 1/1 | 0.96 | 0.05 | 38,38,38,38 | 0 |
| 58 | MG | 1O | 202 | 1/1 | 0.96 | 0.10 | 42,42,42,42 | 0 |
| 58 | MG | 1A | 3974 | 1/1 | 0.96 | 0.10 | 36,36,36,36 | 0 |
| 58 | MG | 1A | 3975 | 1/1 | 0.96 | 0.05 | 41,41,41,41 | 0 |
| 58 | MG | 2A | 3715 | 1/1 | 0.96 | 0.07 | 20,20,20,20 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58 | MG | 1A | 3504 | 1/1 | 0.96 | 0.14 | 31,31,31,31 | 0 |
| 58 | MG | 2A | 3396 | 1/1 | 0.96 | 0.16 | 50,50,50,50 | 0 |
| 58 | MG | 1A | 3350 | 1/1 | 0.96 | 0.13 | 33,33,33,33 | 0 |
| 58 | MG | 1P | 203 | 1/1 | 0.96 | 0.28 | 24,24,24,24 | 0 |
| 58 | MG | 2a | 1681 | 1/1 | 0.96 | 0.06 | 41,41,41,41 | 0 |
| 58 | MG | 1Q | 204 | 1/1 | 0.96 | 0.07 | 43,43,43,43 | 0 |
| 58 | MG | 1A | 3806 | 1/1 | 0.96 | 0.04 | 13,13,13,13 | 0 |
| 58 | MG | 2A | 3159 | 1/1 | 0.96 | 0.12 | 42,42,42,42 | 0 |
| 58 | MG | 1a | 1744 | 1/1 | 0.96 | 0.06 | 38,38,38,38 | 0 |
| 58 | MG | 1A | 3626 | 1/1 | 0.96 | 0.04 | 29,29,29,29 | 0 |
| 58 | MG | 1A | 3221 | 1/1 | 0.96 | 0.07 | 40,40,40,40 | 0 |
| 58 | MG | 1A | 3630 | 1/1 | 0.96 | 0.07 | 39,39,39,39 | 0 |
| 58 | MG | 1A | 3636 | 1/1 | 0.96 | 0.11 | 44,44,44,44 | 0 |
| 58 | MG | 1A | 3427 | 1/1 | 0.96 | 0.07 | 40,40,40,40 | 0 |
| 58 | MG | 1A | 3355 | 1/1 | 0.96 | 0.18 | 29,29,29,29 | 0 |
| 58 | MG | 1A | 3165 | 1/1 | 0.96 | 0.25 | 26,26,26,26 | 0 |
| 58 | MG | 2a | 1694 | 1/1 | 0.96 | 0.25 | 35,35,35,35 | 0 |
| 58 | MG | 1a | 1755 | 1/1 | 0.96 | 0.08 | 38,38,38,38 | 0 |
| 58 | MG | 1A | 3818 | 1/1 | 0.96 | 0.08 | 22,22,22,22 | 0 |
| 58 | MG | 1A | 3067 | 1/1 | 0.96 | 0.09 | 30,30,30,30 | 0 |
| 58 | MG | 1A | 3281 | 1/1 | 0.96 | 0.08 | 25,25,25,25 | 0 |
| 58 | MG | 1A | 3432 | 1/1 | 0.96 | 0.07 | 32,32,32,32 | 0 |
| 58 | MG | 2A | 3418 | 1/1 | 0.96 | 0.16 | 34,34,34,34 | 0 |
| 58 | MG | 1A | 3647 | 1/1 | 0.96 | 0.06 | 24,24,24,24 | 0 |
| 58 | MG | 1U | 205 | 1/1 | 0.96 | 0.20 | 27,27,27,27 | 0 |
| 58 | MG | 1A | 3283 | 1/1 | 0.96 | 0.13 | 22,22,22,22 | 0 |
| 58 | MG | 2A | 3423 | 1/1 | 0.96 | 0.20 | 52,52,52,52 | 0 |
| 58 | MG | 1A | 3289 | 1/1 | 0.96 | 0.09 | 37,37,37,37 | 0 |
| 58 | MG | 1a | 1767 | 1/1 | 0.96 | 0.14 | 60,60,60,60 | 0 |
| 58 | MG | 2a | 1709 | 1/1 | 0.96 | 0.07 | 50,50,50,50 | 0 |
| 58 | MG | 2A | 3428 | 1/1 | 0.96 | 0.15 | 41,41,41,41 | 0 |
| 58 | MG | 2a | 1711 | 1/1 | 0.96 | 0.07 | 45,45,45,45 | 0 |
| 58 | MG | 1A | 3521 | 1/1 | 0.96 | 0.15 | 27,27,27,27 | 0 |
| 58 | MG | 1V | 203 | 1/1 | 0.96 | 0.18 | 24,24,24,24 | 0 |
| 58 | MG | 1A | 3999 | 1/1 | 0.96 | 0.07 | 35,35,35,35 | 0 |
| 58 | MG | 1A | 3655 | 1/1 | 0.96 | 0.06 | 22,22,22,22 | 0 |
| 58 | MG | 1A | 4002 | 1/1 | 0.96 | 0.08 | 48,48,48,48 | 0 |
| 58 | MG | 1A | 3436 | 1/1 | 0.96 | 0.06 | 35,35,35,35 | 0 |
| 58 | MG | 1A | 4004 | 1/1 | 0.96 | 0.05 | 9,9,9,9 | 0 |
| 58 | MG | 1A | 3290 | 1/1 | 0.96 | 0.10 | 26,26,26,26 | 0 |
| 58 | MG | 2A | 3764 | 1/1 | 0.96 | 0.05 | 46,46,46,46 | 0 |
| 58 | MG | 2A | 3193 | 1/1 | 0.96 | 0.08 | 46,46,46,46 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58 | MG | 1a | 1783 | 1/1 | 0.96 | 0.05 | 36,36,36,36 | 0 |
| 58 | MG | 2a | 1723 | 1/1 | 0.96 | 0.07 | 38,38,38,38 | 0 |
| 58 | MG | 1A | 3832 | 1/1 | 0.96 | 0.10 | 31,31,31,31 | 0 |
| 58 | MG | 2A | 3196 | 1/1 | 0.96 | 0.10 | 48,48,48,48 | 0 |
| 58 | MG | 2A | 3197 | 1/1 | 0.96 | 0.26 | 43,43,43,43 | 0 |
| 58 | MG | 1X | 103 | 1/1 | 0.96 | 0.16 | 29,29,29,29 | 0 |
| 58 | MG | 1A | 3525 | 1/1 | 0.96 | 0.07 | 35,35,35,35 | 0 |
| 58 | MG | 2A | 3774 | 1/1 | 0.96 | 0.07 | 50,50,50,50 | 0 |
| 58 | MG | 1A | 3090 | 1/1 | 0.96 | 0.13 | 43,43,43,43 | 0 |
| 58 | MG | 1a | 1795 | 1/1 | 0.96 | 0.13 | 67,67,67,67 | 0 |
| 58 | MG | 1A | 4011 | 1/1 | 0.96 | 0.11 | 31,31,31,31 | 0 |
| 58 | MG | 2a | 1735 | 1/1 | 0.96 | 0.20 | 48,48,48,48 | 0 |
| 58 | MG | 1A | 3663 | 1/1 | 0.96 | 0.06 | 19,19,19,19 | 0 |
| 58 | MG | 1A | 4013 | 1/1 | 0.96 | 0.05 | 17,17,17,17 | 0 |
| 58 | MG | 1Z | 3702 | 1/1 | 0.96 | 0.07 | 34,34,34,34 | 0 |
| 58 | MG | 1A | 4015 | 1/1 | 0.96 | 0.07 | 20,20,20,20 | 0 |
| 58 | MG | 2A | 3783 | 1/1 | 0.96 | 0.06 | 61,61,61,61 | 0 |
| 58 | MG | 2A | 3784 | 1/1 | 0.96 | 0.16 | 46,46,46,46 | 0 |
| 58 | MG | 1a | 1803 | 1/1 | 0.96 | 0.06 | 37,37,37,37 | 0 |
| 58 | MG | 10 | 104 | 1/1 | 0.96 | 0.15 | 39,39,39,39 | 0 |
| 58 | MG | 2a | 1744 | 1/1 | 0.96 | 0.23 | 48,48,48,48 | 0 |
| 58 | MG | 1a | 1806 | 1/1 | 0.96 | 0.14 | 35,35,35,35 | 0 |
| 58 | MG | 1A | 3439 | 1/1 | 0.96 | 0.24 | 28,28,28,28 | 0 |
| 58 | MG | 1A | 3528 | 1/1 | 0.96 | 0.10 | 66,66,66,66 | 0 |
| 58 | MG | 2A | 3791 | 1/1 | 0.96 | 0.07 | 21,21,21,21 | 0 |
| 58 | MG | 1A | 3054 | 1/1 | 0.96 | 0.06 | 38,38,38,38 | 0 |
| 58 | MG | 2A | 3459 | 1/1 | 0.96 | 0.07 | 32,32,32,32 | 0 |
| 58 | MG | 2A | 3460 | 1/1 | 0.96 | 0.10 | 47,47,47,47 | 0 |
| 58 | MG | 2A | 3795 | 1/1 | 0.96 | 0.05 | 32,32,32,32 | 0 |
| 58 | MG | 1A | 3294 | 1/1 | 0.96 | 0.06 | 45,45,45,45 | 0 |
| 58 | MG | 1A | 3366 | 1/1 | 0.96 | 0.08 | 39,39,39,39 | 0 |
| 58 | MG | 11 | 102 | 1/1 | 0.96 | 0.07 | 36,36,36,36 | 0 |
| 58 | MG | 1A | 3232 | 1/1 | 0.96 | 0.19 | 25,25,25,25 | 0 |
| 58 | MG | 1A | 3057 | 1/1 | 0.96 | 0.07 | 31,31,31,31 | 0 |
| 58 | MG | 1A | 3843 | 1/1 | 0.96 | 0.05 | 31,31,31,31 | 0 |
| 58 | MG | 12 | 101 | 1/1 | 0.96 | 0.06 | 43,43,43,43 | 0 |
| 58 | MG | 2A | 3469 | 1/1 | 0.96 | 0.23 | 36,36,36,36 | 0 |
| 58 | MG | 2a | 1765 | 1/1 | 0.96 | 0.06 | 55,55,55,55 | 0 |
| 58 | MG | 12 | 102 | 1/1 | 0.96 | 0.10 | 33,33,33,33 | 0 |
| 58 | MG | 2A | 3471 | 1/1 | 0.96 | 0.12 | 45,45,45,45 | 0 |
| 58 | MG | 2A | 3807 | 1/1 | 0.96 | 0.12 | 49,49,49,49 | 0 |
| 58 | MG | 1A | 3299 | 1/1 | 0.96 | 0.06 | 43,43,43,43 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58 | MG | 1d | 301 | 1/1 | 0.96 | 0.28 | 49,49,49,49 | 0 |
| 58 | MG | 1A | 4028 | 1/1 | 0.96 | 0.08 | 48,48,48,48 | 0 |
| 58 | MG | 15 | 105 | 1/1 | 0.96 | 0.26 | 41,41,41,41 | 0 |
| 58 | MG | 1f | 201 | 1/1 | 0.96 | 0.15 | 34,34,34,34 | 0 |
| 58 | MG | 1A | 4029 | 1/1 | 0.96 | 0.06 | 33,33,33,33 | 0 |
| 58 | MG | 1A | 4030 | 1/1 | 0.96 | 0.07 | 62,62,62,62 | 0 |
| 58 | MG | 2A | 3816 | 1/1 | 0.96 | 0.04 | 41,41,41,41 | 0 |
| 58 | MG | 1A | 3845 | 1/1 | 0.96 | 0.08 | 27,27,27,27 | 0 |
| 58 | MG | 2A | 3818 | 1/1 | 0.96 | 0.08 | 44,44,44,44 | 0 |
| 58 | MG | 1A | 3446 | 1/1 | 0.96 | 0.15 | 26,26,26,26 | 0 |
| 58 | MG | 2A | 3232 | 1/1 | 0.96 | 0.09 | 39,39,39,39 | 0 |
| 58 | MG | 2a | 1791 | 1/1 | 0.96 | 0.14 | 47,47,47,47 | 0 |
| 58 | MG | 1A | 3118 | 1/1 | 0.96 | 0.27 | 31,31,31,31 | 0 |
| 58 | MG | 2A | 3235 | 1/1 | 0.96 | 0.15 | 41,41,41,41 | 0 |
| 58 | MG | 1A | 3686 | 1/1 | 0.96 | 0.08 | 27,27,27,27 | 0 |
| 58 | MG | 1p | 101 | 1/1 | 0.96 | 0.10 | 54,54,54,54 | 0 |
| 58 | MG | 2a | 1797 | 1/1 | 0.96 | 0.06 | 55,55,55,55 | 0 |
| 58 | MG | 2A | 3828 | 1/1 | 0.96 | 0.10 | 45,45,45,45 | 0 |
| 58 | MG | 2A | 3829 | 1/1 | 0.96 | 0.07 | 28,28,28,28 | 0 |
| 58 | MG | 1A | 3538 | 1/1 | 0.96 | 0.19 | 35,35,35,35 | 0 |
| 58 | MG | 2A | 3834 | 1/1 | 0.96 | 0.08 | 45,45,45,45 | 0 |
| 58 | MG | 19 | 101 | 1/1 | 0.96 | 0.10 | 38,38,38,38 | 0 |
| 58 | MG | 1A | 3691 | 1/1 | 0.96 | 0.09 | 29,29,29,29 | 0 |
| 58 | MG | 1A | 3093 | 1/1 | 0.96 | 0.07 | 42,42,42,42 | 0 |
| 58 | MG | 1a | 1603 | 1/1 | 0.96 | 0.07 | 38,38,38,38 | 0 |
| 58 | MG | 2A | 3495 | 1/1 | 0.96 | 0.11 | 29,29,29,29 | 0 |
| 58 | MG | 1A | 3372 | 1/1 | 0.96 | 0.09 | 45,45,45,45 | 0 |
| 58 | MG | 1A | 3451 | 1/1 | 0.96 | 0.19 | 33,33,33,33 | 0 |
| 58 | MG | 1A | 3698 | 1/1 | 0.96 | 0.10 | 34,34,34,34 | 0 |
| 58 | MG | 2A | 3247 | 1/1 | 0.96 | 0.09 | 47,47,47,47 | 0 |
| 58 | MG | 1A | 3094 | 1/1 | 0.96 | 0.07 | 17,17,17,17 | 0 |
| 58 | MG | 1A | 4047 | 1/1 | 0.96 | 0.04 | 27,27,27,27 | 0 |
| 58 | MG | 2a | 1814 | 1/1 | 0.96 | 0.06 | 46,46,46,46 | 0 |
| 58 | MG | 1A | 3123 | 1/1 | 0.96 | 0.20 | 37,37,37,37 | 0 |
| 58 | MG | 2A | 3507 | 1/1 | 0.96 | 0.07 | 50,50,50,50 | 0 |
| 58 | MG | 1a | 1611 | 1/1 | 0.96 | 0.07 | 34,34,34,34 | 0 |
| 58 | MG | 1A | 3704 | 1/1 | 0.96 | 0.05 | 14,14,14,14 | 0 |
| 58 | MG | 2a | 1819 | 1/1 | 0.96 | 0.14 | 51,51,51,51 | 0 |
| 58 | MG | 2A | 3510 | 1/1 | 0.96 | 0.09 | 22,22,22,22 | 0 |
| 58 | MG | 2a | 1821 | 1/1 | 0.96 | 0.06 | 58,58,58,58 | 0 |
| 58 | MG | 2A | 3254 | 1/1 | 0.96 | 0.08 | 45,45,45,45 | 0 |
| 58 | MG | 1A | 3707 | 1/1 | 0.96 | 0.06 | 18,18,18,18 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58 | MG | 2A | 3858 | 1/1 | 0.96 | 0.13 | 43,43,43,43 | 0 |
| 58 | MG | 1A | 3708 | 1/1 | 0.96 | 0.10 | 19,19,19,19 | 0 |
| 58 | MG | 1A | 3866 | 1/1 | 0.96 | 0.05 | 34,34,34,34 | 0 |
| 58 | MG | 2A | 3518 | 1/1 | 0.96 | 0.07 | 31,31,31,31 | 0 |
| 58 | MG | 1A | 4054 | 1/1 | 0.96 | 0.07 | 34,34,34,34 | 0 |
| 58 | MG | 1A | 3545 | 1/1 | 0.96 | 0.12 | 27,27,27,27 | 0 |
| 58 | MG | 2A | 3864 | 1/1 | 0.96 | 0.08 | 45,45,45,45 | 0 |
| 58 | MG | 2a | 1832 | 1/1 | 0.96 | 0.16 | 44,44,44,44 | 0 |
| 58 | MG | 2A | 3865 | 1/1 | 0.96 | 0.08 | 40,40,40,40 | 0 |
| 58 | MG | 1x | 112 | 1/1 | 0.96 | 0.15 | 39,39,39,39 | 0 |
| 58 | MG | 1x | 113 | 1/1 | 0.96 | 0.17 | 45,45,45,45 | 0 |
| 58 | MG | 1A | 3240 | 1/1 | 0.96 | 0.11 | 22,22,22,22 | 0 |
| 58 | MG | 1a | 1620 | 1/1 | 0.96 | 0.06 | 38,38,38,38 | 0 |
| 58 | MG | 2A | 3528 | 1/1 | 0.96 | 0.06 | 47,47,47,47 | 0 |
| 58 | MG | 1A | 3310 | 1/1 | 0.96 | 0.07 | 25,25,25,25 | 0 |
| 58 | MG | 2A | 3531 | 1/1 | 0.96 | 0.06 | 22,22,22,22 | 0 |
| 58 | MG | 2A | 3873 | 1/1 | 0.96 | 0.06 | 37,37,37,37 | 0 |
| 58 | MG | 2A | 3533 | 1/1 | 0.96 | 0.10 | 46,46,46,46 | 0 |
| 58 | MG | 2A | 3004 | 1/1 | 0.96 | 0.14 | 41,41,41,41 | 0 |
| 58 | MG | 1A | 3246 | 1/1 | 0.96 | 0.22 | 31,31,31,31 | 0 |
| 58 | MG | 2i | 201 | 1/1 | 0.96 | 0.05 | 41,41,41,41 | 0 |
| 58 | MG | 2A | 3006 | 1/1 | 0.96 | 0.10 | 51,51,51,51 | 0 |
| 58 | MG | 1A | 3059 | 1/1 | 0.96 | 0.06 | 32,32,32,32 | 0 |
| 58 | MG | 1A | 3183 | 1/1 | 0.96 | 0.10 | 29,29,29,29 | 0 |
| 58 | MG | 2l | 203 | 1/1 | 0.96 | 0.06 | 42,42,42,42 | 0 |
| 58 | MG | 1A | 3028 | 1/1 | 0.96 | 0.17 | 15,15,15,15 | 0 |
| 58 | MG | 2A | 3274 | 1/1 | 0.96 | 0.06 | 38,38,38,38 | 0 |
| 58 | MG | 2A | 3011 | 1/1 | 0.96 | 0.06 | 36,36,36,36 | 0 |
| 58 | MG | 2q | 201 | 1/1 | 0.96 | 0.06 | 55,55,55,55 | 0 |
| 58 | MG | 2A | 3012 | 1/1 | 0.96 | 0.05 | 30,30,30,30 | 0 |
| 58 | MG | 2A | 3014 | 1/1 | 0.96 | 0.06 | 30,30,30,30 | 0 |
| 58 | MG | 2A | 3546 | 1/1 | 0.96 | 0.05 | 32,32,32,32 | 0 |
| 58 | MG | 1A | 3132 | 1/1 | 0.96 | 0.04 | 25,25,25,25 | 0 |
| 58 | MG | 1a | 1629 | 1/1 | 0.96 | 0.30 | 45,45,45,45 | 0 |
| 58 | MG | 1A | 3134 | 1/1 | 0.96 | 0.09 | 25,25,25,25 | 0 |
| 58 | MG | 1a | 1631 | 1/1 | 0.96 | 0.15 | 42,42,42,42 | 0 |
| 58 | MG | 2A | 3282 | 1/1 | 0.96 | 0.16 | 46,46,46,46 | 0 |
| 58 | MG | 1A | 3317 | 1/1 | 0.96 | 0.10 | 40,40,40,40 | 0 |
| 58 | MG | 1A | 3318 | 1/1 | 0.96 | 0.17 | 43,43,43,43 | 0 |
| 58 | MG | 1A | 3882 | 1/1 | 0.96 | 0.11 | 23,23,23,23 | 0 |
| 58 | MG | 2A | 3025 | 1/1 | 0.96 | 0.07 | 35,35,35,35 | 0 |
| 58 | MG | 2B | 213 | 1/1 | 0.96 | 0.04 | 40,40,40,40 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58 | MG | 2A | 3288 | 1/1 | 0.96 | 0.18 | 54,54,54,54 | 0 |
| 58 | MG | 2B | 216 | 1/1 | 0.96 | 0.14 | 54,54,54,54 | 0 |
| 58 | MG | 2A | 3566 | 1/1 | 0.96 | 0.04 | 38,38,38,38 | 0 |
| 58 | MG | 2A | 3026 | 1/1 | 0.96 | 0.11 | 36,36,36,36 | 0 |
| 58 | MG | 1A | 3467 | 1/1 | 0.96 | 0.06 | 51,51,51,51 | 0 |
| 58 | MG | 1A | 3884 | 1/1 | 0.96 | 0.05 | 28,28,28,28 | 0 |
| 58 | MG | 2A | 3573 | 1/1 | 0.96 | 0.14 | 52,52,52,52 | 0 |
| 58 | MG | 2A | 3574 | 1/1 | 0.96 | 0.05 | 37,37,37,37 | 0 |
| 58 | MG | 1A | 4081 | 1/1 | 0.96 | 0.09 | 31,31,31,31 | 0 |
| 58 | MG | 1A | 3562 | 1/1 | 0.96 | 0.18 | 18,18,18,18 | 0 |
| 58 | MG | 2A | 3577 | 1/1 | 0.96 | 0.10 | 36,36,36,36 | 0 |
| 58 | MG | 2A | 3578 | 1/1 | 0.96 | 0.08 | 26,26,26,26 | 0 |
| 58 | MG | 2E | 304 | 1/1 | 0.96 | 0.14 | 39,39,39,39 | 0 |
| 58 | MG | 2A | 3033 | 1/1 | 0.96 | 0.12 | 32,32,32,32 | 0 |
| 58 | MG | 2E | 307 | 1/1 | 0.96 | 0.07 | 29,29,29,29 | 0 |
| 58 | MG | 1A | 3887 | 1/1 | 0.96 | 0.05 | 11,11,11,11 | 0 |
| 58 | MG | 2A | 3296 | 1/1 | 0.96 | 0.11 | 54,54,54,54 | 0 |
| 58 | MG | 1N | 205 | 1/1 | 0.97 | 0.27 | 41,41,41,41 | 0 |
| 58 | MG | 1A | 3683 | 1/1 | 0.97 | 0.04 | 16,16,16,16 | 0 |
| 58 | MG | 2A | 3631 | 1/1 | 0.97 | 0.07 | 39,39,39,39 | 0 |
| 58 | MG | 2A | 3632 | 1/1 | 0.97 | 0.07 | 26,26,26,26 | 0 |
| 58 | MG | 1A | 3465 | 1/1 | 0.97 | 0.06 | 34,34,34,34 | 0 |
| 58 | MG | 1A | 3994 | 1/1 | 0.97 | 0.05 | 16,16,16,16 | 0 |
| 58 | MG | 1a | 1717 | 1/1 | 0.97 | 0.14 | 40,40,40,40 | 0 |
| 58 | MG | 1a | 1718 | 1/1 | 0.97 | 0.14 | 32,32,32,32 | 0 |
| 58 | MG | 2A | 3638 | 1/1 | 0.97 | 0.04 | 27,27,27,27 | 0 |
| 58 | MG | 2A | 3639 | 1/1 | 0.97 | 0.06 | 44,44,44,44 | 0 |
| 58 | MG | 1A | 3258 | 1/1 | 0.97 | 0.09 | 21,21,21,21 | 0 |
| 58 | MG | 1A | 3390 | 1/1 | 0.97 | 0.10 | 42,42,42,42 | 0 |
| 58 | MG | 2A | 3643 | 1/1 | 0.97 | 0.07 | 20,20,20,20 | 0 |
| 58 | MG | 1A | 3104 | 1/1 | 0.97 | 0.07 | 15,15,15,15 | 0 |
| 58 | MG | 2A | 3115 | 1/1 | 0.97 | 0.11 | 36,36,36,36 | 0 |
| 58 | MG | 1a | 1724 | 1/1 | 0.97 | 0.12 | 49,49,49,49 | 0 |
| 58 | MG | 1A | 3041 | 1/1 | 0.97 | 0.05 | 22,22,22,22 | 0 |
| 58 | MG | 1A | 3394 | 1/1 | 0.97 | 0.13 | 16,16,16,16 | 0 |
| 58 | MG | 2A | 3121 | 1/1 | 0.97 | 0.17 | 39,39,39,39 | 0 |
| 58 | MG | 1a | 1727 | 1/1 | 0.97 | 0.05 | 44,44,44,44 | 0 |
| 58 | MG | 1P | 202 | 1/1 | 0.97 | 0.23 | 20,20,20,20 | 0 |
| 58 | MG | 1A | 3471 | 1/1 | 0.97 | 0.38 | 35,35,35,35 | 0 |
| 58 | MG | 1Q | 201 | 1/1 | 0.97 | 0.08 | 29,29,29,29 | 0 |
| 58 | MG | 1Q | 203 | 1/1 | 0.97 | 0.09 | 26,26,26,26 | 0 |
| 58 | MG | 2A | 3368 | 1/1 | 0.97 | 0.07 | 43,43,43,43 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58 | MG | 28 | 102 | 1/1 | 0.97 | 0.13 | 39,39,39,39 | 0 |
| 58 | MG | 2A | 3129 | 1/1 | 0.97 | 0.15 | 47,47,47,47 | 0 |
| 58 | MG | 2A | 3130 | 1/1 | 0.97 | 0.11 | 38,38,38,38 | 0 |
| 58 | MG | 1A | 4001 | 1/1 | 0.97 | 0.04 | 31,31,31,31 | 0 |
| 58 | MG | 1A | 3697 | 1/1 | 0.97 | 0.07 | 35,35,35,35 | 0 |
| 58 | MG | 2A | 3661 | 1/1 | 0.97 | 0.06 | 47,47,47,47 | 0 |
| 58 | MG | 1a | 1736 | 1/1 | 0.97 | 0.07 | 46,46,46,46 | 0 |
| 58 | MG | 1Q | 206 | 1/1 | 0.97 | 0.09 | 45,45,45,45 | 0 |
| 58 | MG | 1A | 3472 | 1/1 | 0.97 | 0.12 | 33,33,33,33 | 0 |
| 58 | MG | 1A | 3556 | 1/1 | 0.97 | 0.09 | 48,48,48,48 | 0 |
| 58 | MG | 2A | 3138 | 1/1 | 0.97 | 0.21 | 34,34,34,34 | 0 |
| 58 | MG | 2A | 3667 | 1/1 | 0.97 | 0.04 | 25,25,25,25 | 0 |
| 58 | MG | 1A | 3701 | 1/1 | 0.97 | 0.06 | 12,12,12,12 | 0 |
| 58 | MG | 2A | 3141 | 1/1 | 0.97 | 0.16 | 31,31,31,31 | 0 |
| 58 | MG | 2A | 3381 | 1/1 | 0.97 | 0.17 | 31,31,31,31 | 0 |
| 58 | MG | 1R | 203 | 1/1 | 0.97 | 0.16 | 27,27,27,27 | 0 |
| 58 | MG | 2A | 3673 | 1/1 | 0.97 | 0.06 | 37,37,37,37 | 0 |
| 58 | MG | 1R | 204 | 1/1 | 0.97 | 0.16 | 29,29,29,29 | 0 |
| 58 | MG | 1A | 4006 | 1/1 | 0.97 | 0.05 | 13,13,13,13 | 0 |
| 58 | MG | 1A | 3323 | 1/1 | 0.97 | 0.14 | 23,23,23,23 | 0 |
| 58 | MG | 1A | 3703 | 1/1 | 0.97 | 0.08 | 19,19,19,19 | 0 |
| 58 | MG | 1A | 3849 | 1/1 | 0.97 | 0.07 | 41,41,41,41 | 0 |
| 58 | MG | 1A | 3558 | 1/1 | 0.97 | 0.12 | 26,26,26,26 | 0 |
| 58 | MG | 2A | 3150 | 1/1 | 0.97 | 0.05 | 27,27,27,27 | 0 |
| 58 | MG | 1A | 3851 | 1/1 | 0.97 | 0.05 | 40,40,40,40 | 0 |
| 58 | MG | 2a | 1622 | 1/1 | 0.97 | 0.06 | 60,60,60,60 | 0 |
| 58 | MG | 1A | 3324 | 1/1 | 0.97 | 0.07 | 50,50,50,50 | 0 |
| 58 | MG | 2A | 3684 | 1/1 | 0.97 | 0.08 | 32,32,32,32 | 0 |
| 58 | MG | 2A | 3153 | 1/1 | 0.97 | 0.16 | 53,53,53,53 | 0 |
| 58 | MG | 1A | 3261 | 1/1 | 0.97 | 0.12 | 16,16,16,16 | 0 |
| 58 | MG | 1A | 3107 | 1/1 | 0.97 | 0.11 | 23,23,23,23 | 0 |
| 58 | MG | 2A | 3156 | 1/1 | 0.97 | 0.04 | 43,43,43,43 | 0 |
| 58 | MG | 2A | 3689 | 1/1 | 0.97 | 0.07 | 46,46,46,46 | 0 |
| 58 | MG | 1A | 3565 | 1/1 | 0.97 | 0.14 | 23,23,23,23 | 0 |
| 58 | MG | 1A | 4019 | 1/1 | 0.97 | 0.04 | 30,30,30,30 | 0 |
| 58 | MG | 1A | 3150 | 1/1 | 0.97 | 0.07 | 27,27,27,27 | 0 |
| 58 | MG | 2A | 3693 | 1/1 | 0.97 | 0.07 | 44,44,44,44 | 0 |
| 58 | MG | 1A | 3012 | 1/1 | 0.97 | 0.06 | 23,23,23,23 | 0 |
| 58 | MG | 1V | 201 | 1/1 | 0.97 | 0.14 | 15,15,15,15 | 0 |
| 58 | MG | 1A | 3205 | 1/1 | 0.97 | 0.15 | 30,30,30,30 | 0 |
| 58 | MG | 2A | 3164 | 1/1 | 0.97 | 0.08 | 43,43,43,43 | 0 |
| 58 | MG | 1a | 1762 | 1/1 | 0.97 | 0.05 | 40,40,40,40 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58 | MG | 1A | 3331 | 1/1 | 0.97 | 0.21 | 36,36,36,36 | 0 |
| 58 | MG | 1a | 1764 | 1/1 | 0.97 | 0.07 | 42,42,42,42 | 0 |
| 58 | MG | 1A | 3571 | 1/1 | 0.97 | 0.12 | 21,21,21,21 | 0 |
| 58 | MG | 1W | 201 | 1/1 | 0.97 | 0.05 | 41,41,41,41 | 0 |
| 58 | MG | 1A | 3022 | 1/1 | 0.97 | 0.15 | 27,27,27,27 | 0 |
| 58 | MG | 1W | 203 | 1/1 | 0.97 | 0.09 | 42,42,42,42 | 0 |
| 58 | MG | 1a | 1770 | 1/1 | 0.97 | 0.06 | 49,49,49,49 | 0 |
| 58 | MG | 1a | 1772 | 1/1 | 0.97 | 0.05 | 58,58,58,58 | 0 |
| 58 | MG | 1W | 204 | 1/1 | 0.97 | 0.09 | 22,22,22,22 | 0 |
| 58 | MG | 2A | 3414 | 1/1 | 0.97 | 0.19 | 35,35,35,35 | 0 |
| 58 | MG | 2A | 3415 | 1/1 | 0.97 | 0.14 | 38,38,38,38 | 0 |
| 58 | MG | 2A | 3175 | 1/1 | 0.97 | 0.12 | 43,43,43,43 | 0 |
| 58 | MG | 1A | 3155 | 1/1 | 0.97 | 0.12 | 23,23,23,23 | 0 |
| 58 | MG | 2A | 3713 | 1/1 | 0.97 | 0.08 | 38,38,38,38 | 0 |
| 58 | MG | 1a | 1776 | 1/1 | 0.97 | 0.05 | 56,56,56,56 | 0 |
| 58 | MG | 1A | 3577 | 1/1 | 0.97 | 0.13 | 32,32,32,32 | 0 |
| 58 | MG | 1A | 3208 | 1/1 | 0.97 | 0.12 | 23,23,23,23 | 0 |
| 58 | MG | 1A | 3721 | 1/1 | 0.97 | 0.07 | 36,36,36,36 | 0 |
| 58 | MG | 2A | 3422 | 1/1 | 0.97 | 0.28 | 40,40,40,40 | 0 |
| 58 | MG | 1X | 102 | 1/1 | 0.97 | 0.08 | 27,27,27,27 | 0 |
| 58 | MG | 2a | 1659 | 1/1 | 0.97 | 0.28 | 44,44,44,44 | 0 |
| 58 | MG | 1A | 3581 | 1/1 | 0.97 | 0.07 | 27,27,27,27 | 0 |
| 58 | MG | 1X | 106 | 1/1 | 0.97 | 0.06 | 57,57,57,57 | 0 |
| 58 | MG | 2A | 3185 | 1/1 | 0.97 | 0.08 | 24,24,24,24 | 0 |
| 58 | MG | 2A | 3725 | 1/1 | 0.97 | 0.10 | 29,29,29,29 | 0 |
| 58 | MG | 2a | 1665 | 1/1 | 0.97 | 0.07 | 54,54,54,54 | 0 |
| 58 | MG | 1A | 3158 | 1/1 | 0.97 | 0.09 | 37,37,37,37 | 0 |
| 58 | MG | 2A | 3187 | 1/1 | 0.97 | 0.09 | 40,40,40,40 | 0 |
| 58 | MG | 2A | 3732 | 1/1 | 0.97 | 0.10 | 37,37,37,37 | 0 |
| 58 | MG | 2a | 1669 | 1/1 | 0.97 | 0.06 | 44,44,44,44 | 0 |
| 58 | MG | 1a | 1789 | 1/1 | 0.97 | 0.04 | 36,36,36,36 | 0 |
| 58 | MG | 1A | 4033 | 1/1 | 0.97 | 0.04 | 31,31,31,31 | 0 |
| 58 | MG | 1A | 3485 | 1/1 | 0.97 | 0.05 | 33,33,33,33 | 0 |
| 58 | MG | 2a | 1673 | 1/1 | 0.97 | 0.06 | 32,32,32,32 | 0 |
| 58 | MG | 2a | 1674 | 1/1 | 0.97 | 0.05 | 29,29,29,29 | 0 |
| 58 | MG | 2a | 1676 | 1/1 | 0.97 | 0.06 | 36,36,36,36 | 0 |
| 58 | MG | 1A | 3587 | 1/1 | 0.97 | 0.06 | 25,25,25,25 | 0 |
| 58 | MG | 1a | 1796 | 1/1 | 0.97 | 0.04 | 54,54,54,54 | 0 |
| 58 | MG | 2A | 3738 | 1/1 | 0.97 | 0.20 | 64,64,64,64 | 0 |
| 58 | MG | 1A | 4037 | 1/1 | 0.97 | 0.04 | 38,38,38,38 | 0 |
| 58 | MG | 1A | 3588 | 1/1 | 0.97 | 0.08 | 37,37,37,37 | 0 |
| 58 | MG | 2a | 1683 | 1/1 | 0.97 | 0.06 | 40,40,40,40 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58 | MG | 10 | 101 | 1/1 | 0.97 | 0.08 | 28,28,28,28 | 0 |
| 58 | MG | 1A | 4039 | 1/1 | 0.97 | 0.12 | 27,27,27,27 | 0 |
| 58 | MG | 1A | 3110 | 1/1 | 0.97 | 0.30 | 27,27,27,27 | 0 |
| 58 | MG | 1A | 4041 | 1/1 | 0.97 | 0.07 | 36,36,36,36 | 0 |
| 58 | MG | 1A | 3877 | 1/1 | 0.97 | 0.17 | 21,21,21,21 | 0 |
| 58 | MG | 1A | 3729 | 1/1 | 0.97 | 0.04 | 24,24,24,24 | 0 |
| 58 | MG | 1A | 3879 | 1/1 | 0.97 | 0.22 | 25,25,25,25 | 0 |
| 58 | MG | 2A | 3751 | 1/1 | 0.97 | 0.10 | 40,40,40,40 | 0 |
| 58 | MG | 1a | 1808 | 1/1 | 0.97 | 0.16 | 51,51,51,51 | 0 |
| 58 | MG | 1A | 3880 | 1/1 | 0.97 | 0.10 | 35,35,35,35 | 0 |
| 58 | MG | 1A | 3730 | 1/1 | 0.97 | 0.12 | 45,45,45,45 | 0 |
| 58 | MG | 1A | 3114 | 1/1 | 0.97 | 0.14 | 21,21,21,21 | 0 |
| 58 | MG | 1A | 3339 | 1/1 | 0.97 | 0.07 | 39,39,39,39 | 0 |
| 58 | MG | 1A | 3086 | 1/1 | 0.97 | 0.35 | 26,26,26,26 | 0 |
| 58 | MG | 1A | 3341 | 1/1 | 0.97 | 0.04 | 34,34,34,34 | 0 |
| 58 | MG | 1A | 3886 | 1/1 | 0.97 | 0.06 | 38,38,38,38 | 0 |
| 58 | MG | 13 | 102 | 1/1 | 0.97 | 0.12 | 32,32,32,32 | 0 |
| 58 | MG | 1A | 3417 | 1/1 | 0.97 | 0.15 | 32,32,32,32 | 0 |
| 58 | MG | 1A | 4053 | 1/1 | 0.97 | 0.04 | 25,25,25,25 | 0 |
| 58 | MG | 2a | 1703 | 1/1 | 0.97 | 0.12 | 42,42,42,42 | 0 |
| 58 | MG | 1A | 3596 | 1/1 | 0.97 | 0.12 | 23,23,23,23 | 0 |
| 58 | MG | 1A | 3493 | 1/1 | 0.97 | 0.06 | 45,45,45,45 | 0 |
| 58 | MG | 1A | 3418 | 1/1 | 0.97 | 0.11 | 23,23,23,23 | 0 |
| 58 | MG | 1A | 3063 | 1/1 | 0.97 | 0.26 | 44,44,44,44 | 0 |
| 58 | MG | 1A | 3600 | 1/1 | 0.97 | 0.12 | 37,37,37,37 | 0 |
| 58 | MG | 1A | 3894 | 1/1 | 0.97 | 0.09 | 12,12,12,12 | 0 |
| 58 | MG | 1A | 3220 | 1/1 | 0.97 | 0.12 | 20,20,20,20 | 0 |
| 58 | MG | 2A | 3771 | 1/1 | 0.97 | 0.08 | 30,30,30,30 | 0 |
| 58 | MG | 18 | 103 | 1/1 | 0.97 | 0.09 | 33,33,33,33 | 0 |
| 58 | MG | 1A | 3497 | 1/1 | 0.97 | 0.15 | 35,35,35,35 | 0 |
| 58 | MG | 1A | 4065 | 1/1 | 0.97 | 0.04 | 26,26,26,26 | 0 |
| 58 | MG | 1A | 4066 | 1/1 | 0.97 | 0.05 | 13,13,13,13 | 0 |
| 58 | MG | 2A | 3226 | 1/1 | 0.97 | 0.19 | 30,30,30,30 | 0 |
| 58 | MG | 1A | 3276 | 1/1 | 0.97 | 0.04 | 31,31,31,31 | 0 |
| 58 | MG | 1A | 3898 | 1/1 | 0.97 | 0.06 | 11,11,11,11 | 0 |
| 58 | MG | 1A | 3277 | 1/1 | 0.97 | 0.14 | 21,21,21,21 | 0 |
| 58 | MG | 1A | 4074 | 1/1 | 0.97 | 0.10 | 27,27,27,27 | 0 |
| 58 | MG | 1A | 3605 | 1/1 | 0.97 | 0.05 | 16,16,16,16 | 0 |
| 58 | MG | 2A | 3782 | 1/1 | 0.97 | 0.09 | 33,33,33,33 | 0 |
| 58 | MG | 1w | 102 | 1/1 | 0.97 | 0.07 | 34,34,34,34 | 0 |
| 58 | MG | 2A | 3478 | 1/1 | 0.97 | 0.07 | 16,16,16,16 | 0 |
| 58 | MG | 1A | 3064 | 1/1 | 0.97 | 0.09 | 33,33,33,33 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58 | MG | 2a | 1727 | 1/1 | 0.97 | 0.10 | 39,39,39,39 | 0 |
| 58 | MG | 2A | 3786 | 1/1 | 0.97 | 0.04 | 30,30,30,30 | 0 |
| 58 | MG | 2A | 3480 | 1/1 | 0.97 | 0.08 | 35,35,35,35 | 0 |
| 58 | MG | 1w | 105 | 1/1 | 0.97 | 0.05 | 41,41,41,41 | 0 |
| 58 | MG | 1A | 3501 | 1/1 | 0.97 | 0.12 | 24,24,24,24 | 0 |
| 58 | MG | 1A | 3608 | 1/1 | 0.97 | 0.07 | 17,17,17,17 | 0 |
| 58 | MG | 1A | 4080 | 1/1 | 0.97 | 0.06 | 35,35,35,35 | 0 |
| 58 | MG | 1A | 3065 | 1/1 | 0.97 | 0.07 | 30,30,30,30 | 0 |
| 58 | MG | 1a | 1613 | 1/1 | 0.97 | 0.12 | 21,21,21,21 | 0 |
| 58 | MG | 1A | 3223 | 1/1 | 0.97 | 0.08 | 41,41,41,41 | 0 |
| 58 | MG | 1A | 3352 | 1/1 | 0.97 | 0.18 | 28,28,28,28 | 0 |
| 58 | MG | 1A | 4084 | 1/1 | 0.97 | 0.08 | 22,22,22,22 | 0 |
| 58 | MG | 1A | 3910 | 1/1 | 0.97 | 0.05 | 46,46,46,46 | 0 |
| 58 | MG | 2A | 3245 | 1/1 | 0.97 | 0.18 | 37,37,37,37 | 0 |
| 58 | MG | 2A | 3492 | 1/1 | 0.97 | 0.13 | 45,45,45,45 | 0 |
| 58 | MG | 1A | 4087 | 1/1 | 0.97 | 0.05 | 30,30,30,30 | 0 |
| 58 | MG | 1A | 3284 | 1/1 | 0.97 | 0.25 | 37,37,37,37 | 0 |
| 58 | MG | 2A | 3248 | 1/1 | 0.97 | 0.06 | 47,47,47,47 | 0 |
| 58 | MG | 2A | 3497 | 1/1 | 0.97 | 0.11 | 32,32,32,32 | 0 |
| 58 | MG | 1A | 3286 | 1/1 | 0.97 | 0.24 | 25,25,25,25 | 0 |
| 58 | MG | 1A | 3915 | 1/1 | 0.97 | 0.19 | 21,21,21,21 | 0 |
| 58 | MG | 1A | 3916 | 1/1 | 0.97 | 0.14 | 15,15,15,15 | 0 |
| 58 | MG | 2a | 1750 | 1/1 | 0.97 | 0.06 | 42,42,42,42 | 0 |
| 58 | MG | 2a | 1751 | 1/1 | 0.97 | 0.05 | 58,58,58,58 | 0 |
| 58 | MG | 2A | 3501 | 1/1 | 0.97 | 0.05 | 61,61,61,61 | 0 |
| 58 | MG | 1a | 1623 | 1/1 | 0.97 | 0.05 | 37,37,37,37 | 0 |
| 58 | MG | 1a | 1624 | 1/1 | 0.97 | 0.15 | 42,42,42,42 | 0 |
| 58 | MG | 1A | 3225 | 1/1 | 0.97 | 0.09 | 22,22,22,22 | 0 |
| 58 | MG | 1A | 3617 | 1/1 | 0.97 | 0.05 | 13,13,13,13 | 0 |
| 58 | MG | 2A | 3506 | 1/1 | 0.97 | 0.07 | 30,30,30,30 | 0 |
| 58 | MG | 1A | 3017 | 1/1 | 0.97 | 0.09 | 43,43,43,43 | 0 |
| 58 | MG | 1A | 3291 | 1/1 | 0.97 | 0.10 | 30,30,30,30 | 0 |
| 58 | MG | 1A | 3170 | 1/1 | 0.97 | 0.06 | 31,31,31,31 | 0 |
| 58 | MG | 1A | 3008 | 1/1 | 0.97 | 0.05 | 13,13,13,13 | 0 |
| 58 | MG | 1A | 3514 | 1/1 | 0.97 | 0.12 | 37,37,37,37 | 0 |
| 58 | MG | 1A | 3515 | 1/1 | 0.97 | 0.32 | 34,34,34,34 | 0 |
| 58 | MG | 2a | 1770 | 1/1 | 0.97 | 0.05 | 46,46,46,46 | 0 |
| 58 | MG | 2A | 3514 | 1/1 | 0.97 | 0.07 | 36,36,36,36 | 0 |
| 58 | MG | 2A | 3824 | 1/1 | 0.97 | 0.07 | 19,19,19,19 | 0 |
| 58 | MG | 1a | 1633 | 1/1 | 0.97 | 0.09 | 45,45,45,45 | 0 |
| 58 | MG | 2a | 1774 | 1/1 | 0.97 | 0.10 | 43,43,43,43 | 0 |
| 58 | MG | 2a | 1775 | 1/1 | 0.97 | 0.04 | 56,56,56,56 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58 | MG | 1A | 3030 | 1/1 | 0.97 | 0.16 | 14,14,14,14 | 0 |
| 58 | MG | 2A | 3013 | 1/1 | 0.97 | 0.06 | 39,39,39,39 | 0 |
| 58 | MG | 1A | 3779 | 1/1 | 0.97 | 0.06 | 31,31,31,31 | 0 |
| 58 | MG | 1a | 1637 | 1/1 | 0.97 | 0.09 | 43,43,43,43 | 0 |
| 58 | MG | 2A | 3269 | 1/1 | 0.97 | 0.07 | 35,35,35,35 | 0 |
| 58 | MG | 1A | 3296 | 1/1 | 0.97 | 0.07 | 23,23,23,23 | 0 |
| 58 | MG | 2a | 1783 | 1/1 | 0.97 | 0.07 | 39,39,39,39 | 0 |
| 58 | MG | 1a | 1639 | 1/1 | 0.97 | 0.06 | 34,34,34,34 | 0 |
| 58 | MG | 2A | 3836 | 1/1 | 0.97 | 0.05 | 54,54,54,54 | 0 |
| 58 | MG | 2a | 1786 | 1/1 | 0.97 | 0.04 | 45,45,45,45 | 0 |
| 58 | MG | 2A | 3019 | 1/1 | 0.97 | 0.06 | 30,30,30,30 | 0 |
| 58 | MG | 1A | 3783 | 1/1 | 0.97 | 0.06 | 38,38,38,38 | 0 |
| 58 | MG | 1A | 3631 | 1/1 | 0.97 | 0.04 | 19,19,19,19 | 0 |
| 58 | MG | 1A | 4105 | 1/1 | 0.97 | 0.19 | 41,41,41,41 | 0 |
| 58 | MG | 1a | 1643 | 1/1 | 0.97 | 0.12 | 41,41,41,41 | 0 |
| 58 | MG | 1A | 3632 | 1/1 | 0.97 | 0.03 | 25,25,25,25 | 0 |
| 58 | MG | 1A | 3635 | 1/1 | 0.97 | 0.04 | 13,13,13,13 | 0 |
| 58 | MG | 1B | 205 | 1/1 | 0.97 | 0.24 | 47,47,47,47 | 0 |
| 58 | MG | 1B | 207 | 1/1 | 0.97 | 0.20 | 33,33,33,33 | 0 |
| 58 | MG | 1a | 1648 | 1/1 | 0.97 | 0.09 | 41,41,41,41 | 0 |
| 58 | MG | 1A | 3788 | 1/1 | 0.97 | 0.05 | 27,27,27,27 | 0 |
| 58 | MG | 1A | 3938 | 1/1 | 0.97 | 0.06 | 30,30,30,30 | 0 |
| 58 | MG | 2A | 3541 | 1/1 | 0.97 | 0.06 | 38,38,38,38 | 0 |
| 58 | MG | 2A | 3851 | 1/1 | 0.97 | 0.04 | 36,36,36,36 | 0 |
| 58 | MG | 2A | 3852 | 1/1 | 0.97 | 0.07 | 21,21,21,21 | 0 |
| 58 | MG | 1B | 210 | 1/1 | 0.97 | 0.07 | 38,38,38,38 | 0 |
| 58 | MG | 1A | 3789 | 1/1 | 0.97 | 0.05 | 28,28,28,28 | 0 |
| 58 | MG | 2A | 3037 | 1/1 | 0.97 | 0.06 | 31,31,31,31 | 0 |
| 58 | MG | 2a | 1806 | 1/1 | 0.97 | 0.07 | 43,43,43,43 | 0 |
| 58 | MG | 2A | 3545 | 1/1 | 0.97 | 0.05 | 41,41,41,41 | 0 |
| 58 | MG | 1A | 3070 | 1/1 | 0.97 | 0.09 | 14,14,14,14 | 0 |
| 58 | MG | 2A | 3547 | 1/1 | 0.97 | 0.05 | 31,31,31,31 | 0 |
| 58 | MG | 2A | 3548 | 1/1 | 0.97 | 0.06 | 37,37,37,37 | 0 |
| 58 | MG | 1a | 1657 | 1/1 | 0.97 | 0.05 | 42,42,42,42 | 0 |
| 58 | MG | 1A | 3127 | 1/1 | 0.97 | 0.18 | 26,26,26,26 | 0 |
| 58 | MG | 1A | 3128 | 1/1 | 0.97 | 0.11 | 25,25,25,25 | 0 |
| 58 | MG | 2A | 3553 | 1/1 | 0.97 | 0.09 | 27,27,27,27 | 0 |
| 58 | MG | 2A | 3555 | 1/1 | 0.97 | 0.07 | 35,35,35,35 | 0 |
| 58 | MG | 1A | 3178 | 1/1 | 0.97 | 0.22 | 25,25,25,25 | 0 |
| 58 | MG | 1B | 217 | 1/1 | 0.97 | 0.06 | 37,37,37,37 | 0 |
| 58 | MG | 1A | 3797 | 1/1 | 0.97 | 0.05 | 15,15,15,15 | 0 |
| 58 | MG | 1B | 219 | 1/1 | 0.97 | 0.08 | 21,21,21,21 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58 | MG | 1A | 3798 | 1/1 | 0.97 | 0.04 | 17,17,17,17 | 0 |
| 58 | MG | 1A | 3949 | 1/1 | 0.97 | 0.07 | 45,45,45,45 | 0 |
| 58 | MG | 1A | 3301 | 1/1 | 0.97 | 0.11 | 28,28,28,28 | 0 |
| 58 | MG | 2a | 1823 | 1/1 | 0.97 | 0.09 | 50,50,50,50 | 0 |
| 58 | MG | 2A | 3564 | 1/1 | 0.97 | 0.06 | 41,41,41,41 | 0 |
| 58 | MG | 1B | 224 | 1/1 | 0.97 | 0.06 | 45,45,45,45 | 0 |
| 58 | MG | 2A | 3875 | 1/1 | 0.97 | 0.18 | 53,53,53,53 | 0 |
| 58 | MG | 2A | 3568 | 1/1 | 0.97 | 0.06 | 26,26,26,26 | 0 |
| 58 | MG | 1A | 3071 | 1/1 | 0.97 | 0.04 | 6,6,6,6 | 0 |
| 58 | MG | 1A | 3953 | 1/1 | 0.97 | 0.05 | 48,48,48,48 | 0 |
| 58 | MG | 1B | 228 | 1/1 | 0.97 | 0.05 | 30,30,30,30 | 0 |
| 58 | MG | 1A | 3954 | 1/1 | 0.97 | 0.07 | 37,37,37,37 | 0 |
| 58 | MG | 1A | 3032 | 1/1 | 0.97 | 0.18 | 20,20,20,20 | 0 |
| 58 | MG | 2a | 1833 | 1/1 | 0.97 | 0.10 | 57,57,57,57 | 0 |
| 58 | MG | 1A | 3304 | 1/1 | 0.97 | 0.07 | 36,36,36,36 | 0 |
| 58 | MG | 2A | 3059 | 1/1 | 0.97 | 0.10 | 35,35,35,35 | 0 |
| 58 | MG | 1A | 3245 | 1/1 | 0.97 | 0.14 | 18,18,18,18 | 0 |
| 58 | MG | 1A | 3958 | 1/1 | 0.97 | 0.10 | 43,43,43,43 | 0 |
| 58 | MG | 2A | 3579 | 1/1 | 0.97 | 0.05 | 26,26,26,26 | 0 |
| 58 | MG | 1A | 3649 | 1/1 | 0.97 | 0.06 | 10,10,10,10 | 0 |
| 58 | MG | 1A | 3373 | 1/1 | 0.97 | 0.17 | 35,35,35,35 | 0 |
| 58 | MG | 1B | 237 | 1/1 | 0.97 | 0.04 | 25,25,25,25 | 0 |
| 58 | MG | 1D | 305 | 1/1 | 0.97 | 0.07 | 33,33,33,33 | 0 |
| 58 | MG | 1A | 3808 | 1/1 | 0.97 | 0.04 | 33,33,33,33 | 0 |
| 58 | MG | 2f | 201 | 1/1 | 0.97 | 0.18 | 35,35,35,35 | 0 |
| 58 | MG | 2A | 3585 | 1/1 | 0.97 | 0.15 | 37,37,37,37 | 0 |
| 58 | MG | 1D | 308 | 1/1 | 0.97 | 0.14 | 38,38,38,38 | 0 |
| 58 | MG | 1A | 3133 | 1/1 | 0.97 | 0.12 | 48,48,48,48 | 0 |
| 58 | MG | 1A | 3375 | 1/1 | 0.97 | 0.06 | 37,37,37,37 | 0 |
| 58 | MG | 1A | 3656 | 1/1 | 0.97 | 0.04 | 17,17,17,17 | 0 |
| 58 | MG | 1A | 3965 | 1/1 | 0.97 | 0.10 | 51,51,51,51 | 0 |
| 58 | MG | 2B | 215 | 1/1 | 0.97 | 0.10 | 44,44,44,44 | 0 |
| 58 | MG | 1A | 3814 | 1/1 | 0.97 | 0.06 | 35,35,35,35 | 0 |
| 58 | MG | 1A | 3967 | 1/1 | 0.97 | 0.07 | 30,30,30,30 | 0 |
| 58 | MG | 1A | 3376 | 1/1 | 0.97 | 0.06 | 31,31,31,31 | 0 |
| 58 | MG | 1A | 3098 | 1/1 | 0.97 | 0.06 | 25,25,25,25 | 0 |
| 58 | MG | 1A | 3186 | 1/1 | 0.97 | 0.05 | 46,46,46,46 | 0 |
| 58 | MG | 1A | 3033 | 1/1 | 0.97 | 0.22 | 20,20,20,20 | 0 |
| 58 | MG | 1A | 3661 | 1/1 | 0.97 | 0.06 | 18,18,18,18 | 0 |
| 58 | MG | 1F | 303 | 1/1 | 0.97 | 0.16 | 26,26,26,26 | 0 |
| 58 | MG | 1F | 304 | 1/1 | 0.97 | 0.05 | 43,43,43,43 | 0 |
| 58 | MG | 1A | 3034 | 1/1 | 0.97 | 0.20 | 25,25,25,25 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58 | MG | 1F | 309 | 1/1 | 0.97 | 0.05 | 32,32,32,32 | 0 |
| 58 | MG | 1A | 3040 | 1/1 | 0.97 | 0.12 | 43,43,43,43 | 0 |
| 58 | MG | 1A | 3080 | 1/1 | 0.97 | 0.10 | 40,40,40,40 | 0 |
| 58 | MG | 1a | 1699 | 1/1 | 0.97 | 0.19 | 44,44,44,44 | 0 |
| 58 | MG | 1A | 3193 | 1/1 | 0.97 | 0.08 | 28,28,28,28 | 0 |
| 58 | MG | 1A | 3542 | 1/1 | 0.97 | 0.18 | 33,33,33,33 | 0 |
| 58 | MG | 2E | 310 | 1/1 | 0.97 | 0.07 | 30,30,30,30 | 0 |
| 58 | MG | 1A | 3827 | 1/1 | 0.97 | 0.05 | 29,29,29,29 | 0 |
| 58 | MG | 2A | 3093 | 1/1 | 0.97 | 0.18 | 36,36,36,36 | 0 |
| 58 | MG | 1A | 3141 | 1/1 | 0.97 | 0.13 | 27,27,27,27 | 0 |
| 58 | MG | 1A | 3196 | 1/1 | 0.97 | 0.27 | 27,27,27,27 | 0 |
| 58 | MG | 1A | 3675 | 1/1 | 0.97 | 0.07 | 16,16,16,16 | 0 |
| 58 | MG | 2A | 3617 | 1/1 | 0.97 | 0.05 | 38,38,38,38 | 0 |
| 58 | MG | 2A | 3618 | 1/1 | 0.97 | 0.12 | 28,28,28,28 | 0 |
| 58 | MG | 2F | 307 | 1/1 | 0.97 | 0.21 | 35,35,35,35 | 0 |
| 58 | MG | 2F | 308 | 1/1 | 0.97 | 0.11 | 35,35,35,35 | 0 |
| 58 | MG | 2A | 3098 | 1/1 | 0.97 | 0.07 | 33,33,33,33 | 0 |
| 58 | MG | 1A | 3387 | 1/1 | 0.97 | 0.19 | 18,18,18,18 | 0 |
| 58 | MG | 1A | 3677 | 1/1 | 0.97 | 0.07 | 12,12,12,12 | 0 |
| 58 | MG | 1A | 3546 | 1/1 | 0.97 | 0.05 | 18,18,18,18 | 0 |
| 58 | MG | 1A | 3197 | 1/1 | 0.97 | 0.30 | 18,18,18,18 | 0 |
| 58 | MG | 1A | 3989 | 1/1 | 0.97 | 0.10 | 47,47,47,47 | 0 |
| 58 | MG | 1N | 204 | 1/1 | 0.97 | 0.04 | 27,27,27,27 | 0 |
| 59 | K | 2x | 101 | 1/1 | 0.97 | 0.05 | 41,41,41,41 | 0 |
| 58 | MG | 2A | 3348 | 1/1 | 0.97 | 0.07 | 44,44,44,44 | 0 |
| 58 | MG | 2A | 3425 | 1/1 | 0.98 | 0.09 | 27,27,27,27 | 0 |
| 58 | MG | 1A | 3785 | 1/1 | 0.98 | 0.04 | 17,17,17,17 | 0 |
| 58 | MG | 1A | 3239 | 1/1 | 0.98 | 0.12 | 21,21,21,21 | 0 |
| 58 | MG | 1A | 3305 | 1/1 | 0.98 | 0.04 | 19,19,19,19 | 0 |
| 58 | MG | 1A | 3936 | 1/1 | 0.98 | 0.08 | 57,57,57,57 | 0 |
| 58 | MG | 1A | 3646 | 1/1 | 0.98 | 0.06 | 12,12,12,12 | 0 |
| 58 | MG | 1a | 1610 | 1/1 | 0.98 | 0.05 | 34,34,34,34 | 0 |
| 58 | MG | 1A | 3939 | 1/1 | 0.98 | 0.07 | 18,18,18,18 | 0 |
| 58 | MG | 1A | 3144 | 1/1 | 0.98 | 0.04 | 5,5,5,5 | 0 |
| 58 | MG | 1A | 3942 | 1/1 | 0.98 | 0.03 | 48,48,48,48 | 0 |
| 58 | MG | 1A | 3241 | 1/1 | 0.98 | 0.07 | 31,31,31,31 | 0 |
| 58 | MG | 1B | 206 | 1/1 | 0.98 | 0.04 | 41,41,41,41 | 0 |
| 58 | MG | 1A | 3792 | 1/1 | 0.98 | 0.05 | 14,14,14,14 | 0 |
| 58 | MG | 1A | 3309 | 1/1 | 0.98 | 0.10 | 41,41,41,41 | 0 |
| 58 | MG | 1A | 3794 | 1/1 | 0.98 | 0.10 | 38,38,38,38 | 0 |
| 58 | MG | 1A | 3650 | 1/1 | 0.98 | 0.04 | 18,18,18,18 | 0 |
| 58 | MG | 1B | 211 | 1/1 | 0.98 | 0.26 | 34,34,34,34 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58 | MG | 1A | 3242 | 1/1 | 0.98 | 0.07 | 22,22,22,22 | 0 |
| 58 | MG | 1A | 3652 | 1/1 | 0.98 | 0.04 | 30,30,30,30 | 0 |
| 58 | MG | 1A | 3950 | 1/1 | 0.98 | 0.04 | 33,33,33,33 | 0 |
| 58 | MG | 1v | 102 | 1/1 | 0.98 | 0.05 | 37,37,37,37 | 0 |
| 58 | MG | 1A | 3243 | 1/1 | 0.98 | 0.04 | 23,23,23,23 | 0 |
| 58 | MG | 1A | 3799 | 1/1 | 0.98 | 0.07 | 10,10,10,10 | 0 |
| 58 | MG | 2A | 3448 | 1/1 | 0.98 | 0.19 | 40,40,40,40 | 0 |
| 58 | MG | 1A | 3145 | 1/1 | 0.98 | 0.05 | 38,38,38,38 | 0 |
| 58 | MG | 2A | 3450 | 1/1 | 0.98 | 0.19 | 28,28,28,28 | 0 |
| 58 | MG | 1w | 104 | 1/1 | 0.98 | 0.05 | 51,51,51,51 | 0 |
| 58 | MG | 1A | 3801 | 1/1 | 0.98 | 0.05 | 24,24,24,24 | 0 |
| 58 | MG | 1A | 3097 | 1/1 | 0.98 | 0.09 | 28,28,28,28 | 0 |
| 58 | MG | 2A | 3217 | 1/1 | 0.98 | 0.14 | 37,37,37,37 | 0 |
| 58 | MG | 1B | 220 | 1/1 | 0.98 | 0.04 | 24,24,24,24 | 0 |
| 58 | MG | 2A | 3722 | 1/1 | 0.98 | 0.06 | 40,40,40,40 | 0 |
| 58 | MG | 1A | 3463 | 1/1 | 0.98 | 0.10 | 30,30,30,30 | 0 |
| 58 | MG | 1A | 3021 | 1/1 | 0.98 | 0.10 | 15,15,15,15 | 0 |
| 58 | MG | 1A | 3149 | 1/1 | 0.98 | 0.22 | 18,18,18,18 | 0 |
| 58 | MG | 1A | 3190 | 1/1 | 0.98 | 0.14 | 23,23,23,23 | 0 |
| 58 | MG | 2A | 3728 | 1/1 | 0.98 | 0.04 | 28,28,28,28 | 0 |
| 58 | MG | 2A | 3729 | 1/1 | 0.98 | 0.04 | 26,26,26,26 | 0 |
| 58 | MG | 1A | 3119 | 1/1 | 0.98 | 0.15 | 22,22,22,22 | 0 |
| 58 | MG | 1A | 3662 | 1/1 | 0.98 | 0.05 | 14,14,14,14 | 0 |
| 58 | MG | 1a | 1636 | 1/1 | 0.98 | 0.08 | 23,23,23,23 | 0 |
| 58 | MG | 1B | 227 | 1/1 | 0.98 | 0.04 | 26,26,26,26 | 0 |
| 58 | MG | 1A | 3810 | 1/1 | 0.98 | 0.21 | 18,18,18,18 | 0 |
| 58 | MG | 1A | 3192 | 1/1 | 0.98 | 0.15 | 30,30,30,30 | 0 |
| 58 | MG | 1x | 110 | 1/1 | 0.98 | 0.11 | 43,43,43,43 | 0 |
| 58 | MG | 1A | 3099 | 1/1 | 0.98 | 0.12 | 10,10,10,10 | 0 |
| 58 | MG | 2A | 3740 | 1/1 | 0.98 | 0.05 | 36,36,36,36 | 0 |
| 58 | MG | 1A | 3253 | 1/1 | 0.98 | 0.26 | 31,31,31,31 | 0 |
| 58 | MG | 1A | 3194 | 1/1 | 0.98 | 0.21 | 20,20,20,20 | 0 |
| 58 | MG | 2A | 3233 | 1/1 | 0.98 | 0.06 | 38,38,38,38 | 0 |
| 58 | MG | 1A | 3392 | 1/1 | 0.98 | 0.21 | 18,18,18,18 | 0 |
| 58 | MG | 1A | 3152 | 1/1 | 0.98 | 0.24 | 23,23,23,23 | 0 |
| 58 | MG | 2A | 3002 | 1/1 | 0.98 | 0.23 | 35,35,35,35 | 0 |
| 58 | MG | 2A | 3747 | 1/1 | 0.98 | 0.05 | 33,33,33,33 | 0 |
| 58 | MG | 1A | 3969 | 1/1 | 0.98 | 0.08 | 17,17,17,17 | 0 |
| 58 | MG | 2A | 3476 | 1/1 | 0.98 | 0.06 | 39,39,39,39 | 0 |
| 58 | MG | 2a | 1660 | 1/1 | 0.98 | 0.05 | 52,52,52,52 | 0 |
| 58 | MG | 1B | 236 | 1/1 | 0.98 | 0.05 | 35,35,35,35 | 0 |
| 58 | MG | 1A | 3018 | 1/1 | 0.98 | 0.10 | 20,20,20,20 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58 | MG | 1D | 301 | 1/1 | 0.98 | 0.17 | 22,22,22,22 | 0 |
| 58 | MG | 1A | 3971 | 1/1 | 0.98 | 0.05 | 22,22,22,22 | 0 |
| 58 | MG | 1A | 3154 | 1/1 | 0.98 | 0.27 | 20,20,20,20 | 0 |
| 58 | MG | 1A | 3325 | 1/1 | 0.98 | 0.16 | 25,25,25,25 | 0 |
| 58 | MG | 1A | 3561 | 1/1 | 0.98 | 0.12 | 21,21,21,21 | 0 |
| 58 | MG | 1a | 1653 | 1/1 | 0.98 | 0.03 | 36,36,36,36 | 0 |
| 58 | MG | 1a | 1654 | 1/1 | 0.98 | 0.12 | 33,33,33,33 | 0 |
| 58 | MG | 1a | 1655 | 1/1 | 0.98 | 0.09 | 39,39,39,39 | 0 |
| 58 | MG | 2A | 3015 | 1/1 | 0.98 | 0.11 | 38,38,38,38 | 0 |
| 58 | MG | 1D | 310 | 1/1 | 0.98 | 0.24 | 19,19,19,19 | 0 |
| 58 | MG | 1A | 3821 | 1/1 | 0.98 | 0.06 | 35,35,35,35 | 0 |
| 58 | MG | 1A | 3678 | 1/1 | 0.98 | 0.04 | 12,12,12,12 | 0 |
| 58 | MG | 2a | 1675 | 1/1 | 0.98 | 0.14 | 35,35,35,35 | 0 |
| 58 | MG | 1E | 302 | 1/1 | 0.98 | 0.08 | 31,31,31,31 | 0 |
| 58 | MG | 2A | 3765 | 1/1 | 0.98 | 0.04 | 39,39,39,39 | 0 |
| 58 | MG | 1E | 303 | 1/1 | 0.98 | 0.08 | 18,18,18,18 | 0 |
| 58 | MG | 2A | 3021 | 1/1 | 0.98 | 0.07 | 16,16,16,16 | 0 |
| 58 | MG | 2a | 1680 | 1/1 | 0.98 | 0.09 | 37,37,37,37 | 0 |
| 58 | MG | 1A | 3680 | 1/1 | 0.98 | 0.05 | 21,21,21,21 | 0 |
| 58 | MG | 1A | 3198 | 1/1 | 0.98 | 0.15 | 28,28,28,28 | 0 |
| 58 | MG | 2A | 3496 | 1/1 | 0.98 | 0.12 | 35,35,35,35 | 0 |
| 58 | MG | 1A | 3085 | 1/1 | 0.98 | 0.10 | 22,22,22,22 | 0 |
| 58 | MG | 1A | 3564 | 1/1 | 0.98 | 0.21 | 26,26,26,26 | 0 |
| 58 | MG | 2A | 3259 | 1/1 | 0.98 | 0.04 | 48,48,48,48 | 0 |
| 58 | MG | 1A | 3156 | 1/1 | 0.98 | 0.04 | 26,26,26,26 | 0 |
| 58 | MG | 2A | 3027 | 1/1 | 0.98 | 0.12 | 24,24,24,24 | 0 |
| 58 | MG | 1A | 3685 | 1/1 | 0.98 | 0.06 | 11,11,11,11 | 0 |
| 58 | MG | 2A | 3263 | 1/1 | 0.98 | 0.05 | 50,50,50,50 | 0 |
| 58 | MG | 1A | 3124 | 1/1 | 0.98 | 0.13 | 26,26,26,26 | 0 |
| 58 | MG | 2A | 3030 | 1/1 | 0.98 | 0.12 | 33,33,33,33 | 0 |
| 58 | MG | 1A | 3984 | 1/1 | 0.98 | 0.03 | 22,22,22,22 | 0 |
| 58 | MG | 1F | 301 | 1/1 | 0.98 | 0.08 | 27,27,27,27 | 0 |
| 58 | MG | 1A | 3125 | 1/1 | 0.98 | 0.05 | 34,34,34,34 | 0 |
| 58 | MG | 1A | 3160 | 1/1 | 0.98 | 0.09 | 29,29,29,29 | 0 |
| 58 | MG | 1F | 305 | 1/1 | 0.98 | 0.07 | 25,25,25,25 | 0 |
| 58 | MG | 1A | 3692 | 1/1 | 0.98 | 0.09 | 9,9,9,9 | 0 |
| 58 | MG | 2A | 3038 | 1/1 | 0.98 | 0.10 | 13,13,13,13 | 0 |
| 58 | MG | 2A | 3513 | 1/1 | 0.98 | 0.07 | 24,24,24,24 | 0 |
| 58 | MG | 1F | 308 | 1/1 | 0.98 | 0.17 | 18,18,18,18 | 0 |
| 58 | MG | 1A | 3056 | 1/1 | 0.98 | 0.04 | 24,24,24,24 | 0 |
| 58 | MG | 1A | 3333 | 1/1 | 0.98 | 0.05 | 31,31,31,31 | 0 |
| 58 | MG | 2A | 3517 | 1/1 | 0.98 | 0.12 | 34,34,34,34 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58 | MG | 2a | 1705 | 1/1 | 0.98 | 0.05 | 49,49,49,49 | 0 |
| 58 | MG | 1A | 3572 | 1/1 | 0.98 | 0.04 | 12,12,12,12 | 0 |
| 58 | MG | 1A | 3696 | 1/1 | 0.98 | 0.06 | 12,12,12,12 | 0 |
| 58 | MG | 2A | 3044 | 1/1 | 0.98 | 0.04 | 35,35,35,35 | 0 |
| 58 | MG | 2A | 3521 | 1/1 | 0.98 | 0.06 | 39,39,39,39 | 0 |
| 58 | MG | 2A | 3796 | 1/1 | 0.98 | 0.04 | 37,37,37,37 | 0 |
| 58 | MG | 1A | 3087 | 1/1 | 0.98 | 0.23 | 30,30,30,30 | 0 |
| 58 | MG | 2A | 3523 | 1/1 | 0.98 | 0.05 | 25,25,25,25 | 0 |
| 58 | MG | 1A | 3486 | 1/1 | 0.98 | 0.05 | 21,21,21,21 | 0 |
| 58 | MG | 1A | 3408 | 1/1 | 0.98 | 0.11 | 36,36,36,36 | 0 |
| 58 | MG | 1A | 3700 | 1/1 | 0.98 | 0.11 | 16,16,16,16 | 0 |
| 58 | MG | 2A | 3049 | 1/1 | 0.98 | 0.10 | 14,14,14,14 | 0 |
| 58 | MG | 1A | 3578 | 1/1 | 0.98 | 0.11 | 24,24,24,24 | 0 |
| 58 | MG | 2A | 3285 | 1/1 | 0.98 | 0.09 | 44,44,44,44 | 0 |
| 58 | MG | 2A | 3532 | 1/1 | 0.98 | 0.06 | 39,39,39,39 | 0 |
| 58 | MG | 1A | 3579 | 1/1 | 0.98 | 0.15 | 23,23,23,23 | 0 |
| 58 | MG | 1A | 3163 | 1/1 | 0.98 | 0.15 | 25,25,25,25 | 0 |
| 58 | MG | 2A | 3808 | 1/1 | 0.98 | 0.07 | 48,48,48,48 | 0 |
| 58 | MG | 1A | 3164 | 1/1 | 0.98 | 0.14 | 21,21,21,21 | 0 |
| 58 | MG | 1A | 3706 | 1/1 | 0.98 | 0.04 | 32,32,32,32 | 0 |
| 58 | MG | 1A | 3043 | 1/1 | 0.98 | 0.23 | 29,29,29,29 | 0 |
| 58 | MG | 1A | 3583 | 1/1 | 0.98 | 0.19 | 24,24,24,24 | 0 |
| 58 | MG | 1A | 3584 | 1/1 | 0.98 | 0.34 | 30,30,30,30 | 0 |
| 58 | MG | 1A | 3130 | 1/1 | 0.98 | 0.31 | 25,25,25,25 | 0 |
| 58 | MG | 2a | 1729 | 1/1 | 0.98 | 0.13 | 33,33,33,33 | 0 |
| 58 | MG | 1A | 3586 | 1/1 | 0.98 | 0.04 | 28,28,28,28 | 0 |
| 58 | MG | 1A | 3105 | 1/1 | 0.98 | 0.12 | 31,31,31,31 | 0 |
| 58 | MG | 1A | 3414 | 1/1 | 0.98 | 0.04 | 39,39,39,39 | 0 |
| 58 | MG | 1A | 3854 | 1/1 | 0.98 | 0.10 | 14,14,14,14 | 0 |
| 58 | MG | 1A | 3855 | 1/1 | 0.98 | 0.10 | 30,30,30,30 | 0 |
| 58 | MG | 1A | 3415 | 1/1 | 0.98 | 0.10 | 33,33,33,33 | 0 |
| 58 | MG | 2A | 3821 | 1/1 | 0.98 | 0.05 | 22,22,22,22 | 0 |
| 58 | MG | 1A | 4014 | 1/1 | 0.98 | 0.03 | 15,15,15,15 | 0 |
| 58 | MG | 1A | 3168 | 1/1 | 0.98 | 0.12 | 26,26,26,26 | 0 |
| 58 | MG | 1A | 4016 | 1/1 | 0.98 | 0.07 | 15,15,15,15 | 0 |
| 58 | MG | 1A | 3591 | 1/1 | 0.98 | 0.06 | 35,35,35,35 | 0 |
| 58 | MG | 2A | 3551 | 1/1 | 0.98 | 0.03 | 25,25,25,25 | 0 |
| 58 | MG | 2A | 3069 | 1/1 | 0.98 | 0.04 | 23,23,23,23 | 0 |
| 58 | MG | 1A | 3717 | 1/1 | 0.98 | 0.05 | 7,7,7,7 | 0 |
| 58 | MG | 2A | 3554 | 1/1 | 0.98 | 0.05 | 22,22,22,22 | 0 |
| 58 | MG | 1A | 3213 | 1/1 | 0.98 | 0.06 | 32,32,32,32 | 0 |
| 58 | MG | 1A | 3044 | 1/1 | 0.98 | 0.12 | 25,25,25,25 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58 | MG | 1A | 3862 | 1/1 | 0.98 | 0.18 | 29,29,29,29 | 0 |
| 58 | MG | 2A | 3558 | 1/1 | 0.98 | 0.08 | 20,20,20,20 | 0 |
| 58 | MG | 1A | 3215 | 1/1 | 0.98 | 0.21 | 23,23,23,23 | 0 |
| 58 | MG | 1A | 3864 | 1/1 | 0.98 | 0.05 | 35,35,35,35 | 0 |
| 58 | MG | 1A | 3420 | 1/1 | 0.98 | 0.06 | 34,34,34,34 | 0 |
| 58 | MG | 1A | 3344 | 1/1 | 0.98 | 0.17 | 48,48,48,48 | 0 |
| 58 | MG | 1A | 3345 | 1/1 | 0.98 | 0.09 | 31,31,31,31 | 0 |
| 58 | MG | 1A | 3216 | 1/1 | 0.98 | 0.03 | 20,20,20,20 | 0 |
| 58 | MG | 1A | 3869 | 1/1 | 0.98 | 0.11 | 19,19,19,19 | 0 |
| 58 | MG | 2A | 3567 | 1/1 | 0.98 | 0.05 | 24,24,24,24 | 0 |
| 58 | MG | 1A | 3217 | 1/1 | 0.98 | 0.11 | 36,36,36,36 | 0 |
| 58 | MG | 2a | 1758 | 1/1 | 0.98 | 0.05 | 50,50,50,50 | 0 |
| 58 | MG | 1A | 3279 | 1/1 | 0.98 | 0.08 | 28,28,28,28 | 0 |
| 58 | MG | 2A | 3570 | 1/1 | 0.98 | 0.04 | 26,26,26,26 | 0 |
| 58 | MG | 1A | 3218 | 1/1 | 0.98 | 0.05 | 33,33,33,33 | 0 |
| 58 | MG | 1A | 3219 | 1/1 | 0.98 | 0.13 | 32,32,32,32 | 0 |
| 58 | MG | 1A | 3351 | 1/1 | 0.98 | 0.28 | 26,26,26,26 | 0 |
| 58 | MG | 1a | 1719 | 1/1 | 0.98 | 0.07 | 30,30,30,30 | 0 |
| 58 | MG | 2a | 1766 | 1/1 | 0.98 | 0.12 | 32,32,32,32 | 0 |
| 58 | MG | 2a | 1768 | 1/1 | 0.98 | 0.12 | 44,44,44,44 | 0 |
| 58 | MG | 1A | 3731 | 1/1 | 0.98 | 0.06 | 40,40,40,40 | 0 |
| 58 | MG | 1A | 3732 | 1/1 | 0.98 | 0.05 | 25,25,25,25 | 0 |
| 58 | MG | 2A | 3856 | 1/1 | 0.98 | 0.04 | 34,34,34,34 | 0 |
| 58 | MG | 1A | 3046 | 1/1 | 0.98 | 0.03 | 18,18,18,18 | 0 |
| 58 | MG | 1U | 206 | 1/1 | 0.98 | 0.12 | 29,29,29,29 | 0 |
| 58 | MG | 2A | 3094 | 1/1 | 0.98 | 0.13 | 33,33,33,33 | 0 |
| 58 | MG | 1A | 3734 | 1/1 | 0.98 | 0.03 | 13,13,13,13 | 0 |
| 58 | MG | 1U | 208 | 1/1 | 0.98 | 0.12 | 21,21,21,21 | 0 |
| 58 | MG | 2a | 1778 | 1/1 | 0.98 | 0.05 | 54,54,54,54 | 0 |
| 58 | MG | 1A | 3010 | 1/1 | 0.98 | 0.05 | 18,18,18,18 | 0 |
| 58 | MG | 1A | 3354 | 1/1 | 0.98 | 0.21 | 19,19,19,19 | 0 |
| 58 | MG | 2A | 3331 | 1/1 | 0.98 | 0.07 | 38,38,38,38 | 0 |
| 58 | MG | 1A | 3285 | 1/1 | 0.98 | 0.11 | 16,16,16,16 | 0 |
| 58 | MG | 1V | 202 | 1/1 | 0.98 | 0.18 | 30,30,30,30 | 0 |
| 58 | MG | 1A | 3513 | 1/1 | 0.98 | 0.15 | 22,22,22,22 | 0 |
| 58 | MG | 1V | 204 | 1/1 | 0.98 | 0.23 | 22,22,22,22 | 0 |
| 58 | MG | 2A | 3103 | 1/1 | 0.98 | 0.09 | 22,22,22,22 | 0 |
| 58 | MG | 2A | 3590 | 1/1 | 0.98 | 0.08 | 40,40,40,40 | 0 |
| 58 | MG | 2A | 3591 | 1/1 | 0.98 | 0.04 | 48,48,48,48 | 0 |
| 58 | MG | 1A | 3739 | 1/1 | 0.98 | 0.08 | 30,30,30,30 | 0 |
| 58 | MG | 1A | 3135 | 1/1 | 0.98 | 0.10 | 20,20,20,20 | 0 |
| 58 | MG | 1A | 3287 | 1/1 | 0.98 | 0.27 | 20,20,20,20 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58 | MG | 2a | 1792 | 1/1 | 0.98 | 0.10 | 43,43,43,43 | 0 |
| 58 | MG | 1A | 3742 | 1/1 | 0.98 | 0.06 | 50,50,50,50 | 0 |
| 58 | MG | 1A | 3173 | 1/1 | 0.98 | 0.09 | 6,6,6,6 | 0 |
| 58 | MG | 2A | 3599 | 1/1 | 0.98 | 0.05 | 33,33,33,33 | 0 |
| 58 | MG | 1A | 3224 | 1/1 | 0.98 | 0.08 | 25,25,25,25 | 0 |
| 58 | MG | 1A | 3746 | 1/1 | 0.98 | 0.07 | 10,10,10,10 | 0 |
| 58 | MG | 1A | 3518 | 1/1 | 0.98 | 0.35 | 21,21,21,21 | 0 |
| 58 | MG | 1A | 3519 | 1/1 | 0.98 | 0.20 | 27,27,27,27 | 0 |
| 58 | MG | 1A | 3892 | 1/1 | 0.98 | 0.06 | 43,43,43,43 | 0 |
| 58 | MG | 1A | 3136 | 1/1 | 0.98 | 0.07 | 32,32,32,32 | 0 |
| 58 | MG | 1A | 3226 | 1/1 | 0.98 | 0.06 | 30,30,30,30 | 0 |
| 58 | MG | 1a | 1749 | 1/1 | 0.98 | 0.06 | 37,37,37,37 | 0 |
| 58 | MG | 2A | 3117 | 1/1 | 0.98 | 0.05 | 39,39,39,39 | 0 |
| 58 | MG | 1X | 104 | 1/1 | 0.98 | 0.15 | 33,33,33,33 | 0 |
| 58 | MG | 1X | 105 | 1/1 | 0.98 | 0.03 | 25,25,25,25 | 0 |
| 58 | MG | 1A | 3522 | 1/1 | 0.98 | 0.19 | 26,26,26,26 | 0 |
| 58 | MG | 1A | 3620 | 1/1 | 0.98 | 0.04 | 18,18,18,18 | 0 |
| 58 | MG | 1a | 1754 | 1/1 | 0.98 | 0.04 | 41,41,41,41 | 0 |
| 58 | MG | 2A | 3124 | 1/1 | 0.98 | 0.12 | 45,45,45,45 | 0 |
| 58 | MG | 1A | 4060 | 1/1 | 0.98 | 0.12 | 44,44,44,44 | 0 |
| 58 | MG | 2A | 3126 | 1/1 | 0.98 | 0.03 | 36,36,36,36 | 0 |
| 58 | MG | 1A | 3621 | 1/1 | 0.98 | 0.03 | 19,19,19,19 | 0 |
| 58 | MG | 1A | 3754 | 1/1 | 0.98 | 0.04 | 25,25,25,25 | 0 |
| 58 | MG | 1A | 3009 | 1/1 | 0.98 | 0.03 | 18,18,18,18 | 0 |
| 58 | MG | 1A | 3035 | 1/1 | 0.98 | 0.07 | 41,41,41,41 | 0 |
| 58 | MG | 1A | 3295 | 1/1 | 0.98 | 0.16 | 15,15,15,15 | 0 |
| 58 | MG | 1A | 3902 | 1/1 | 0.98 | 0.05 | 31,31,31,31 | 0 |
| 58 | MG | 1A | 3903 | 1/1 | 0.98 | 0.05 | 15,15,15,15 | 0 |
| 58 | MG | 1A | 3625 | 1/1 | 0.98 | 0.04 | 18,18,18,18 | 0 |
| 58 | MG | 2A | 3625 | 1/1 | 0.98 | 0.04 | 25,25,25,25 | 0 |
| 58 | MG | 2D | 302 | 1/1 | 0.98 | 0.14 | 38,38,38,38 | 0 |
| 58 | MG | 1A | 4071 | 1/1 | 0.98 | 0.07 | 6,6,6,6 | 0 |
| 58 | MG | 2A | 3136 | 1/1 | 0.98 | 0.04 | 34,34,34,34 | 0 |
| 58 | MG | 2D | 305 | 1/1 | 0.98 | 0.06 | 26,26,26,26 | 0 |
| 58 | MG | 2D | 306 | 1/1 | 0.98 | 0.24 | 30,30,30,30 | 0 |
| 58 | MG | 2A | 3628 | 1/1 | 0.98 | 0.04 | 29,29,29,29 | 0 |
| 58 | MG | 1a | 1765 | 1/1 | 0.98 | 0.10 | 40,40,40,40 | 0 |
| 58 | MG | 1A | 3365 | 1/1 | 0.98 | 0.06 | 37,37,37,37 | 0 |
| 58 | MG | 1A | 3761 | 1/1 | 0.98 | 0.09 | 8,8,8,8 | 0 |
| 58 | MG | 1A | 3907 | 1/1 | 0.98 | 0.06 | 35,35,35,35 | 0 |
| 58 | MG | 2E | 305 | 1/1 | 0.98 | 0.08 | 35,35,35,35 | 0 |
| 58 | MG | 1I | 101 | 1/1 | 0.98 | 0.24 | 23,23,23,23 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58 | MG | 1A | 3177 | 1/1 | 0.98 | 0.14 | 21,21,21,21 | 0 |
| 58 | MG | 1a | 1771 | 1/1 | 0.98 | 0.04 | 49,49,49,49 | 0 |
| 58 | MG | 1A | 3763 | 1/1 | 0.98 | 0.04 | 20,20,20,20 | 0 |
| 58 | MG | 2A | 3377 | 1/1 | 0.98 | 0.03 | 39,39,39,39 | 0 |
| 58 | MG | 2a | 1838 | 1/1 | 0.98 | 0.06 | 49,49,49,49 | 0 |
| 58 | MG | 1l | 104 | 1/1 | 0.98 | 0.04 | 30,30,30,30 | 0 |
| 58 | MG | 1A | 4078 | 1/1 | 0.98 | 0.03 | 19,19,19,19 | 0 |
| 58 | MG | 1A | 3629 | 1/1 | 0.98 | 0.05 | 11,11,11,11 | 0 |
| 58 | MG | 2A | 3149 | 1/1 | 0.98 | 0.11 | 27,27,27,27 | 0 |
| 58 | MG | 1a | 1777 | 1/1 | 0.98 | 0.05 | 56,56,56,56 | 0 |
| 58 | MG | 1A | 3113 | 1/1 | 0.98 | 0.12 | 25,25,25,25 | 0 |
| 58 | MG | 1A | 3233 | 1/1 | 0.98 | 0.21 | 24,24,24,24 | 0 |
| 58 | MG | 1a | 1780 | 1/1 | 0.98 | 0.05 | 40,40,40,40 | 0 |
| 58 | MG | 2A | 3648 | 1/1 | 0.98 | 0.08 | 44,44,44,44 | 0 |
| 58 | MG | 13 | 101 | 1/1 | 0.98 | 0.11 | 18,18,18,18 | 0 |
| 58 | MG | 1A | 3914 | 1/1 | 0.98 | 0.05 | 31,31,31,31 | 0 |
| 58 | MG | 13 | 103 | 1/1 | 0.98 | 0.07 | 33,33,33,33 | 0 |
| 58 | MG | 1a | 1784 | 1/1 | 0.98 | 0.05 | 57,57,57,57 | 0 |
| 58 | MG | 1a | 1785 | 1/1 | 0.98 | 0.05 | 40,40,40,40 | 0 |
| 58 | MG | 1a | 1786 | 1/1 | 0.98 | 0.04 | 44,44,44,44 | 0 |
| 58 | MG | 2A | 3160 | 1/1 | 0.98 | 0.12 | 37,37,37,37 | 0 |
| 58 | MG | 15 | 101 | 1/1 | 0.98 | 0.23 | 28,28,28,28 | 0 |
| 58 | MG | 1A | 3179 | 1/1 | 0.98 | 0.07 | 19,19,19,19 | 0 |
| 58 | MG | 1A | 3633 | 1/1 | 0.98 | 0.05 | 13,13,13,13 | 0 |
| 58 | MG | 15 | 104 | 1/1 | 0.98 | 0.15 | 20,20,20,20 | 0 |
| 58 | MG | 1a | 1791 | 1/1 | 0.98 | 0.04 | 53,53,53,53 | 0 |
| 58 | MG | 1a | 1792 | 1/1 | 0.98 | 0.03 | 33,33,33,33 | 0 |
| 58 | MG | 1A | 3769 | 1/1 | 0.98 | 0.06 | 17,17,17,17 | 0 |
| 58 | MG | 1a | 1794 | 1/1 | 0.98 | 0.03 | 51,51,51,51 | 0 |
| 58 | MG | 1A | 3634 | 1/1 | 0.98 | 0.04 | 20,20,20,20 | 0 |
| 58 | MG | 15 | 107 | 1/1 | 0.98 | 0.04 | 18,18,18,18 | 0 |
| 58 | MG | 1A | 3771 | 1/1 | 0.98 | 0.07 | 17,17,17,17 | 0 |
| 58 | MG | 1A | 3922 | 1/1 | 0.98 | 0.09 | 42,42,42,42 | 0 |
| 58 | MG | 16 | 101 | 1/1 | 0.98 | 0.05 | 32,32,32,32 | 0 |
| 58 | MG | 1a | 1800 | 1/1 | 0.98 | 0.07 | 52,52,52,52 | 0 |
| 58 | MG | 1A | 3772 | 1/1 | 0.98 | 0.04 | 21,21,21,21 | 0 |
| 58 | MG | 17 | 101 | 1/1 | 0.98 | 0.11 | 23,23,23,23 | 0 |
| 58 | MG | 2A | 3672 | 1/1 | 0.98 | 0.10 | 37,37,37,37 | 0 |
| 58 | MG | 17 | 102 | 1/1 | 0.98 | 0.20 | 31,31,31,31 | 0 |
| 58 | MG | 2A | 3178 | 1/1 | 0.98 | 0.08 | 19,19,19,19 | 0 |
| 58 | MG | 1A | 3036 | 1/1 | 0.98 | 0.09 | 21,21,21,21 | 0 |
| 58 | MG | 2A | 3412 | 1/1 | 0.98 | 0.06 | 24,24,24,24 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58 | MG | 1a | 1805 | 1/1 | 0.98 | 0.06 | 47,47,47,47 | 0 |
| 58 | MG | 2A | 3678 | 1/1 | 0.98 | 0.07 | 25,25,25,25 | 0 |
| 58 | MG | 1A | 3532 | 1/1 | 0.98 | 0.08 | 39,39,39,39 | 0 |
| 58 | MG | 1A | 3637 | 1/1 | 0.98 | 0.04 | 20,20,20,20 | 0 |
| 58 | MG | 18 | 104 | 1/1 | 0.98 | 0.04 | 28,28,28,28 | 0 |
| 58 | MG | 1A | 3182 | 1/1 | 0.98 | 0.07 | 28,28,28,28 | 0 |
| 58 | MG | 1A | 3778 | 1/1 | 0.98 | 0.05 | 40,40,40,40 | 0 |
| 58 | MG | 1A | 3450 | 1/1 | 0.98 | 0.18 | 27,27,27,27 | 0 |
| 58 | MG | 1A | 3038 | 1/1 | 0.98 | 0.11 | 28,28,28,28 | 0 |
| 58 | MG | 1A | 3082 | 1/1 | 0.98 | 0.15 | 22,22,22,22 | 0 |
| 59 | K | 1A | 3569 | 1/1 | 0.98 | 0.04 | 29,29,29,29 | 0 |
| 58 | MG | 2A | 3189 | 1/1 | 0.98 | 0.08 | 37,37,37,37 | 0 |
| 60 | ZN | 14 | 501 | 1/1 | 0.98 | 0.05 | 79,79,79,79 | 0 |
| 60 | ZN | 1n | 102 | 1/1 | 0.98 | 0.03 | 47,47,47,47 | 0 |
| 60 | ZN | 2Y | 501 | 1/1 | 0.98 | 0.04 | 70,70,70,70 | 0 |
| 58 | MG | 1A | 3643 | 1/1 | 0.98 | 0.05 | 9,9,9,9 | 0 |
| 58 | MG | 2a | 1760 | 1/1 | 0.99 | 0.04 | 62,62,62,62 | 0 |
| 58 | MG | 1A | 3288 | 1/1 | 0.99 | 0.20 | 31,31,31,31 | 0 |
| 58 | MG | 2A | 3739 | 1/1 | 0.99 | 0.05 | 38,38,38,38 | 0 |
| 58 | MG | 1A | 3129 | 1/1 | 0.99 | 0.26 | 29,29,29,29 | 0 |
| 58 | MG | 1A | 3638 | 1/1 | 0.99 | 0.03 | 12,12,12,12 | 0 |
| 58 | MG | 1A | 3075 | 1/1 | 0.99 | 0.03 | 23,23,23,23 | 0 |
| 58 | MG | 1A | 3229 | 1/1 | 0.99 | 0.12 | 30,30,30,30 | 0 |
| 58 | MG | 2a | 1767 | 1/1 | 0.99 | 0.05 | 28,28,28,28 | 0 |
| 58 | MG | 1A | 3510 | 1/1 | 0.99 | 0.04 | 26,26,26,26 | 0 |
| 58 | MG | 2a | 1769 | 1/1 | 0.99 | 0.04 | 46,46,46,46 | 0 |
| 58 | MG | 18 | 102 | 1/1 | 0.99 | 0.10 | 24,24,24,24 | 0 |
| 58 | MG | 1A | 4106 | 1/1 | 0.99 | 0.04 | 42,42,42,42 | 0 |
| 58 | MG | 1B | 201 | 1/1 | 0.99 | 0.07 | 36,36,36,36 | 0 |
| 58 | MG | 1B | 202 | 1/1 | 0.99 | 0.11 | 34,34,34,34 | 0 |
| 58 | MG | 1A | 3824 | 1/1 | 0.99 | 0.06 | 25,25,25,25 | 0 |
| 58 | MG | 1A | 3048 | 1/1 | 0.99 | 0.15 | 25,25,25,25 | 0 |
| 58 | MG | 1A | 3231 | 1/1 | 0.99 | 0.14 | 19,19,19,19 | 0 |
| 58 | MG | 1A | 3434 | 1/1 | 0.99 | 0.06 | 34,34,34,34 | 0 |
| 58 | MG | 1A | 3397 | 1/1 | 0.99 | 0.10 | 22,22,22,22 | 0 |
| 58 | MG | 1Q | 202 | 1/1 | 0.99 | 0.07 | 22,22,22,22 | 0 |
| 58 | MG | 1A | 3204 | 1/1 | 0.99 | 0.08 | 24,24,24,24 | 0 |
| 58 | MG | 1A | 3111 | 1/1 | 0.99 | 0.21 | 22,22,22,22 | 0 |
| 58 | MG | 1A | 3705 | 1/1 | 0.99 | 0.03 | 5,5,5,5 | 0 |
| 58 | MG | 1A | 3180 | 1/1 | 0.99 | 0.06 | 21,21,21,21 | 0 |
| 58 | MG | 1A | 3112 | 1/1 | 0.99 | 0.04 | 29,29,29,29 | 0 |
| 58 | MG | 1A | 3559 | 1/1 | 0.99 | 0.15 | 22,22,22,22 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58 | MG | 1A | 3157 | 1/1 | 0.99 | 0.13 | 22,22,22,22 | 0 |
| 58 | MG | 1a | 1711 | 1/1 | 0.99 | 0.08 | 29,29,29,29 | 0 |
| 58 | MG | 1A | 3403 | 1/1 | 0.99 | 0.04 | 26,26,26,26 | 0 |
| 58 | MG | 1A | 3653 | 1/1 | 0.99 | 0.04 | 23,23,23,23 | 0 |
| 58 | MG | 2A | 3640 | 1/1 | 0.99 | 0.06 | 26,26,26,26 | 0 |
| 58 | MG | 1A | 3039 | 1/1 | 0.99 | 0.28 | 22,22,22,22 | 0 |
| 58 | MG | 1A | 3078 | 1/1 | 0.99 | 0.17 | 24,24,24,24 | 0 |
| 58 | MG | 1A | 3013 | 1/1 | 0.99 | 0.06 | 12,12,12,12 | 0 |
| 58 | MG | 1A | 3609 | 1/1 | 0.99 | 0.08 | 31,31,31,31 | 0 |
| 58 | MG | 1A | 3007 | 1/1 | 0.99 | 0.04 | 29,29,29,29 | 0 |
| 58 | MG | 1A | 3270 | 1/1 | 0.99 | 0.05 | 30,30,30,30 | 0 |
| 58 | MG | 2A | 3076 | 1/1 | 0.99 | 0.15 | 28,28,28,28 | 0 |
| 58 | MG | 2A | 3527 | 1/1 | 0.99 | 0.03 | 20,20,20,20 | 0 |
| 58 | MG | 1U | 201 | 1/1 | 0.99 | 0.19 | 16,16,16,16 | 0 |
| 58 | MG | 2A | 3078 | 1/1 | 0.99 | 0.10 | 20,20,20,20 | 0 |
| 58 | MG | 2A | 3530 | 1/1 | 0.99 | 0.06 | 30,30,30,30 | 0 |
| 58 | MG | 1A | 3781 | 1/1 | 0.99 | 0.03 | 15,15,15,15 | 0 |
| 58 | MG | 1A | 3042 | 1/1 | 0.99 | 0.12 | 13,13,13,13 | 0 |
| 58 | MG | 1a | 1723 | 1/1 | 0.99 | 0.04 | 42,42,42,42 | 0 |
| 58 | MG | 1A | 3003 | 1/1 | 0.99 | 0.05 | 19,19,19,19 | 0 |
| 58 | MG | 2A | 3083 | 1/1 | 0.99 | 0.05 | 44,44,44,44 | 0 |
| 58 | MG | 1A | 3614 | 1/1 | 0.99 | 0.08 | 25,25,25,25 | 0 |
| 58 | MG | 1A | 3306 | 1/1 | 0.99 | 0.05 | 18,18,18,18 | 0 |
| 58 | MG | 1A | 3912 | 1/1 | 0.99 | 0.03 | 32,32,32,32 | 0 |
| 58 | MG | 1A | 3031 | 1/1 | 0.99 | 0.13 | 20,20,20,20 | 0 |
| 58 | MG | 2A | 3424 | 1/1 | 0.99 | 0.05 | 25,25,25,25 | 0 |
| 58 | MG | 1U | 209 | 1/1 | 0.99 | 0.22 | 24,24,24,24 | 0 |
| 58 | MG | 1a | 1730 | 1/1 | 0.99 | 0.04 | 22,22,22,22 | 0 |
| 58 | MG | 1a | 1731 | 1/1 | 0.99 | 0.10 | 25,25,25,25 | 0 |
| 58 | MG | 1A | 4055 | 1/1 | 0.99 | 0.04 | 19,19,19,19 | 0 |
| 58 | MG | 1A | 3244 | 1/1 | 0.99 | 0.24 | 23,23,23,23 | 0 |
| 58 | MG | 1A | 4057 | 1/1 | 0.99 | 0.07 | 43,43,43,43 | 0 |
| 58 | MG | 1A | 3573 | 1/1 | 0.99 | 0.14 | 31,31,31,31 | 0 |
| 58 | MG | 1A | 3667 | 1/1 | 0.99 | 0.06 | 21,21,21,21 | 0 |
| 58 | MG | 1A | 3917 | 1/1 | 0.99 | 0.03 | 26,26,26,26 | 0 |
| 58 | MG | 1V | 205 | 1/1 | 0.99 | 0.10 | 17,17,17,17 | 0 |
| 58 | MG | 1A | 3918 | 1/1 | 0.99 | 0.03 | 20,20,20,20 | 0 |
| 58 | MG | 1a | 1740 | 1/1 | 0.99 | 0.06 | 23,23,23,23 | 0 |
| 58 | MG | 1A | 3790 | 1/1 | 0.99 | 0.03 | 22,22,22,22 | 0 |
| 58 | MG | 1A | 3120 | 1/1 | 0.99 | 0.17 | 25,25,25,25 | 0 |
| 58 | MG | 1D | 302 | 1/1 | 0.99 | 0.06 | 31,31,31,31 | 0 |
| 58 | MG | 1D | 303 | 1/1 | 0.99 | 0.05 | 25,25,25,25 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58 | MG | 1a | 1745 | 1/1 | 0.99 | 0.03 | 44,44,44,44 | 0 |
| 58 | MG | 1D | 304 | 1/1 | 0.99 | 0.04 | 7,7,7,7 | 0 |
| 58 | MG | 1A | 3055 | 1/1 | 0.99 | 0.07 | 37,37,37,37 | 0 |
| 58 | MG | 1W | 206 | 1/1 | 0.99 | 0.03 | 22,22,22,22 | 0 |
| 58 | MG | 1D | 306 | 1/1 | 0.99 | 0.04 | 19,19,19,19 | 0 |
| 58 | MG | 1A | 3990 | 1/1 | 0.99 | 0.05 | 14,14,14,14 | 0 |
| 58 | MG | 1A | 3670 | 1/1 | 0.99 | 0.03 | 10,10,10,10 | 0 |
| 58 | MG | 1A | 3992 | 1/1 | 0.99 | 0.08 | 24,24,24,24 | 0 |
| 58 | MG | 2A | 3565 | 1/1 | 0.99 | 0.06 | 24,24,24,24 | 0 |
| 58 | MG | 1A | 3671 | 1/1 | 0.99 | 0.05 | 19,19,19,19 | 0 |
| 58 | MG | 1A | 4069 | 1/1 | 0.99 | 0.03 | 27,27,27,27 | 0 |
| 58 | MG | 1A | 4070 | 1/1 | 0.99 | 0.04 | 34,34,34,34 | 0 |
| 58 | MG | 1E | 301 | 1/1 | 0.99 | 0.23 | 20,20,20,20 | 0 |
| 58 | MG | 1A | 3576 | 1/1 | 0.99 | 0.18 | 32,32,32,32 | 0 |
| 58 | MG | 1A | 3673 | 1/1 | 0.99 | 0.04 | 27,27,27,27 | 0 |
| 58 | MG | 1E | 304 | 1/1 | 0.99 | 0.13 | 22,22,22,22 | 0 |
| 58 | MG | 2A | 3009 | 1/1 | 0.99 | 0.05 | 29,29,29,29 | 0 |
| 58 | MG | 2A | 3120 | 1/1 | 0.99 | 0.04 | 16,16,16,16 | 0 |
| 58 | MG | 2A | 3696 | 1/1 | 0.99 | 0.10 | 21,21,21,21 | 0 |
| 58 | MG | 1E | 305 | 1/1 | 0.99 | 0.14 | 21,21,21,21 | 0 |
| 58 | MG | 2A | 3823 | 1/1 | 0.99 | 0.07 | 25,25,25,25 | 0 |
| 58 | MG | 1A | 4073 | 1/1 | 0.99 | 0.04 | 12,12,12,12 | 0 |
| 58 | MG | 1A | 3674 | 1/1 | 0.99 | 0.05 | 12,12,12,12 | 0 |
| 58 | MG | 1A | 3143 | 1/1 | 0.99 | 0.10 | 20,20,20,20 | 0 |
| 58 | MG | 1A | 3278 | 1/1 | 0.99 | 0.07 | 31,31,31,31 | 0 |
| 58 | MG | 10 | 103 | 1/1 | 0.99 | 0.14 | 28,28,28,28 | 0 |
| 58 | MG | 1A | 3068 | 1/1 | 0.99 | 0.03 | 19,19,19,19 | 0 |
| 58 | MG | 2A | 3830 | 1/1 | 0.99 | 0.07 | 25,25,25,25 | 0 |
| 58 | MG | 2A | 3831 | 1/1 | 0.99 | 0.04 | 36,36,36,36 | 0 |
| 58 | MG | 1A | 3045 | 1/1 | 0.99 | 0.06 | 23,23,23,23 | 0 |
| 58 | MG | 2A | 3833 | 1/1 | 0.99 | 0.03 | 43,43,43,43 | 0 |
| 58 | MG | 2A | 3466 | 1/1 | 0.99 | 0.06 | 14,14,14,14 | 0 |
| 58 | MG | 1A | 3679 | 1/1 | 0.99 | 0.02 | 11,11,11,11 | 0 |
| 58 | MG | 1E | 313 | 1/1 | 0.99 | 0.08 | 25,25,25,25 | 0 |
| 58 | MG | 1A | 3383 | 1/1 | 0.99 | 0.15 | 21,21,21,21 | 0 |
| 58 | MG | 1A | 3627 | 1/1 | 0.99 | 0.12 | 39,39,39,39 | 0 |
| 58 | MG | 1F | 302 | 1/1 | 0.99 | 0.09 | 13,13,13,13 | 0 |
| 58 | MG | 1A | 3037 | 1/1 | 0.99 | 0.09 | 15,15,15,15 | 0 |
| 58 | MG | 1A | 3460 | 1/1 | 0.99 | 0.13 | 32,32,32,32 | 0 |
| 58 | MG | 1a | 1775 | 1/1 | 0.99 | 0.03 | 42,42,42,42 | 0 |
| 58 | MG | 2A | 3843 | 1/1 | 0.99 | 0.04 | 21,21,21,21 | 0 |
| 58 | MG | 1A | 3743 | 1/1 | 0.99 | 0.03 | 39,39,39,39 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58 | MG | 1F | 306 | 1/1 | 0.99 | 0.03 | 28,28,28,28 | 0 |
| 58 | MG | 2A | 3139 | 1/1 | 0.99 | 0.10 | 27,27,27,27 | 0 |
| 58 | MG | 2A | 3595 | 1/1 | 0.99 | 0.06 | 29,29,29,29 | 0 |
| 58 | MG | 2A | 3596 | 1/1 | 0.99 | 0.03 | 27,27,27,27 | 0 |
| 58 | MG | 1A | 4007 | 1/1 | 0.99 | 0.03 | 22,22,22,22 | 0 |
| 58 | MG | 1A | 4086 | 1/1 | 0.99 | 0.03 | 16,16,16,16 | 0 |
| 58 | MG | 1A | 3937 | 1/1 | 0.99 | 0.03 | 16,16,16,16 | 0 |
| 58 | MG | 1A | 3282 | 1/1 | 0.99 | 0.14 | 21,21,21,21 | 0 |
| 58 | MG | 1A | 3809 | 1/1 | 0.99 | 0.03 | 14,14,14,14 | 0 |
| 58 | MG | 1A | 3058 | 1/1 | 0.99 | 0.02 | 16,16,16,16 | 0 |
| 58 | MG | 2A | 3726 | 1/1 | 0.99 | 0.11 | 26,26,26,26 | 0 |
| 58 | MG | 2A | 3034 | 1/1 | 0.99 | 0.10 | 32,32,32,32 | 0 |
| 58 | MG | 1A | 3941 | 1/1 | 0.99 | 0.05 | 18,18,18,18 | 0 |
| 58 | MG | 1A | 3148 | 1/1 | 0.99 | 0.13 | 14,14,14,14 | 0 |
| 58 | MG | 1A | 3687 | 1/1 | 0.99 | 0.04 | 17,17,17,17 | 0 |
| 58 | MG | 2A | 3731 | 1/1 | 0.99 | 0.03 | 24,24,24,24 | 0 |
| 58 | MG | 1A | 3072 | 1/1 | 0.99 | 0.22 | 21,21,21,21 | 0 |
| 58 | MG | 1A | 3689 | 1/1 | 0.99 | 0.03 | 11,11,11,11 | 0 |
| 60 | ZN | 1Y | 204 | 1/1 | 0.99 | 0.02 | 54,54,54,54 | 0 |
| 58 | MG | 1A | 3690 | 1/1 | 0.99 | 0.04 | 16,16,16,16 | 0 |
| 60 | ZN | 19 | 102 | 1/1 | 0.99 | 0.03 | 31,31,31,31 | 0 |
| 58 | MG | 1A | 3073 | 1/1 | 0.99 | 0.04 | 8,8,8,8 | 0 |
| 58 | MG | 1A | 3023 | 1/1 | 0.99 | 0.06 | 6,6,6,6 | 0 |
| 58 | MG | 1A | 4020 | 1/1 | 0.99 | 0.02 | 21,21,21,21 | 0 |
| 60 | ZN | 25 | 105 | 1/1 | 0.99 | 0.06 | 50,50,50,50 | 0 |
| 60 | ZN | 29 | 102 | 1/1 | 0.99 | 0.03 | 62,62,62,62 | 0 |
| 60 | ZN | 2n | 501 | 1/1 | 0.99 | 0.03 | 68,68,68,68 | 0 |
| 61 | SF4 | 1d | 302 | 8/8 | 0.99 | 0.04 | 45,51,56,57 | 0 |
| 61 | SF4 | 2d | 302 | 8/8 | 0.99 | 0.03 | 45,53,60,64 | 0 |
| 60 | ZN | 15 | 110 | 1/1 | 1.00 | 0.04 | 28,28,28,28 | 0 |
| 60 | ZN | 16 | 103 | 1/1 | 1.00 | 0.02 | 30,30,30,30 | 0 |
| 58 | MG | 1A | 3724 | 1/1 | 1.00 | 0.04 | 5,5,5,5 | 0 |
| 58 | MG | 2A | 3635 | 1/1 | 1.00 | 0.04 | 27,27,27,27 | 0 |
| 58 | MG | 1A | 3780 | 1/1 | 1.00 | 0.02 | 21,21,21,21 | 0 |
| 58 | MG | 1P | 204 | 1/1 | 1.00 | 0.05 | 23,23,23,23 | 0 |
| 58 | MG | 1A | 4036 | 1/1 | 1.00 | 0.02 | 13,13,13,13 | 0 |
| 60 | ZN | 26 | 102 | 1/1 | 1.00 | 0.02 | 43,43,43,43 | 0 |
| 58 | MG | 1A | 3014 | 1/1 | 1.00 | 0.08 | 16,16,16,16 | 0 |
| 58 | MG | 1A | 3777 | 1/1 | 1.00 | 0.02 | 23,23,23,23 | 0 |
| 58 | MG | 1A | 3756 | 1/1 | 1.00 | 0.04 | 10,10,10,10 | 0 |
| 58 | MG | 2A | 3714 | 1/1 | 1.00 | 0.04 | 13,13,13,13 | 0 |

6.5 Other polymers [i](#)

There are no such residues in this entry.