



## Full wwPDB X-ray Structure Validation Report ⓘ

Sep 2, 2026 – 10:06 PM EDT

PDB ID : 9Q6V / pdb\_00009q6v  
Title : Crystal structure of the wild-type *Thermus thermophilus* 70S ribosome in complex with tiamulin-31 triazole derivative and protein Y at 2.85Å resolution  
Authors : Killam, B.Y.; Kopec, I.; Breiner, L.M.; Hoernig, M.; LoPresti, M.; Abdelsattar, A.S.; Abouelkhair, A.A.; Briganti, A.J.; Slowinski, R.P.; Vogelaar, N.J.; Seleem, M.N.; Brown, A.M.; Lowell, A.N.; Polikanov, Y.S.  
Deposited on : 2025-08-22  
Resolution : 2.85 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| MolProbity                     | : | 4-5-2 with Phenix2.0                                             |
| Mogul                          | : | 2022.3.0, CSD as543be (2022)                                     |
| Xtriage (Phenix)               | : | 2.0                                                              |
| EDS                            | : | 3.0                                                              |
| Buster-report                  | : | wwPDB partial adaption of 1.1.7 (2018)                           |
| Percentile statistics          | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| CCP4                           | : | 9.0.015 (Gargrove)                                               |
| Density-Fitness                | : | 1.0.12                                                           |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)                                              |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)                                          |
| Validation Pipeline (wwPDB-VP) | : | 2.50                                                             |

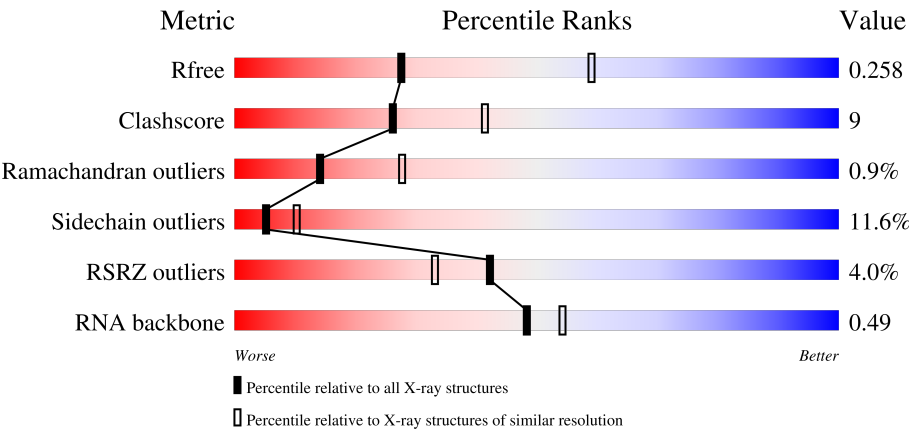
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.85 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<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| R <sub>free</sub>     | 180053                      | 1407 (2.88-2.84)                                      |
| Clashscore            | 190562                      | 1446 (2.88-2.84)                                      |
| Ramachandran outliers | 187476                      | 1406 (2.88-2.84)                                      |
| Sidechain outliers    | 187428                      | 1407 (2.88-2.84)                                      |
| RSRZ outliers         | 180081                      | 1408 (2.88-2.84)                                      |
| RNA backbone          | 3983                        | 1009 (3.06-2.66)                                      |

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  $\geq 3$ , 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>4%</div><div>63%</div><div>29%</div><div>6%</div><div></div></div> |
| 1   | 2A    | 2915   | <div><div>4%</div><div>56%</div><div>34%</div><div>8%</div><div></div></div> |
| 2   | 1B    | 121    | <div><div></div><div>71%</div><div>26%</div><div></div><div></div></div>     |
| 2   | 2B    | 121    | <div><div>%</div><div>60%</div><div>31%</div><div>8%</div><div></div></div>  |

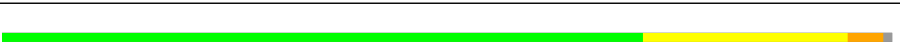
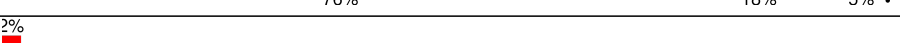
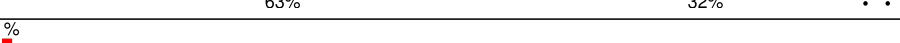
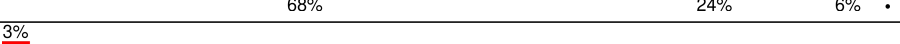
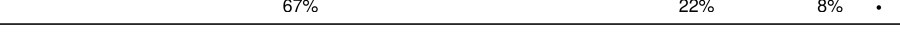
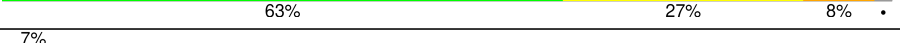
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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 3   | 1D    | 276    |    |
| 3   | 2D    | 276    |    |
| 4   | 1E    | 206    |    |
| 4   | 2E    | 206    |    |
| 5   | 1F    | 210    |    |
| 5   | 2F    | 210    |    |
| 6   | 1G    | 182    |    |
| 6   | 2G    | 182    |    |
| 7   | 1H    | 180    |    |
| 7   | 2H    | 180    |    |
| 8   | 1I    | 148    |    |
| 8   | 2I    | 148    |   |
| 9   | 1N    | 140    |  |
| 9   | 2N    | 140    |  |
| 10  | 1O    | 122    |  |
| 10  | 2O    | 122    |  |
| 11  | 1P    | 150    |  |
| 11  | 2P    | 150    |  |
| 12  | 1Q    | 141    |  |
| 12  | 2Q    | 141    |  |
| 13  | 1R    | 118    |  |
| 13  | 2R    | 118    |  |
| 14  | 1S    | 112    |  |
| 14  | 2S    | 112    |  |
| 15  | 1T    | 146    |  |

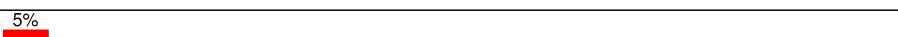
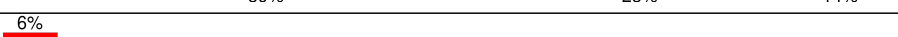
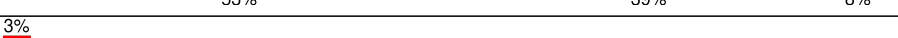
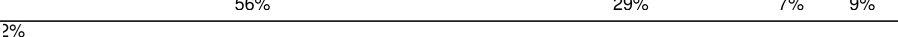
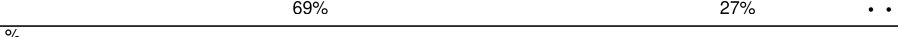
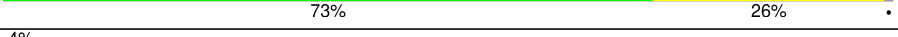
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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 15  | 2T    | 146    |    |
| 16  | 1U    | 118    |    |
| 16  | 2U    | 118    |    |
| 17  | 1V    | 101    |    |
| 17  | 2V    | 101    |    |
| 18  | 1W    | 113    |    |
| 18  | 2W    | 113    |    |
| 19  | 1X    | 96     |    |
| 19  | 2X    | 96     |    |
| 20  | 1Y    | 110    |    |
| 20  | 2Y    | 110    |    |
| 21  | 1Z    | 206    |    |
| 21  | 2Z    | 206    |  |
| 22  | 10    | 85     |  |
| 22  | 20    | 85     |  |
| 23  | 11    | 98     |  |
| 23  | 21    | 98     |  |
| 24  | 12    | 72     |  |
| 24  | 22    | 72     |  |
| 25  | 13    | 60     |  |
| 25  | 23    | 60     |  |
| 26  | 14    | 71     |  |
| 26  | 24    | 71     |  |
| 27  | 15    | 60     |  |
| 27  | 25    | 60     |  |

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

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

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 53  | 1y    | 113    |                  |
| 53  | 2y    | 113    |                  |

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 |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 59  | SF4  | 2d    | 501 | -         | -        | X       | -                |



## 2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 298337 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    | 2872     | Total | C     | N     | O     | P    | 0       | 0       | 0     |
|     |       |          | 61869 | 27540 | 11574 | 19884 | 2871 |         |         |       |
| 1   | 2A    | 2867     | Total | C     | N     | O     | P    | 0       | 0       | 0     |
|     |       |          | 61758 | 27491 | 11552 | 19850 | 2865 |         |         |       |

- 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     |
|     |       |          | 2572  | 1145 | 476 | 832 | 119 |         |         |       |
| 2   | 2B    | 120      | Total | C    | N   | O   | P   | 0       | 0       | 0     |
|     |       |          | 2573  | 1146 | 476 | 832 | 119 |         |         |       |

- 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     |
|     |       |          | 2131  | 1346 | 422 | 360 | 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     |
|     |       |          | 1426  | 916 | 253 | 253 | 4 |         |         |       |
| 6   | 2G    | 181      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1424  | 912 | 259 | 249 | 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    | 173      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1324  | 842 | 247 | 234 | 1 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 8   | 1I    | 147      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1094  | 699 | 191 | 203 | 1 |         |         |       |
| 8   | 2I    | 146      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1076  | 687 | 186 | 202 | 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     |
|     |       |          | 1121  | 722 | 208 | 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     |
|     |       |          | 877   | 553 | 175 | 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     |
|     |       |          | 775   | 498 | 141 | 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     |
|     |       |          | 810   | 520 | 153 | 131 | 6 |         |         |       |
| 20  | 2Y    | 107      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 810   | 519 | 153 | 132 | 6 |         |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 21  | 1Z    | 203      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1587  | 1011 | 282 | 292 | 2 |         |         |       |
| 21  | 2Z    | 201      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1557  | 995  | 274 | 286 | 2 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 22  | 10    | 77       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 608   | 375 | 129 | 103 | 1 |         |         |       |
| 22  | 20    | 77       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 608   | 375 | 129 | 103 | 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     |
|     |       |          | 754   | 475 | 148 | 130 | 1 |         |         |       |
| 23  | 21    | 97       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 759   | 478 | 149 | 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     |
|     |       |          | 592   | 368 | 119 | 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     |
|     |       |          | 546   | 346 | 96 | 99 | 5 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 26  | 24    | 69       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 536   | 342 | 98 | 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     |
|     |       |          | 459   | 288 | 90 | 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    | 1504     | Total | C     | N    | O     | P    | 0       | 0       | 0     |
|     |       |          | 32331 | 14396 | 5990 | 10441 | 1504 |         |         |       |

- 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     |
|     |       |          | 1842  | 1175 | 330 | 332 | 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     |
|     |       |          | 1558  | 979 | 305 | 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     |
|     |       |          | 1665  | 1043 | 329 | 286 | 7 |         |         |       |
| 35  | 2d    | 208      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1668  | 1047 | 330 | 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     |
|     |       |          | 1133  | 716 | 214 | 199 | 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     |
|     |       |          | 814   | 516 | 144 | 151 | 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     |
|     |       |          | 1235  | 769 | 244 | 216 | 6 |         |         |       |
| 38  | 2g    | 155      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1229  | 766 | 241 | 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     |
|     |       |          | 1098  | 694 | 210 | 192 | 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     |
|     |       |          | 986   | 625 | 193 | 168 |         |         |       |
| 40  | 2i    | 126      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 966   | 613 | 186 | 167 |         |         |       |

- 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     |
|     |       |          | 719   | 446 | 142 | 131 |         |         |       |
| 41  | 2j    | 96       | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 710   | 442 | 137 | 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     |
|     |       |          | 834   | 520 | 156 | 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    | 116      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 914   | 564 | 189 | 159 | 2 |         |         |       |
| 44  | 2m    | 114      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 895   | 550 | 186 | 157 | 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     |
|     |       |          | 648   | 415 | 120 | 111 | 2 |         |         |       |
| 50  | 2s    | 83       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 645   | 410 | 118 | 115 | 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     |
|     |       |          | 732   | 449 | 157 | 124 | 2 |         |         |       |
| 51  | 2t    | 98       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 733   | 451 | 154 | 126 | 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 protein called Ribosome-associated inhibitor A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 53  | 1y    | 97       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 764   | 478 | 144 | 139 | 3 |         |         |       |
| 53  | 2y    | 96       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 749   | 468 | 141 | 137 | 3 |         |         |       |

- Molecule 54 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |      | ZeroOcc | AltConf |
|-----|-------|----------|-------|------|---------|---------|
| 54  | 1A    | 1049     | Total | Mg   | 0       | 0       |
|     |       |          | 1049  | 1049 |         |         |
| 54  | 1B    | 30       | Total | Mg   | 0       | 0       |
|     |       |          | 30    | 30   |         |         |
| 54  | 1D    | 21       | Total | Mg   | 0       | 0       |
|     |       |          | 21    | 21   |         |         |
| 54  | 1E    | 8        | Total | Mg   | 0       | 0       |
|     |       |          | 8     | 8    |         |         |
| 54  | 1F    | 18       | Total | Mg   | 0       | 0       |
|     |       |          | 18    | 18   |         |         |
| 54  | 1G    | 4        | Total | Mg   | 0       | 0       |
|     |       |          | 4     | 4    |         |         |
| 54  | 1H    | 3        | Total | Mg   | 0       | 0       |
|     |       |          | 3     | 3    |         |         |
| 54  | 1N    | 2        | Total | Mg   | 0       | 0       |
|     |       |          | 2     | 2    |         |         |
| 54  | 1O    | 2        | Total | Mg   | 0       | 0       |
|     |       |          | 2     | 2    |         |         |
| 54  | 1P    | 6        | Total | Mg   | 0       | 0       |
|     |       |          | 6     | 6    |         |         |
| 54  | 1Q    | 6        | Total | Mg   | 0       | 0       |
|     |       |          | 6     | 6    |         |         |
| 54  | 1R    | 4        | Total | Mg   | 0       | 0       |
|     |       |          | 4     | 4    |         |         |
| 54  | 1S    | 2        | Total | Mg   | 0       | 0       |
|     |       |          | 2     | 2    |         |         |
| 54  | 1T    | 4        | Total | Mg   | 0       | 0       |
|     |       |          | 4     | 4    |         |         |
| 54  | 1U    | 6        | Total | Mg   | 0       | 0       |
|     |       |          | 6     | 6    |         |         |
| 54  | 1V    | 6        | Total | Mg   | 0       | 0       |
|     |       |          | 6     | 6    |         |         |
| 54  | 1W    | 3        | Total | Mg   | 0       | 0       |
|     |       |          | 3     | 3    |         |         |
| 54  | 1X    | 1        | Total | Mg   | 0       | 0       |
|     |       |          | 1     | 1    |         |         |

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| Mol | Chain | Residues | Atoms        |           | ZeroOcc | AltConf |
|-----|-------|----------|--------------|-----------|---------|---------|
| 54  | 1Y    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 54  | 1Z    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 54  | 10    | 7        | Total<br>7   | Mg<br>7   | 0       | 0       |
| 54  | 11    | 5        | Total<br>5   | Mg<br>5   | 0       | 0       |
| 54  | 13    | 3        | Total<br>3   | Mg<br>3   | 0       | 0       |
| 54  | 15    | 8        | Total<br>8   | Mg<br>8   | 0       | 0       |
| 54  | 16    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 54  | 17    | 5        | Total<br>5   | Mg<br>5   | 0       | 0       |
| 54  | 18    | 3        | Total<br>3   | Mg<br>3   | 0       | 0       |
| 54  | 19    | 3        | Total<br>3   | Mg<br>3   | 0       | 0       |
| 54  | 1a    | 282      | Total<br>282 | Mg<br>282 | 0       | 0       |
| 54  | 1b    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 54  | 1d    | 5        | Total<br>5   | Mg<br>5   | 0       | 0       |
| 54  | 1e    | 3        | Total<br>3   | Mg<br>3   | 0       | 0       |
| 54  | 1f    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 54  | 1g    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 54  | 1h    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 54  | 1i    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 54  | 1k    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 54  | 1l    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 54  | 1m    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |

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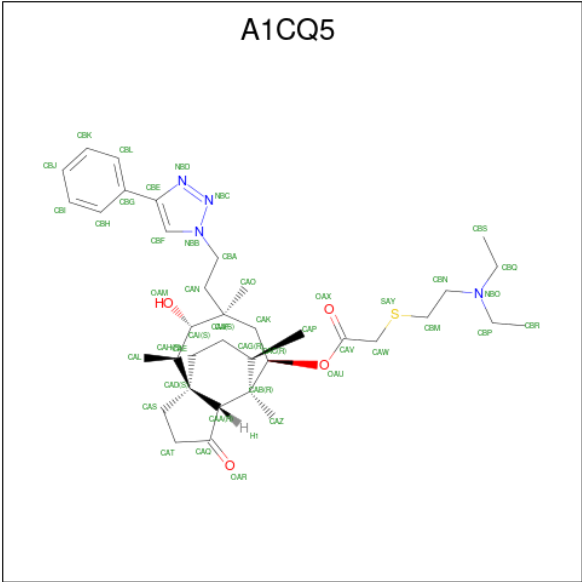
| Mol | Chain | Residues | Atoms        |           | ZeroOcc | AltConf |
|-----|-------|----------|--------------|-----------|---------|---------|
| 54  | 1n    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 54  | 1o    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 54  | 1p    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 54  | 1t    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 54  | 1y    | 4        | Total<br>4   | Mg<br>4   | 0       | 0       |
| 54  | 2A    | 756      | Total<br>756 | Mg<br>756 | 0       | 0       |
| 54  | 2B    | 19       | Total<br>19  | Mg<br>19  | 0       | 0       |
| 54  | 2D    | 11       | Total<br>11  | Mg<br>11  | 0       | 0       |
| 54  | 2E    | 7        | Total<br>7   | Mg<br>7   | 0       | 0       |
| 54  | 2F    | 5        | Total<br>5   | Mg<br>5   | 0       | 0       |
| 54  | 2G    | 3        | Total<br>3   | Mg<br>3   | 0       | 0       |
| 54  | 2I    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 54  | 2N    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 54  | 2O    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 54  | 2P    | 3        | Total<br>3   | Mg<br>3   | 0       | 0       |
| 54  | 2Q    | 4        | Total<br>4   | Mg<br>4   | 0       | 0       |
| 54  | 2R    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 54  | 2T    | 4        | Total<br>4   | Mg<br>4   | 0       | 0       |
| 54  | 2V    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 54  | 2W    | 3        | Total<br>3   | Mg<br>3   | 0       | 0       |
| 54  | 2X    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |

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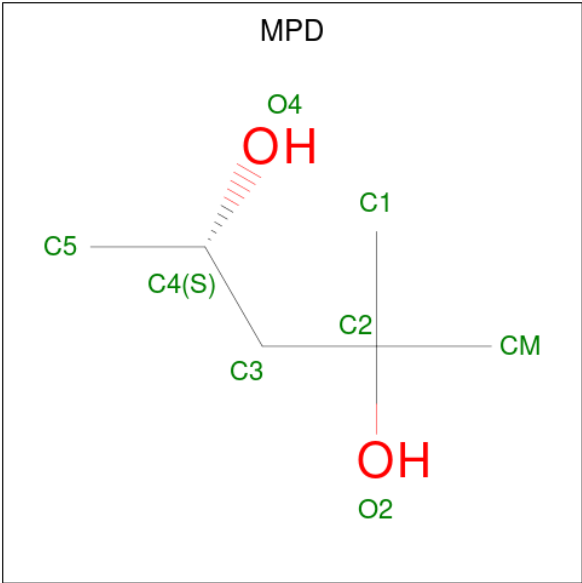
| Mol | Chain | Residues | Atoms               | ZeroOcc | AltConf |
|-----|-------|----------|---------------------|---------|---------|
| 54  | 2Y    | 1        | Total Mg<br>1 1     | 0       | 0       |
| 54  | 20    | 1        | Total Mg<br>1 1     | 0       | 0       |
| 54  | 21    | 2        | Total Mg<br>2 2     | 0       | 0       |
| 54  | 23    | 1        | Total Mg<br>1 1     | 0       | 0       |
| 54  | 25    | 2        | Total Mg<br>2 2     | 0       | 0       |
| 54  | 27    | 2        | Total Mg<br>2 2     | 0       | 0       |
| 54  | 28    | 2        | Total Mg<br>2 2     | 0       | 0       |
| 54  | 2a    | 193      | Total Mg<br>193 193 | 0       | 0       |
| 54  | 2e    | 1        | Total Mg<br>1 1     | 0       | 0       |
| 54  | 2f    | 1        | Total Mg<br>1 1     | 0       | 0       |
| 54  | 2j    | 1        | Total Mg<br>1 1     | 0       | 0       |
| 54  | 2k    | 1        | Total Mg<br>1 1     | 0       | 0       |
| 54  | 2n    | 1        | Total Mg<br>1 1     | 0       | 0       |
| 54  | 2p    | 1        | Total Mg<br>1 1     | 0       | 0       |
| 54  | 2q    | 1        | Total Mg<br>1 1     | 0       | 0       |
| 54  | 2r    | 1        | Total Mg<br>1 1     | 0       | 0       |
| 54  | 2t    | 1        | Total Mg<br>1 1     | 0       | 0       |
| 54  | 2y    | 1        | Total Mg<br>1 1     | 0       | 0       |

- Molecule 55 is (3aS,4R,5S,6S,8R,9R,9aR,10R)-5-hydroxy-4,6,9,10-tetramethyl-1-oxo-6-[2-(4-phenyl-1H-1,2,3-triazol-1-yl)ethyl]decahydro-3a,9-propanocyclopenta[8]annulen-8-yl {[2-(diethylamino)ethyl]sulfanyl}acetate (CCD ID: A1CQ5) (formula: C<sub>36</sub>H<sub>54</sub>N<sub>4</sub>O<sub>4</sub>S) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |    |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|---------|
| 55  | 1A    | 1        | Total | C  | N | O | S | 0       | 0       |
|     |       |          | 45    | 36 | 4 | 4 | 1 |         |         |
| 55  | 2A    | 1        | Total | C  | N | O | S | 0       | 0       |
|     |       |          | 45    | 36 | 4 | 4 | 1 |         |         |

- Molecule 56 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>2</sub>).



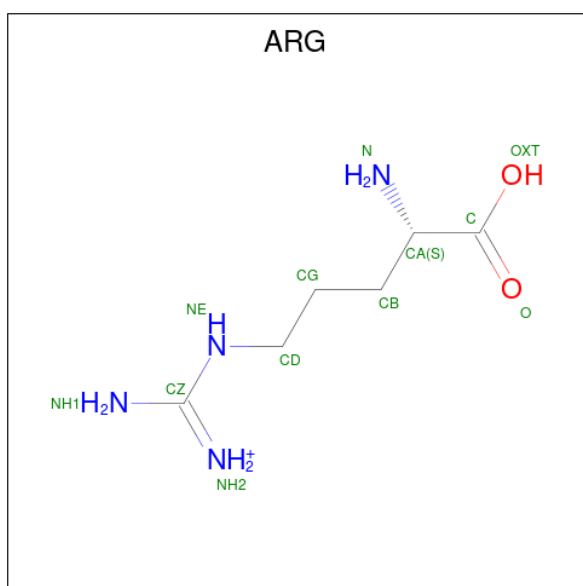
| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 56  | 1A    | 1        | Total | C | O | 0       | 0       |
|     |       |          | 8     | 6 | 2 |         |         |
| 56  | 1O    | 1        | Total | C | O | 0       | 0       |
|     |       |          | 8     | 6 | 2 |         |         |

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| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 56  | 18    | 1        | Total | C | O | 0       | 0       |
|     |       |          | 8     | 6 | 2 |         |         |
| 56  | 1a    | 1        | Total | C | O | 0       | 0       |
|     |       |          | 8     | 6 | 2 |         |         |
| 56  | 2A    | 1        | Total | C | O | 0       | 0       |
|     |       |          | 8     | 6 | 2 |         |         |
| 56  | 2A    | 1        | Total | C | O | 0       | 0       |
|     |       |          | 8     | 6 | 2 |         |         |
| 56  | 2B    | 1        | Total | C | O | 0       | 0       |
|     |       |          | 8     | 6 | 2 |         |         |

- Molecule 57 is ARGinine (CCD ID: ARG) (formula:  $C_6H_{15}N_4O_2$ ).



| Mol | Chain | Residues | Atoms |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---------|---------|
| 57  | 1B    | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 12    | 6 | 4 | 2 |         |         |

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

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 58  | 1Y    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 58  | 14    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 58  | 15    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

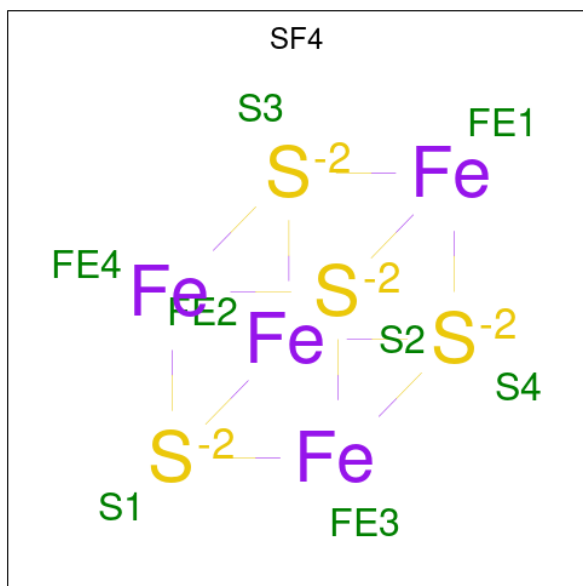
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| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 58  | 16    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 58  | 19    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 58  | 1n    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 58  | 2Y    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 58  | 24    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 58  | 25    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 58  | 26    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 58  | 29    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 58  | 2n    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

- Molecule 59 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula:  $\text{Fe}_4\text{S}_4$ ).



| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 59  | 1d    | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 8     | 4  | 4 |         |         |
| 59  | 2d    | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 8     | 4  | 4 |         |         |

- Molecule 60 is water.

| Mol | Chain | Residues | Atoms                | ZeroOcc | AltConf |
|-----|-------|----------|----------------------|---------|---------|
| 60  | 1A    | 4087     | Total O<br>4087 4087 | 0       | 0       |
| 60  | 1B    | 107      | Total O<br>107 107   | 0       | 0       |
| 60  | 1D    | 109      | Total O<br>109 109   | 0       | 0       |
| 60  | 1E    | 73       | Total O<br>73 73     | 0       | 0       |
| 60  | 1F    | 66       | Total O<br>66 66     | 0       | 0       |
| 60  | 1G    | 19       | Total O<br>19 19     | 0       | 0       |
| 60  | 1H    | 15       | Total O<br>15 15     | 0       | 0       |
| 60  | 1I    | 7        | Total O<br>7 7       | 0       | 0       |
| 60  | 1N    | 53       | Total O<br>53 53     | 0       | 0       |
| 60  | 1O    | 26       | Total O<br>26 26     | 0       | 0       |
| 60  | 1P    | 58       | Total O<br>58 58     | 0       | 0       |
| 60  | 1Q    | 42       | Total O<br>42 42     | 0       | 0       |
| 60  | 1R    | 31       | Total O<br>31 31     | 0       | 0       |
| 60  | 1S    | 8        | Total O<br>8 8       | 0       | 0       |
| 60  | 1T    | 28       | Total O<br>28 28     | 0       | 0       |
| 60  | 1U    | 49       | Total O<br>49 49     | 0       | 0       |
| 60  | 1V    | 42       | Total O<br>42 42     | 0       | 0       |
| 60  | 1W    | 32       | Total O<br>32 32     | 0       | 0       |
| 60  | 1X    | 27       | Total O<br>27 27     | 0       | 0       |
| 60  | 1Y    | 20       | Total O<br>20 20     | 0       | 0       |
| 60  | 1Z    | 10       | Total O<br>10 10     | 0       | 0       |

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| Mol | Chain | Residues | Atoms        |          | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 60  | 10    | 22       | Total<br>22  | O<br>22  | 0       | 0       |
| 60  | 11    | 25       | Total<br>25  | O<br>25  | 0       | 0       |
| 60  | 12    | 12       | Total<br>12  | O<br>12  | 0       | 0       |
| 60  | 13    | 25       | Total<br>25  | O<br>25  | 0       | 0       |
| 60  | 14    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 60  | 15    | 26       | Total<br>26  | O<br>26  | 0       | 0       |
| 60  | 16    | 18       | Total<br>18  | O<br>18  | 0       | 0       |
| 60  | 17    | 16       | Total<br>16  | O<br>16  | 0       | 0       |
| 60  | 18    | 32       | Total<br>32  | O<br>32  | 0       | 0       |
| 60  | 19    | 12       | Total<br>12  | O<br>12  | 0       | 0       |
| 60  | 1a    | 596      | Total<br>596 | O<br>596 | 0       | 0       |
| 60  | 1b    | 2        | Total<br>2   | O<br>2   | 0       | 0       |
| 60  | 1d    | 7        | Total<br>7   | O<br>7   | 0       | 0       |
| 60  | 1e    | 6        | Total<br>6   | O<br>6   | 0       | 0       |
| 60  | 1f    | 2        | Total<br>2   | O<br>2   | 0       | 0       |
| 60  | 1h    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 60  | 1j    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 60  | 1l    | 6        | Total<br>6   | O<br>6   | 0       | 0       |
| 60  | 1m    | 2        | Total<br>2   | O<br>2   | 0       | 0       |
| 60  | 1n    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 60  | 1o    | 3        | Total<br>3   | O<br>3   | 0       | 0       |

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| Mol | Chain | Residues | Atoms         |           | ZeroOcc | AltConf |
|-----|-------|----------|---------------|-----------|---------|---------|
| 60  | 1p    | 3        | Total<br>3    | O<br>3    | 0       | 0       |
| 60  | 1q    | 1        | Total<br>1    | O<br>1    | 0       | 0       |
| 60  | 1t    | 1        | Total<br>1    | O<br>1    | 0       | 0       |
| 60  | 1u    | 2        | Total<br>2    | O<br>2    | 0       | 0       |
| 60  | 1y    | 9        | Total<br>9    | O<br>9    | 0       | 0       |
| 60  | 2A    | 2546     | Total<br>2546 | O<br>2546 | 0       | 0       |
| 60  | 2B    | 60       | Total<br>60   | O<br>60   | 0       | 0       |
| 60  | 2D    | 50       | Total<br>50   | O<br>50   | 0       | 0       |
| 60  | 2E    | 36       | Total<br>36   | O<br>36   | 0       | 0       |
| 60  | 2F    | 25       | Total<br>25   | O<br>25   | 0       | 0       |
| 60  | 2G    | 8        | Total<br>8    | O<br>8    | 0       | 0       |
| 60  | 2H    | 2        | Total<br>2    | O<br>2    | 0       | 0       |
| 60  | 2I    | 4        | Total<br>4    | O<br>4    | 0       | 0       |
| 60  | 2N    | 8        | Total<br>8    | O<br>8    | 0       | 0       |
| 60  | 2O    | 20       | Total<br>20   | O<br>20   | 0       | 0       |
| 60  | 2P    | 30       | Total<br>30   | O<br>30   | 0       | 0       |
| 60  | 2Q    | 18       | Total<br>18   | O<br>18   | 0       | 0       |
| 60  | 2R    | 19       | Total<br>19   | O<br>19   | 0       | 0       |
| 60  | 2S    | 5        | Total<br>5    | O<br>5    | 0       | 0       |
| 60  | 2T    | 10       | Total<br>10   | O<br>10   | 0       | 0       |
| 60  | 2U    | 12       | Total<br>12   | O<br>12   | 0       | 0       |

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| Mol | Chain | Residues | Atoms        |          | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 60  | 2V    | 9        | Total<br>9   | O<br>9   | 0       | 0       |
| 60  | 2W    | 25       | Total<br>25  | O<br>25  | 0       | 0       |
| 60  | 2X    | 9        | Total<br>9   | O<br>9   | 0       | 0       |
| 60  | 2Y    | 7        | Total<br>7   | O<br>7   | 0       | 0       |
| 60  | 2Z    | 11       | Total<br>11  | O<br>11  | 0       | 0       |
| 60  | 20    | 16       | Total<br>16  | O<br>16  | 0       | 0       |
| 60  | 21    | 22       | Total<br>22  | O<br>22  | 0       | 0       |
| 60  | 22    | 2        | Total<br>2   | O<br>2   | 0       | 0       |
| 60  | 23    | 3        | Total<br>3   | O<br>3   | 0       | 0       |
| 60  | 24    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 60  | 25    | 7        | Total<br>7   | O<br>7   | 0       | 0       |
| 60  | 26    | 7        | Total<br>7   | O<br>7   | 0       | 0       |
| 60  | 27    | 13       | Total<br>13  | O<br>13  | 0       | 0       |
| 60  | 28    | 15       | Total<br>15  | O<br>15  | 0       | 0       |
| 60  | 29    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 60  | 2a    | 461      | Total<br>461 | O<br>461 | 0       | 0       |
| 60  | 2d    | 4        | Total<br>4   | O<br>4   | 0       | 0       |
| 60  | 2e    | 2        | Total<br>2   | O<br>2   | 0       | 0       |
| 60  | 2f    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 60  | 2j    | 2        | Total<br>2   | O<br>2   | 0       | 0       |
| 60  | 2l    | 3        | Total<br>3   | O<br>3   | 0       | 0       |

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| Mol | Chain | Residues | Atoms      |        | ZeroOcc | AltConf |
|-----|-------|----------|------------|--------|---------|---------|
| 60  | 2o    | 3        | Total<br>3 | O<br>3 | 0       | 0       |
| 60  | 2p    | 2        | Total<br>2 | O<br>2 | 0       | 0       |
| 60  | 2q    | 1        | Total<br>1 | O<br>1 | 0       | 0       |
| 60  | 2r    | 4        | Total<br>4 | O<br>4 | 0       | 0       |
| 60  | 2t    | 2        | Total<br>2 | O<br>2 | 0       | 0       |
| 60  | 2y    | 4        | Total<br>4 | O<br>4 | 0       | 0       |

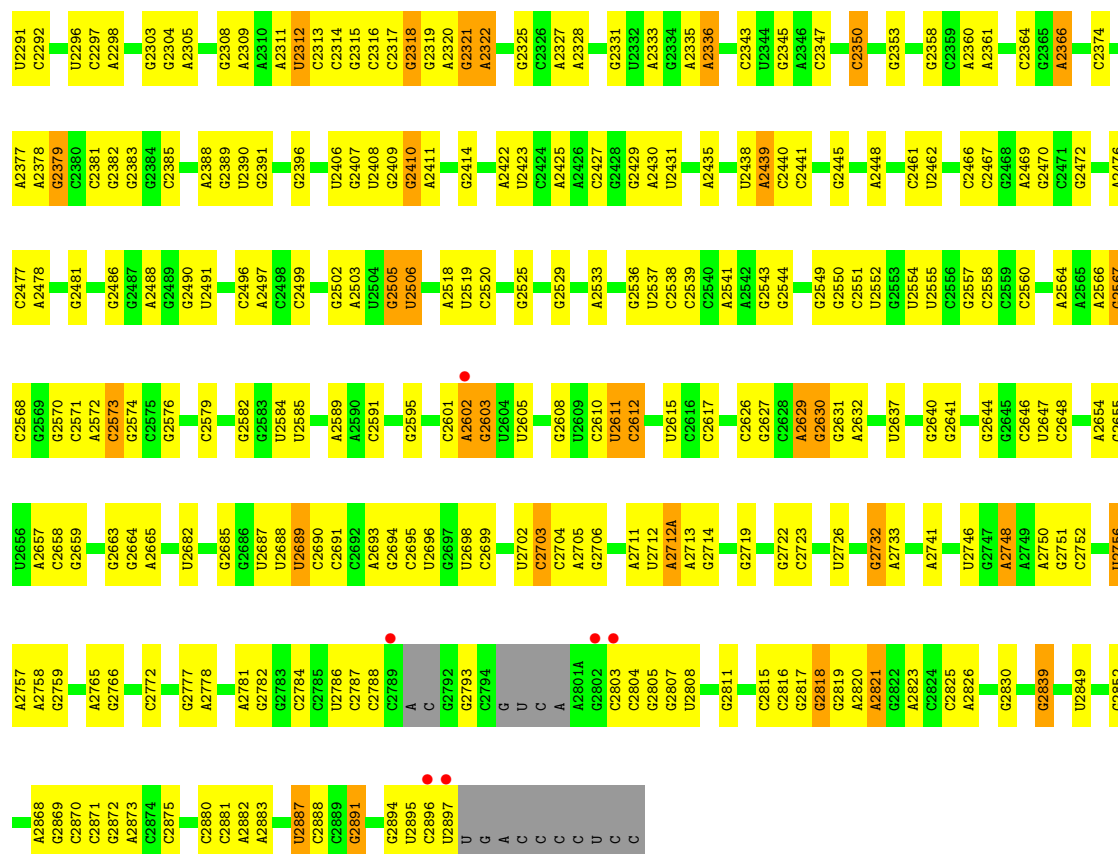


|       |       |       |        |        |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |        |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
|-------|-------|-------|--------|--------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|--------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| G2490 | U2491 | U2492 | U2493  | C2380  | C2381 | G2382 | C2383 | G2384 | C2385 | G2386 | G2405 | U2406 | G2410 | A2411 | G2414 | G2418 | U2419 | A2422 | U2423 | A2424 | A2425 | C2427 | G2428 | G2429 | U2430 | U2431 | A2435 | G2439 | U2440 | C2441 | G2445 | G2446 | G2447 | A2448 | G2452 | A2453 | G2458 | U2459 | A2468 | C2474 | G2475  | A2476 | A2478 | C2483 | G2490 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| C2277 | A2278 | C2283 | C2284  | C2285  | A2286 | G2287 | A2288 | G2289 | G2290 | U2291 | C2292 | G2304 | A2305 | C2306 | G2307 | G2308 | U2312 | C2313 | C2314 | G2315 | G2319 | A2320 | G2325 | C2326 | A2327 | G2328 | G2329 | G2330 | C2331 | G2334 | A2335 | A2336 | G2337 | G2345 | C2346 | C2347 | G2348 | G2349 | C2350 | G2354 | C2355  | C2356 | U2357 | A2361 | C2364 | G2365 | C2371 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| C2179 | U2180 | G2181 | G2182  | C2183  | G2184 | C2185 | G2186 | G2187 | C2188 | U2189 | G2190 | G2191 | G2192 | A2198 | A2199 | C2200 | G2206 | G2207 | A2208 | U2218 | G2219 | G2224 | A2225 | C2226 | U2232 | U2233 | G2234 | G2235 | G2236 | G2237 | G2238 | G2239 | G2242 | U2243 | U2244 | U2245 | G2246 | A2247 | G2251 | G2256 | U2257  | C2258 | U2262 | C2263 | C2264 | A2267 | A2268 | A2273 | A2274 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| A2119 | G2120 | G2121 | U2122  | G2123  | G2124 | G2125 | A2126 | G2127 | C2128 | C2129 | U2130 | G2131 | U2132 | G2133 | A2134 | A2135 | C2136 | C2137 | C2138 | C2139 | G2140 | G2141 | C2142 | C2143 | U2144 | C2145 | C2146 | G2147 | C2148 | G2149 | U2150 | G2151 | G2152 | G2153 | G2154 | G2155 | G2156 | A2157 | A2158 | G2159 | G2160  | C2161 | C2162 | C2163 | C2164 | G2165 | G2166 | U2167 | C2168 | A2169 | U2170 | G2171 | U2172 | U2173 | U2174 | C2175 | A2176 | C2177 | C2178 |       |       |       |       |       |       |
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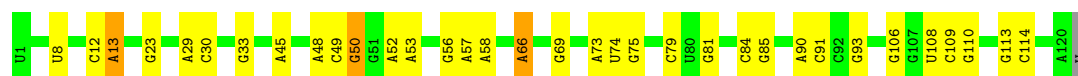




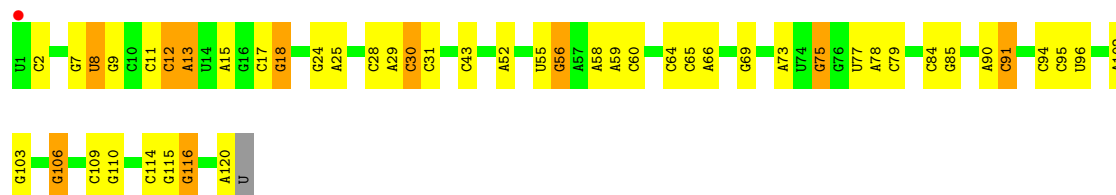
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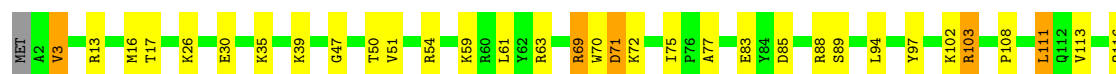
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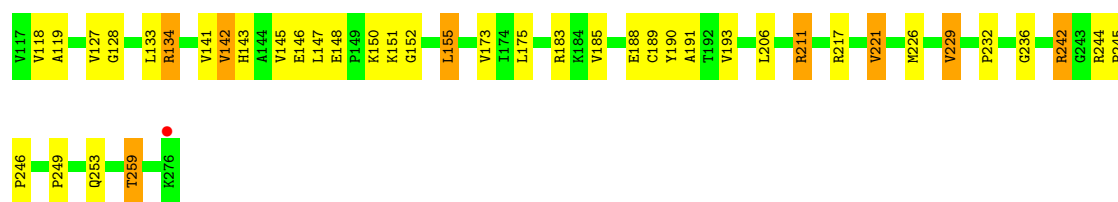


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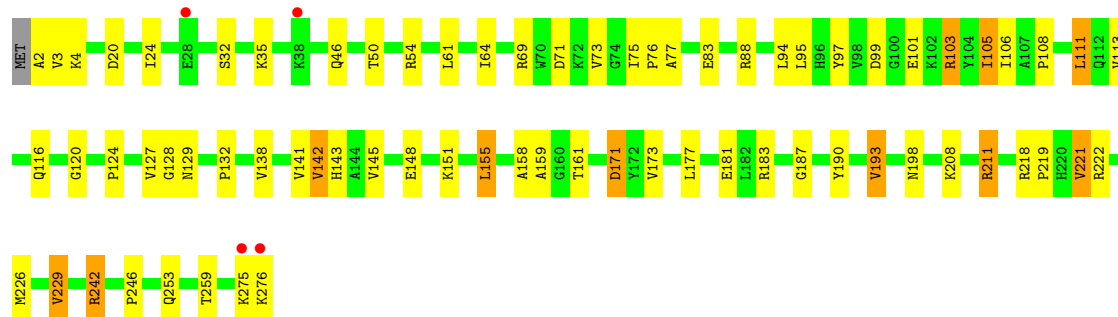
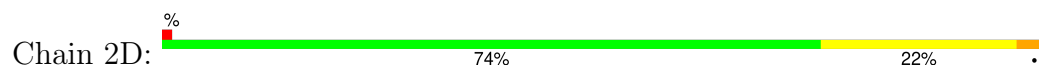


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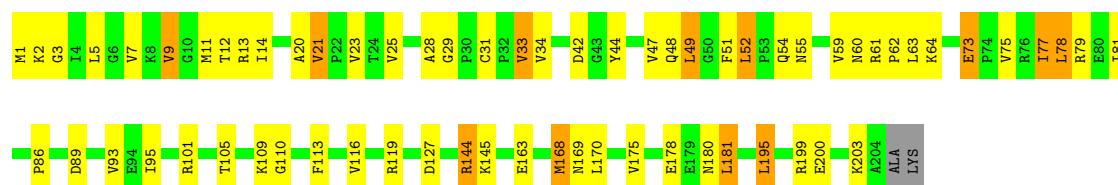




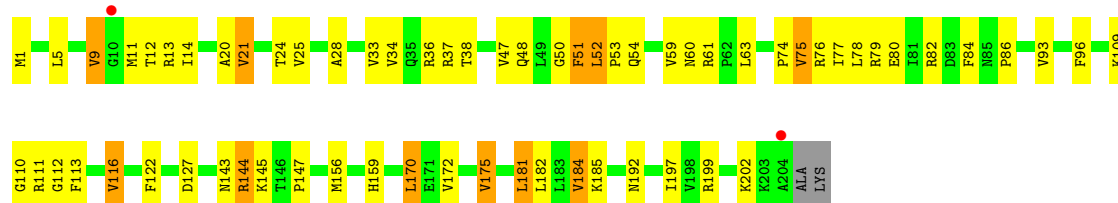
• Molecule 3: 50S ribosomal protein L2



• Molecule 4: 50S ribosomal protein L3



• Molecule 4: 50S ribosomal protein L3

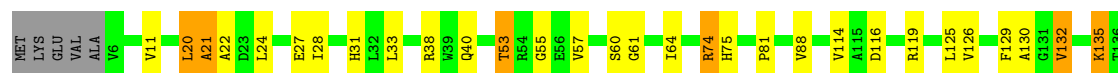


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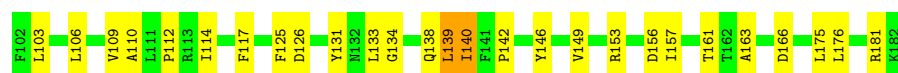
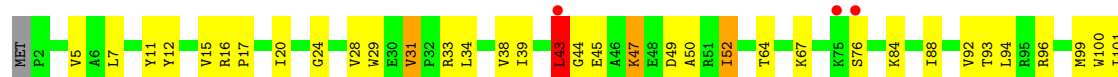




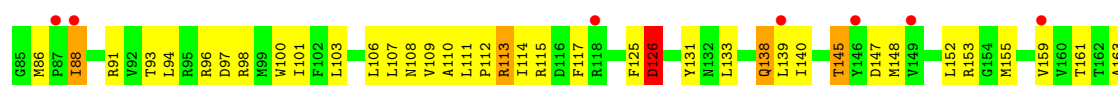
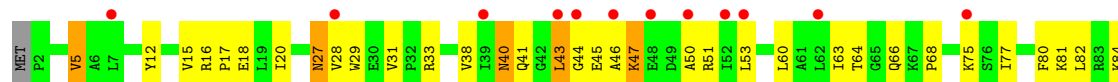
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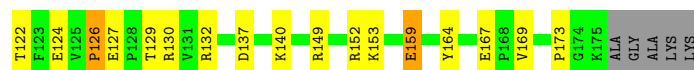
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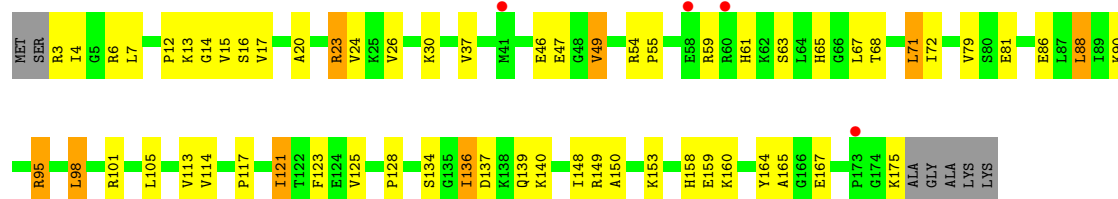
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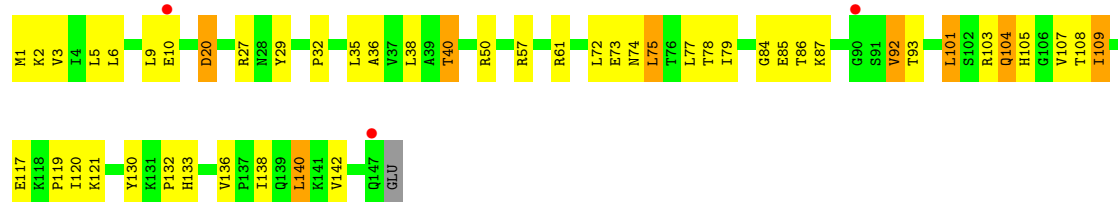
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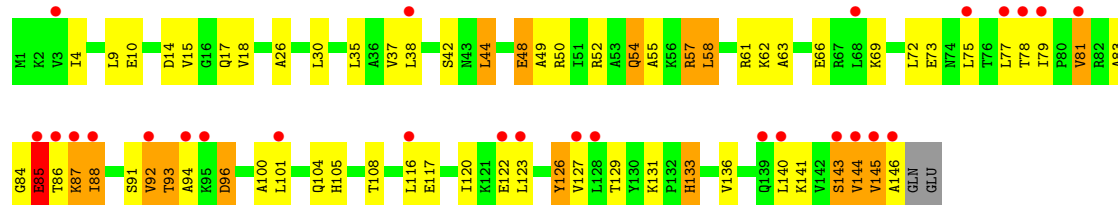
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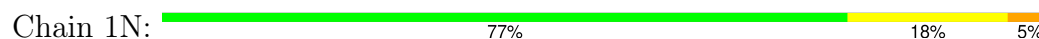
• Molecule 8: 50S ribosomal protein L9



• Molecule 8: 50S ribosomal protein L9



• Molecule 9: 50S ribosomal protein L13



• Molecule 9: 50S ribosomal protein L13



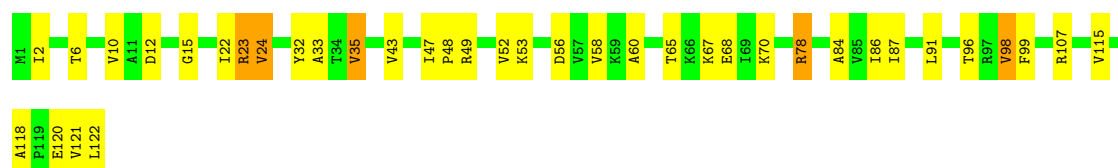
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Chain 1O:  70% 26%



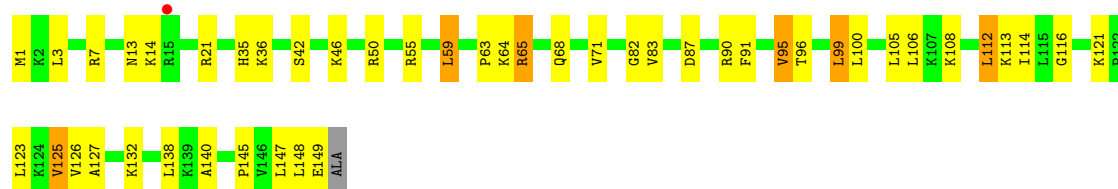
- Molecule 10: 50S ribosomal protein L14

Chain 2O:  69% 27%



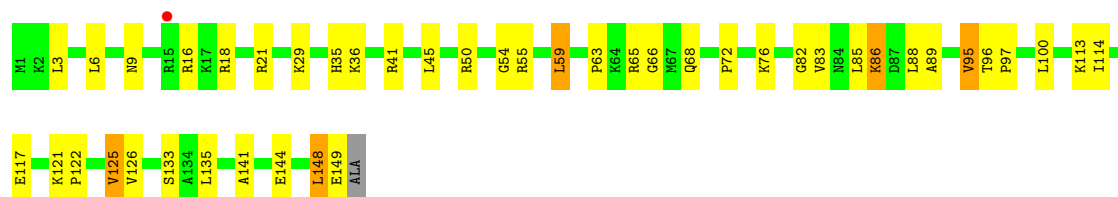
- Molecule 11: 50S ribosomal protein L15

Chain 1P:  69% 27%



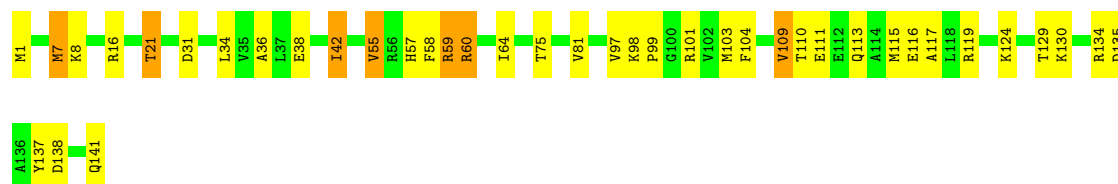
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Chain 2P:  70% 26%

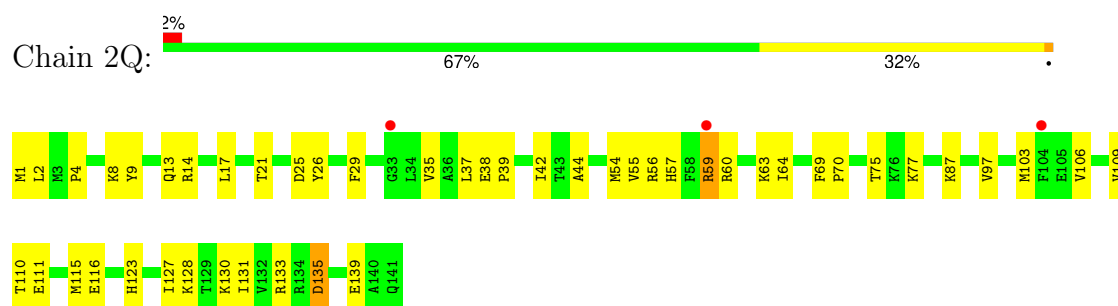


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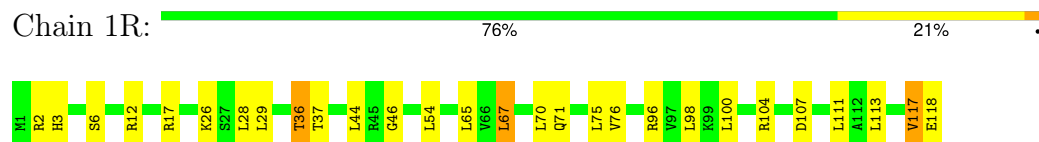
Chain 1Q:  72% 23% 5%



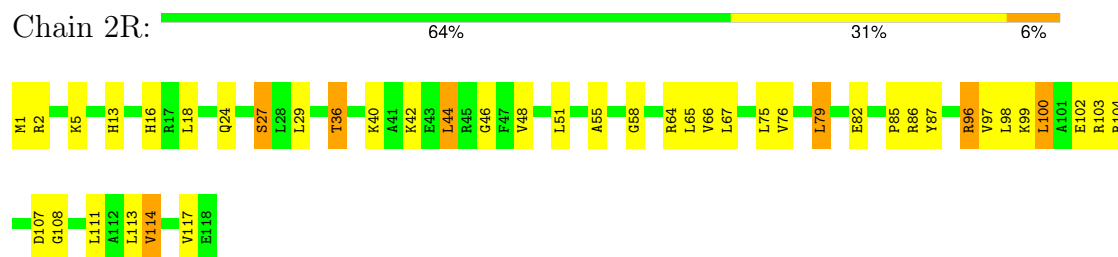
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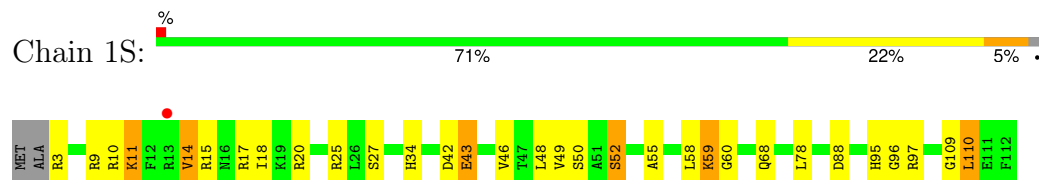
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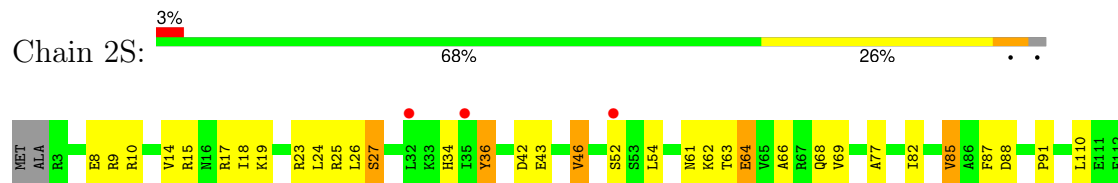
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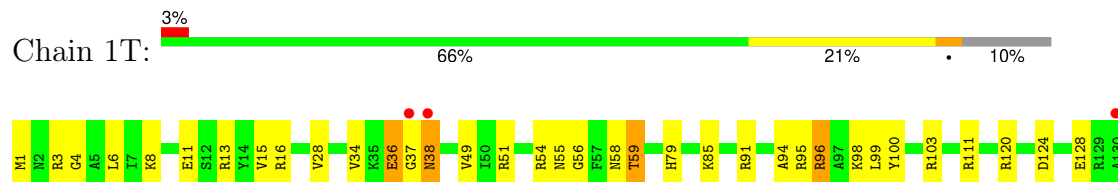
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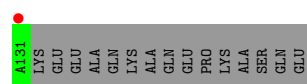
- Molecule 14: 50S ribosomal protein L18



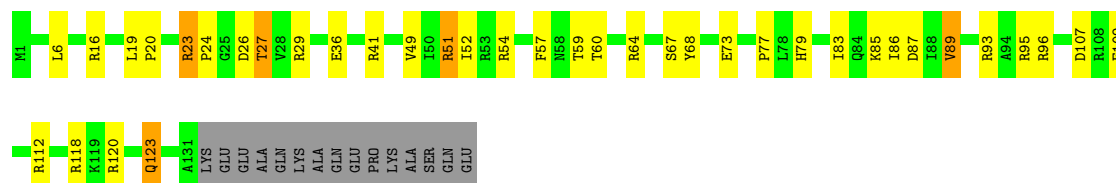
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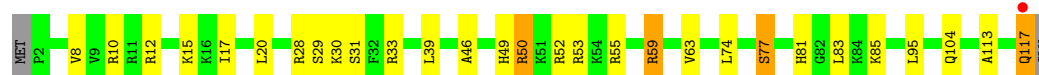
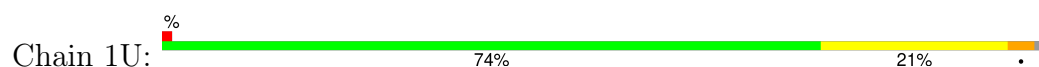




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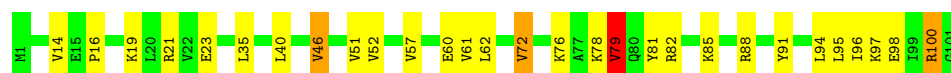
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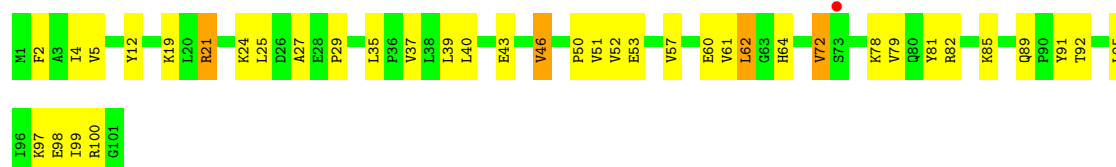
- Molecule 16: 50S ribosomal protein L20



- Molecule 17: 50S ribosomal protein L21



- Molecule 17: 50S ribosomal protein L21



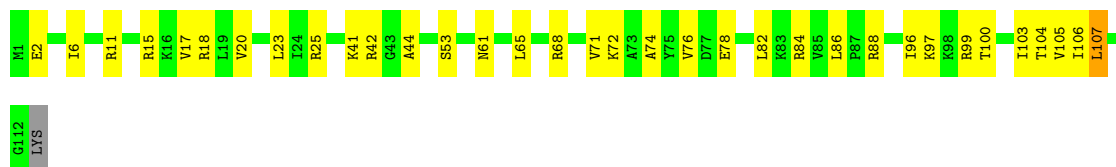
- Molecule 18: 50S ribosomal protein L22





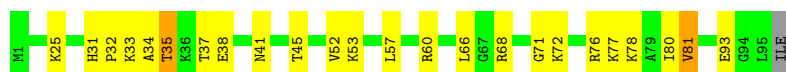
- Molecule 18: 50S ribosomal protein L22

Chain 2W: 69% 29% ..



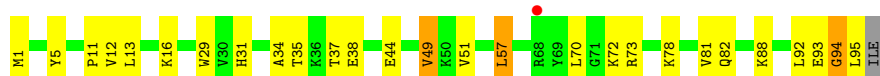
- Molecule 19: 50S ribosomal protein L23

Chain 1X: 74% 23% ..



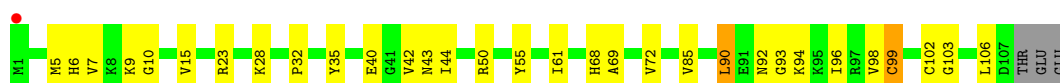
- Molecule 19: 50S ribosomal protein L23

Chain 2X: 71% 25% ..



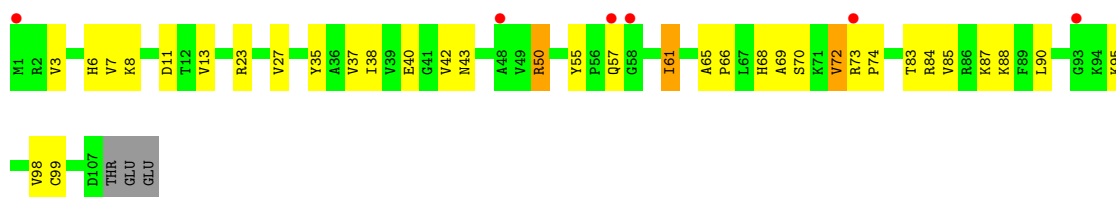
- Molecule 20: 50S ribosomal protein L24

Chain 1Y: 69% 26% ..



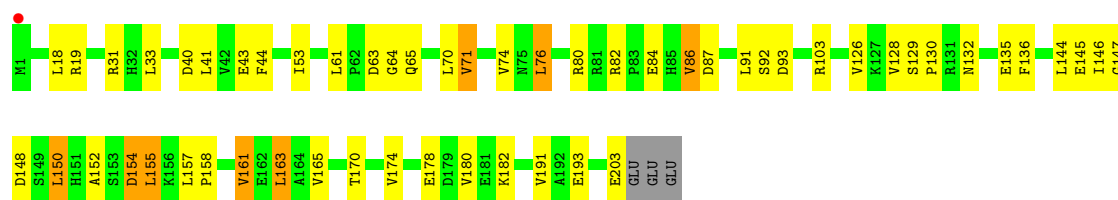
- Molecule 20: 50S ribosomal protein L24

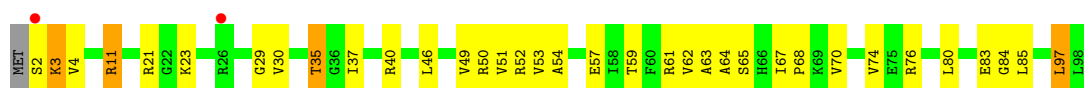
Chain 2Y: 65% 29% ..



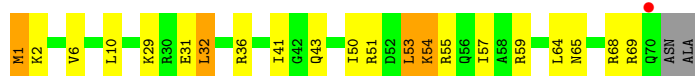
- Molecule 21: 50S ribosomal protein L25

Chain 1Z: 72% 23% ..

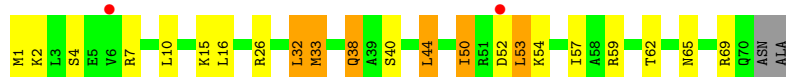




- Molecule 24: 50S ribosomal protein L29



- Molecule 24: 50S ribosomal protein L29



- Molecule 25: 50S ribosomal protein L30



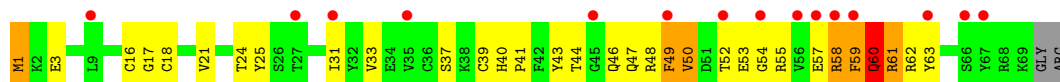
- Molecule 25: 50S ribosomal protein L30



- Molecule 26: 50S ribosomal protein L31

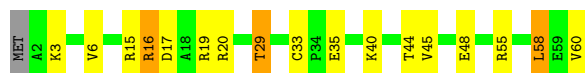


- Molecule 26: 50S ribosomal protein L31



- Molecule 27: 50S ribosomal protein L32

Chain 15:  70% 23% 5% .



- Molecule 27: 50S ribosomal protein L32

Chain 25:  65% 28% 5% .



- Molecule 28: 50S ribosomal protein L33

Chain 16:  76% 20% ..



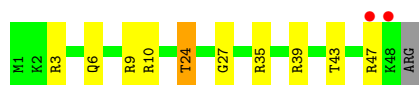
- Molecule 28: 50S ribosomal protein L33

Chain 26:  70% 24% . .



- Molecule 29: 50S ribosomal protein L34

Chain 17:  4% 78% 18% ..



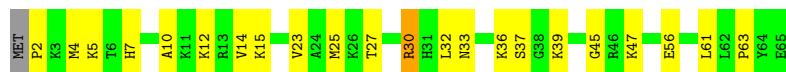
- Molecule 29: 50S ribosomal protein L34

Chain 27:  4% 76% 22% .



- Molecule 30: 50S ribosomal protein L35

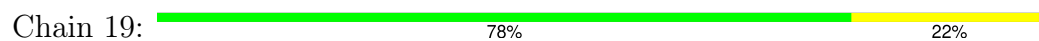
Chain 18:  65% 32% ..



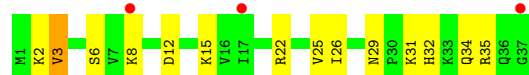
- Molecule 30: 50S ribosomal protein L35



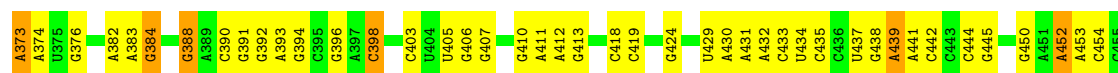
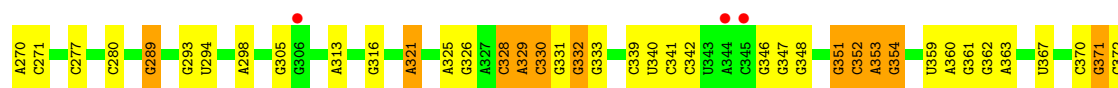
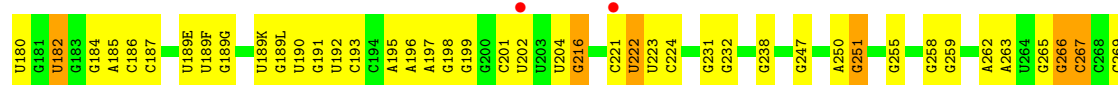
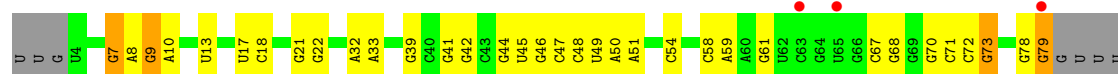
- Molecule 31: 50S ribosomal protein L36

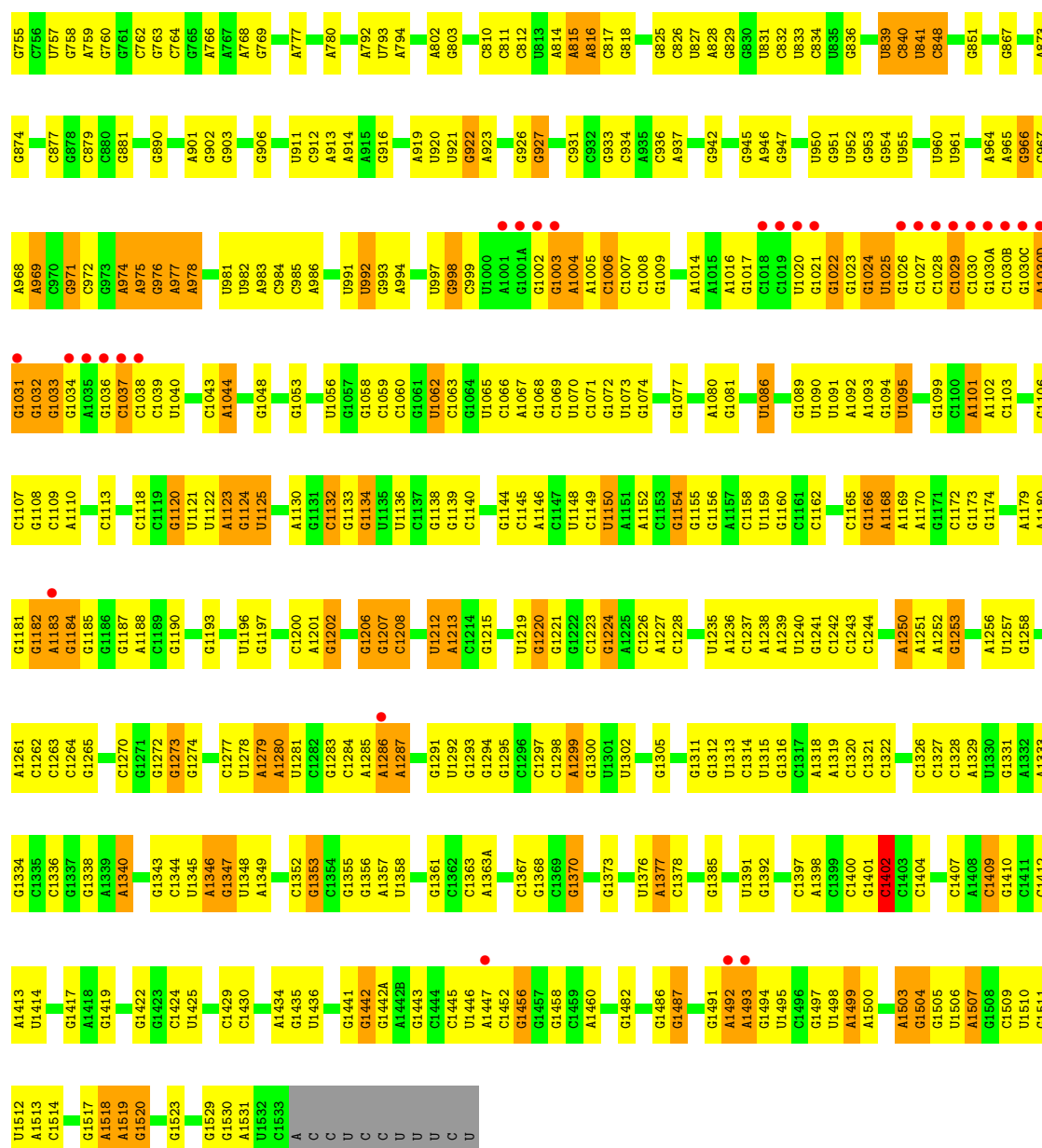


- Molecule 31: 50S ribosomal protein L36

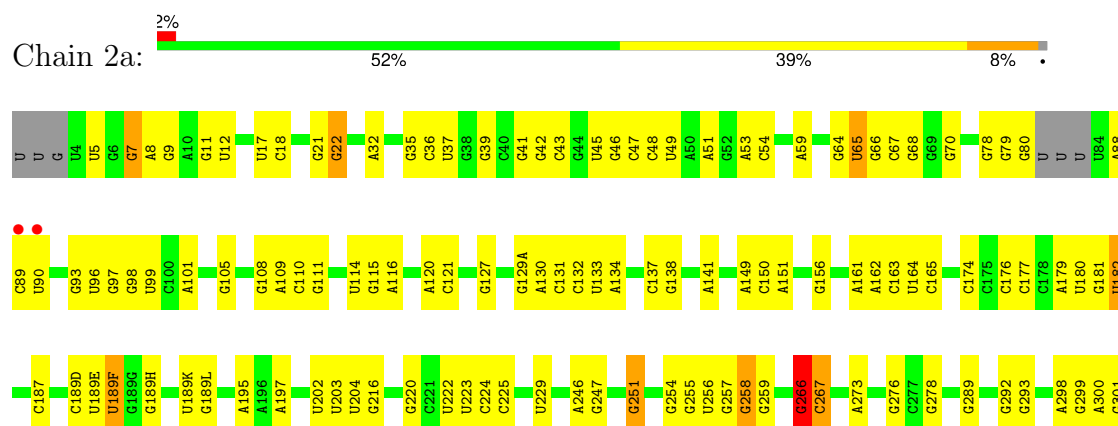


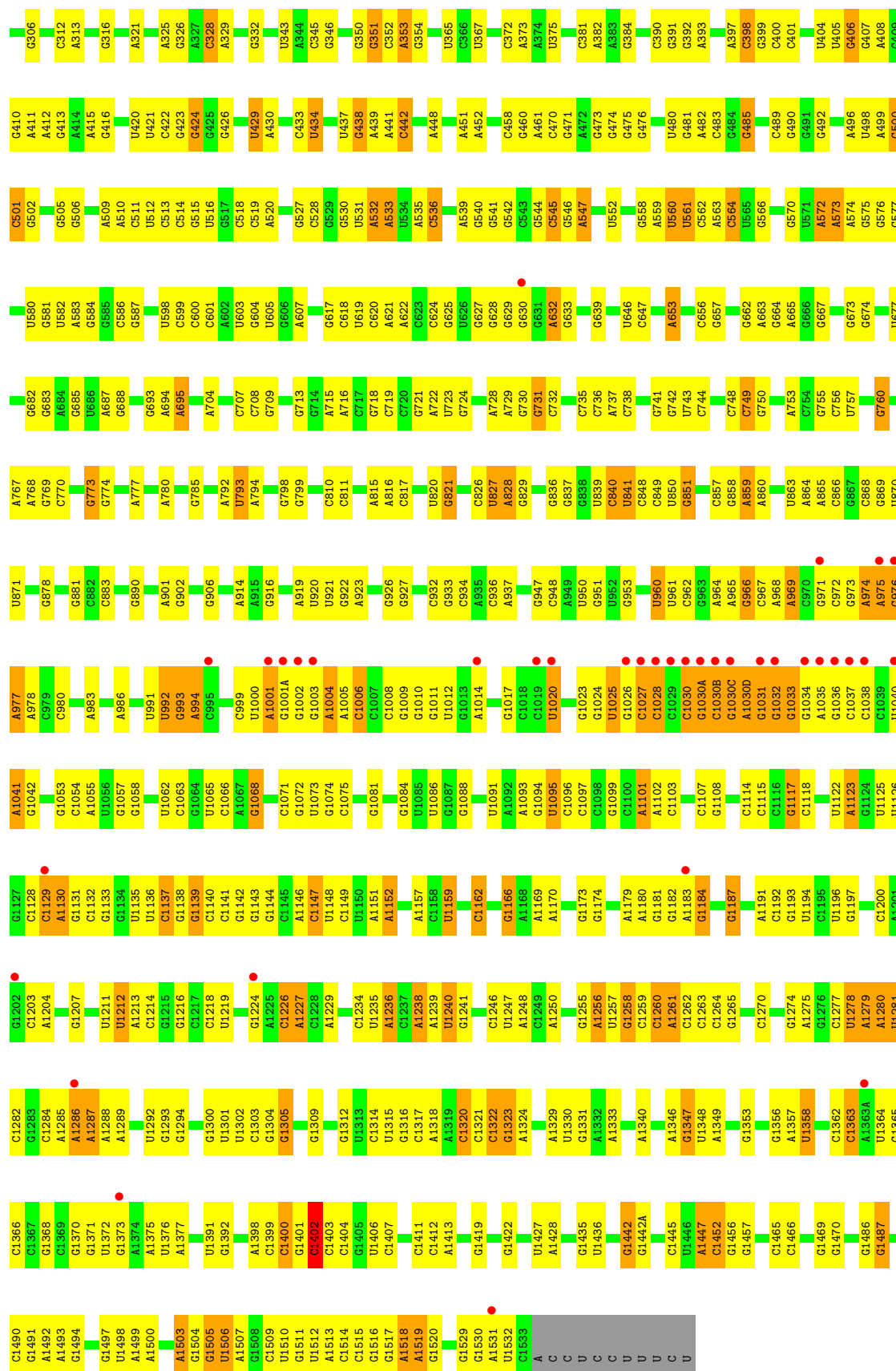
- Molecule 32: 16S Ribosomal RNA





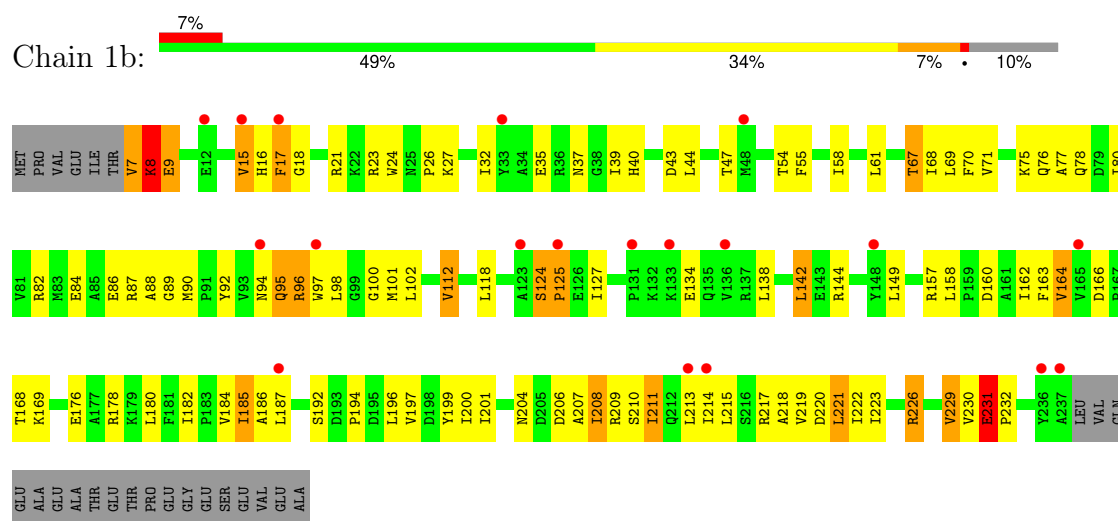
- Molecule 32: 16S Ribosomal RNA



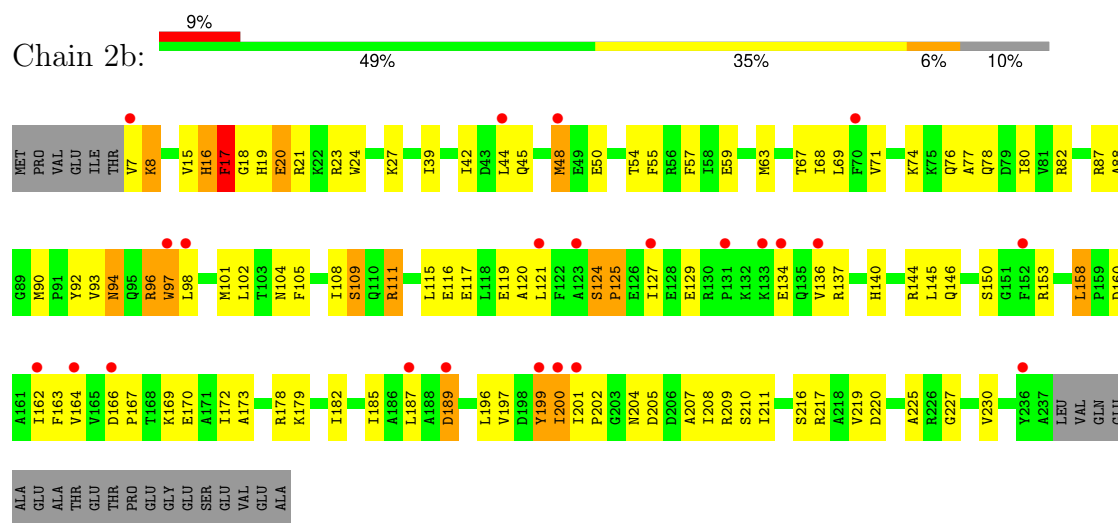


- Molecule 33: 30S ribosomal protein S2

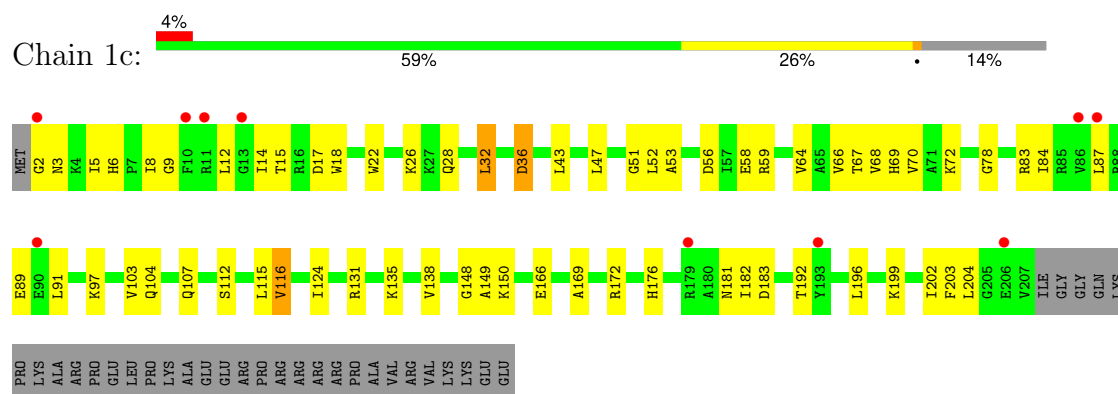




- Molecule 33: 30S ribosomal protein S2

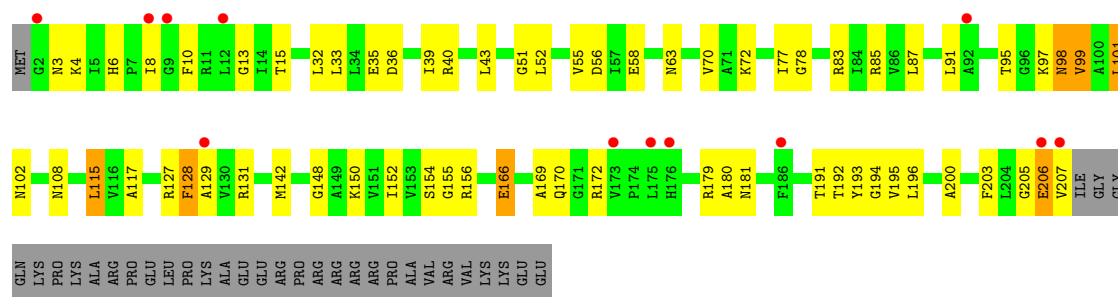


- Molecule 34: 30S ribosomal protein S3

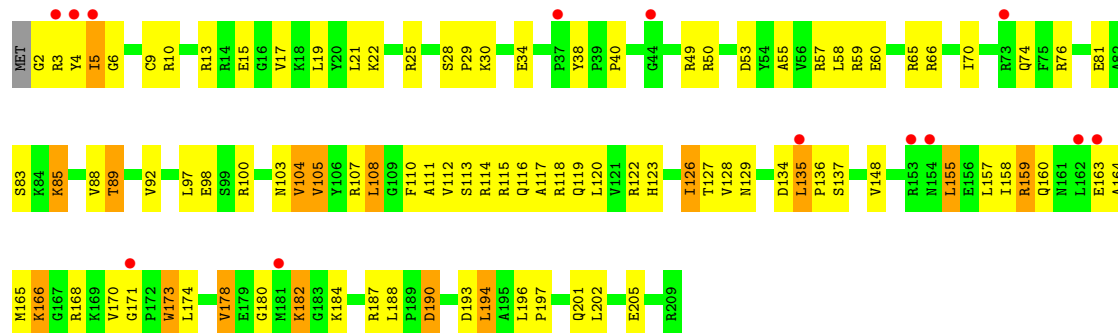


- Molecule 34: 30S ribosomal protein S3

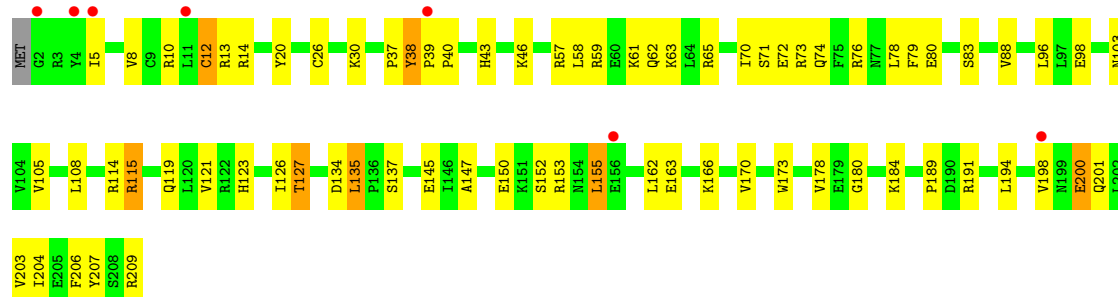




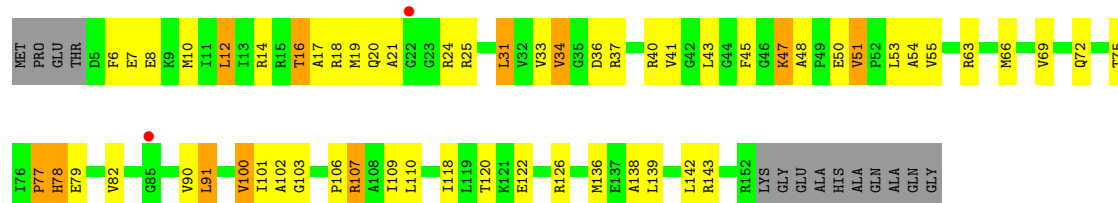
- Molecule 35: 30S ribosomal protein S4



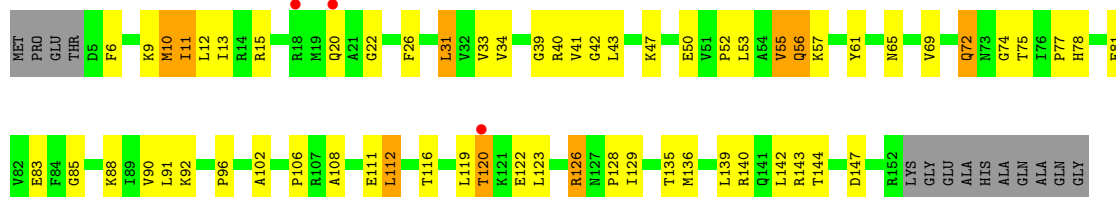
- Molecule 35: 30S ribosomal protein S4



- Molecule 36: 30S ribosomal protein S5



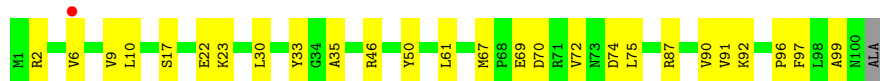
- Molecule 36: 30S ribosomal protein S5



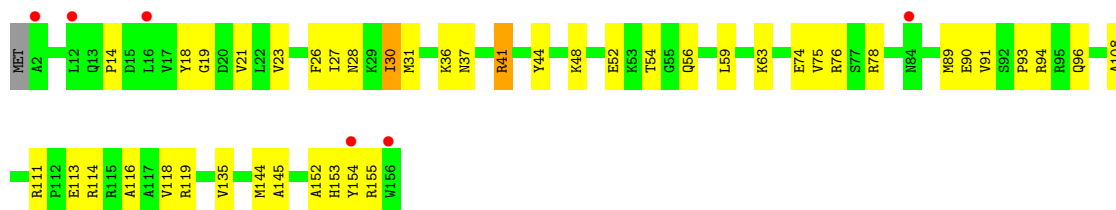
- Molecule 37: 30S ribosomal protein S6



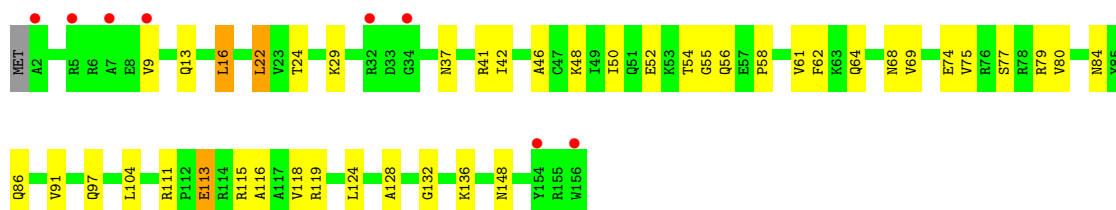
- Molecule 37: 30S ribosomal protein S6



- Molecule 38: 30S ribosomal protein S7

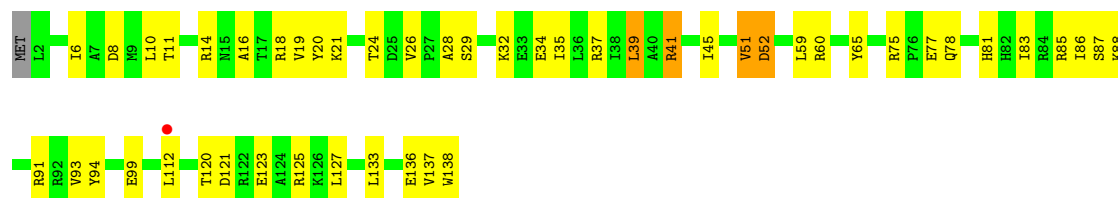


- Molecule 38: 30S ribosomal protein S7

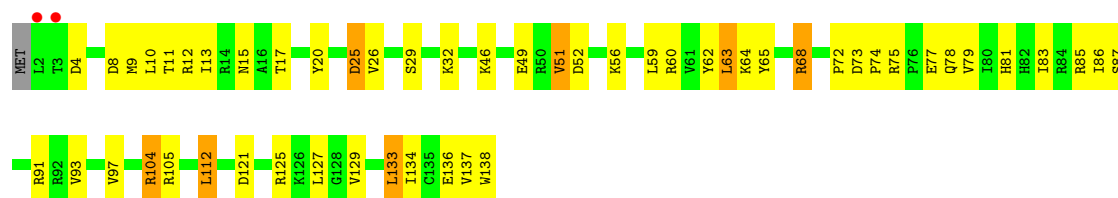


- Molecule 39: 30S ribosomal protein S8

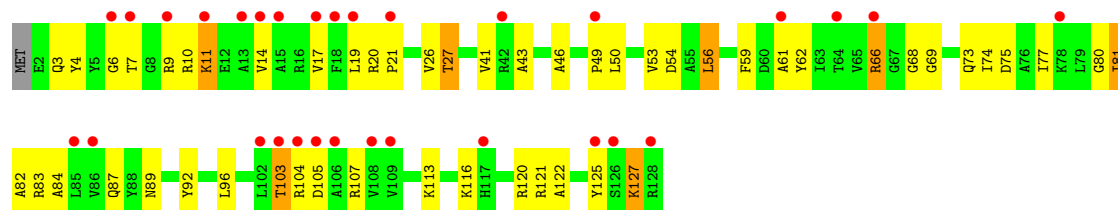




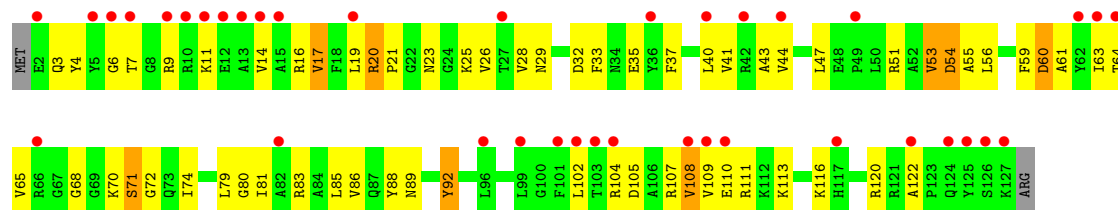
- Molecule 39: 30S ribosomal protein S8



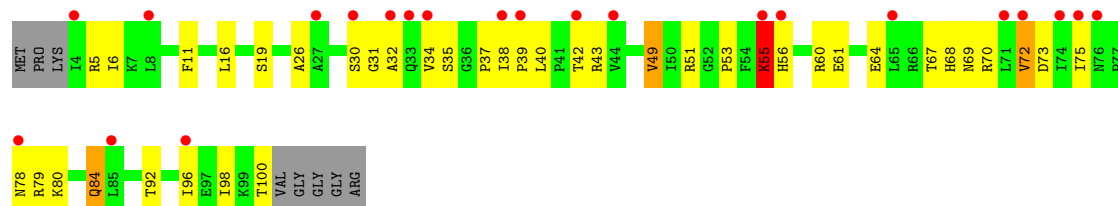
- Molecule 40: 30S ribosomal protein S9



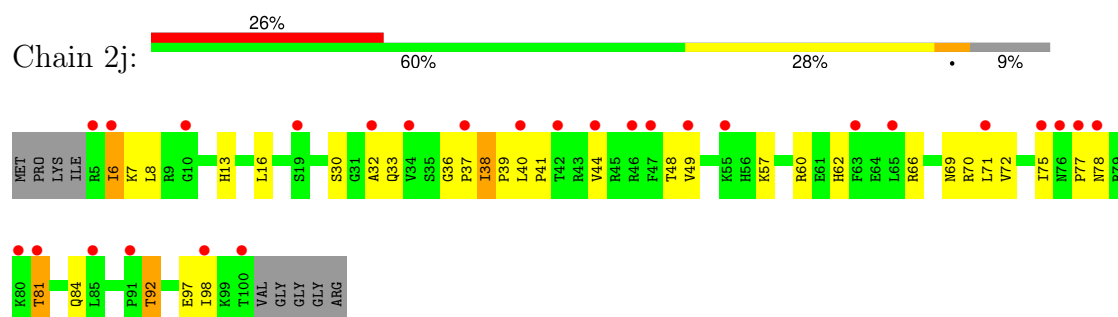
- Molecule 40: 30S ribosomal protein S9



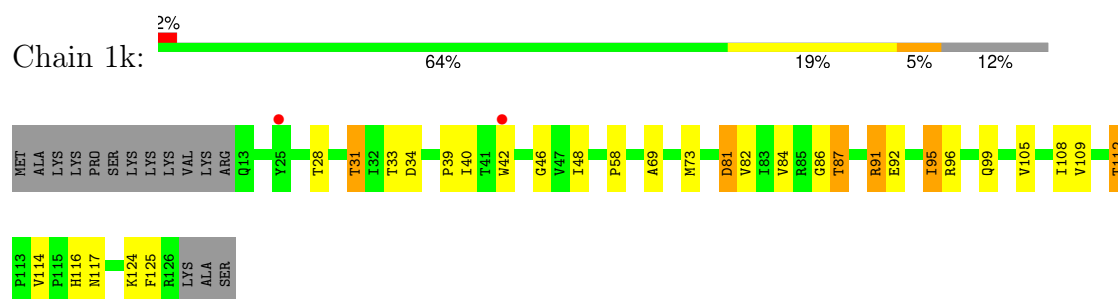
- Molecule 41: 30S ribosomal protein S10



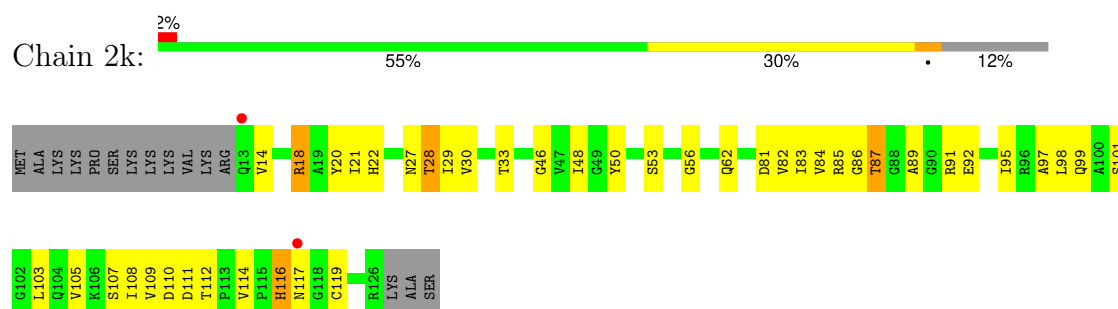
- Molecule 41: 30S ribosomal protein S10



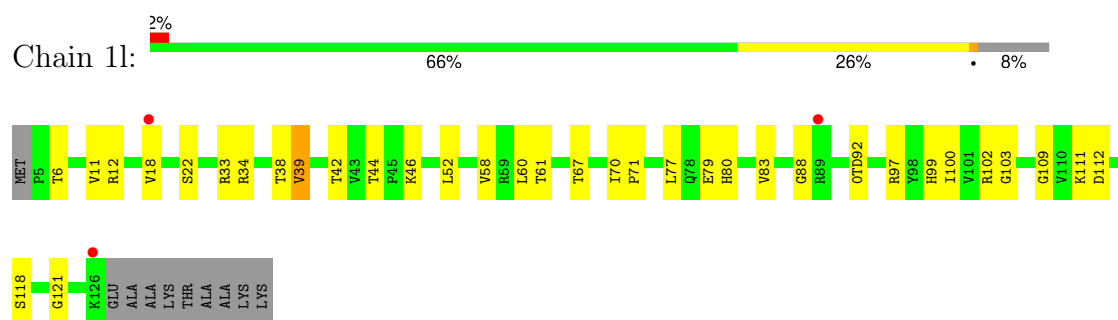
- Molecule 42: 30S ribosomal protein S11



- Molecule 42: 30S ribosomal protein S11

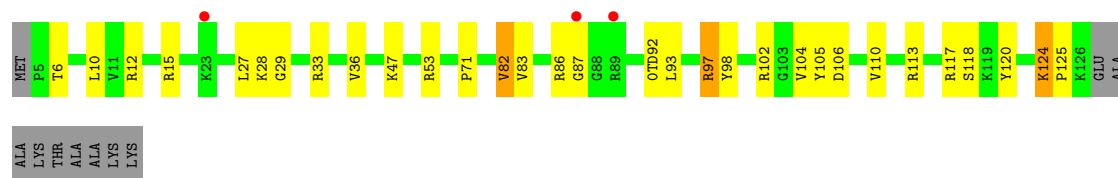


- Molecule 43: 30S ribosomal protein S12

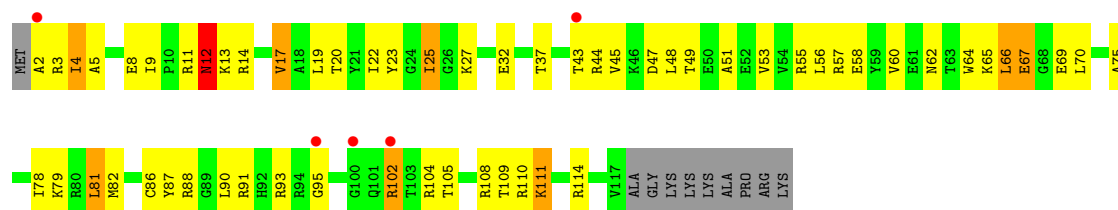


- Molecule 43: 30S ribosomal protein S12

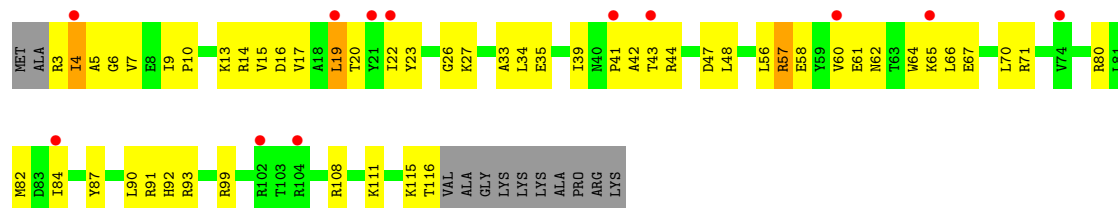




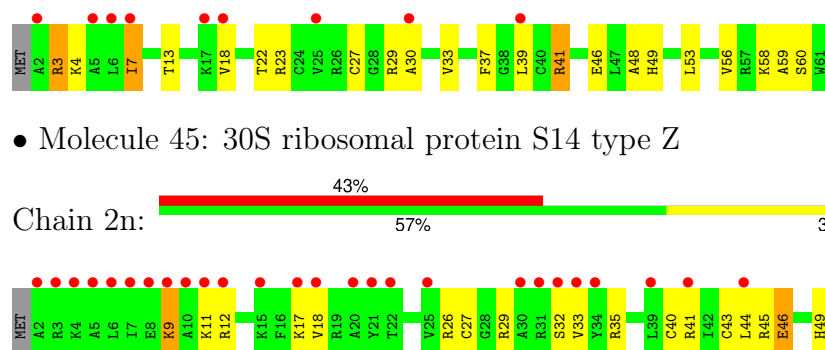
- Molecule 44: 30S ribosomal protein S13



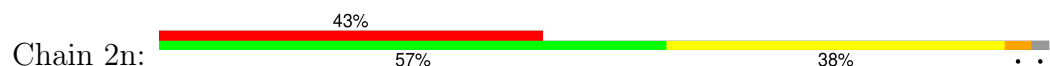
- Molecule 44: 30S ribosomal protein S13



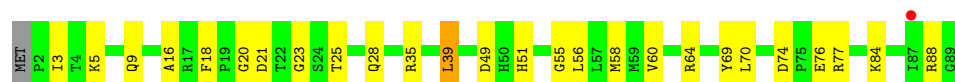
- Molecule 45: 30S ribosomal protein S14 type Z



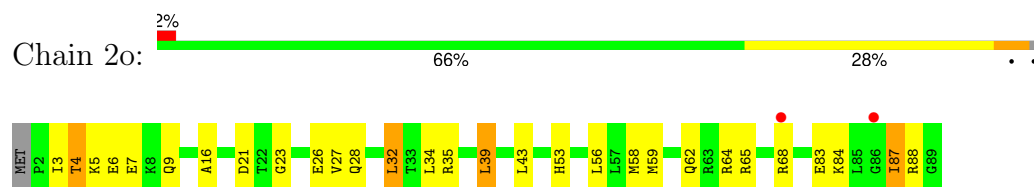
- Molecule 45: 30S ribosomal protein S14 type Z



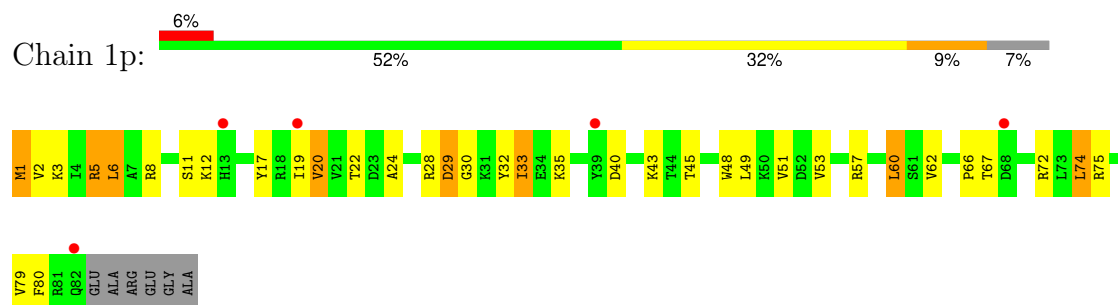
- Molecule 46: 30S ribosomal protein S15



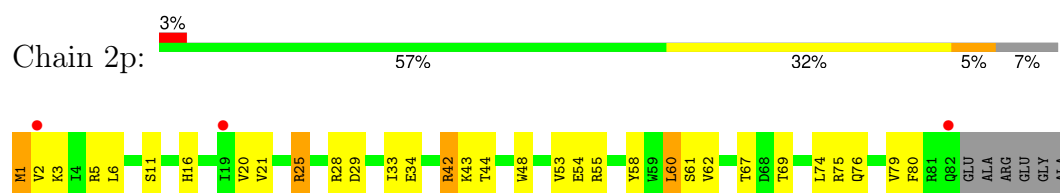
- Molecule 46: 30S ribosomal protein S15



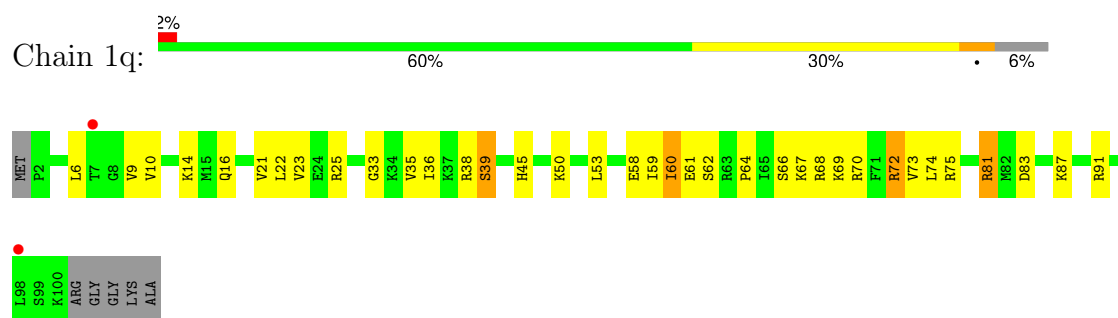
- Molecule 47: 30S ribosomal protein S16



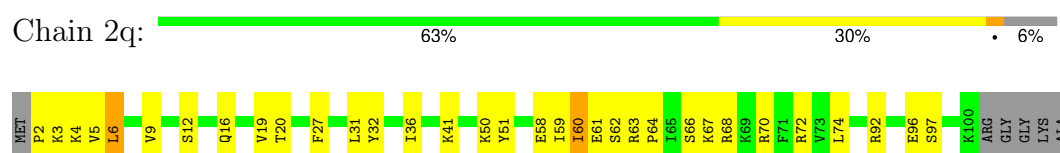
- Molecule 47: 30S ribosomal protein S16



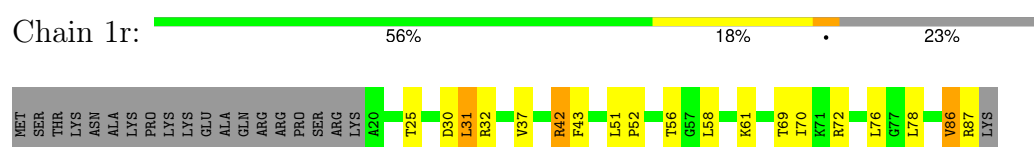
- Molecule 48: 30S ribosomal protein S17



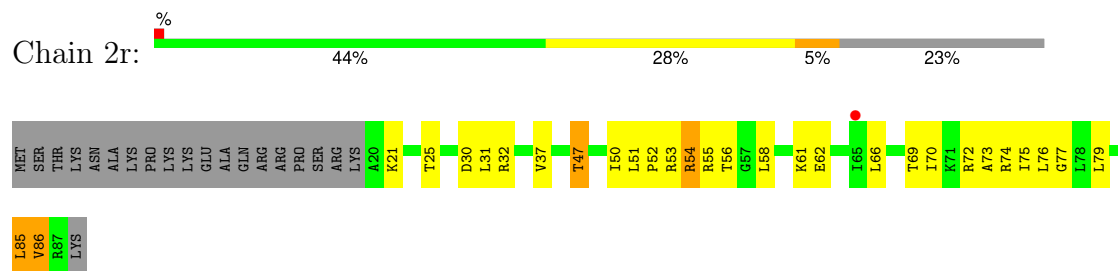
- Molecule 48: 30S ribosomal protein S17



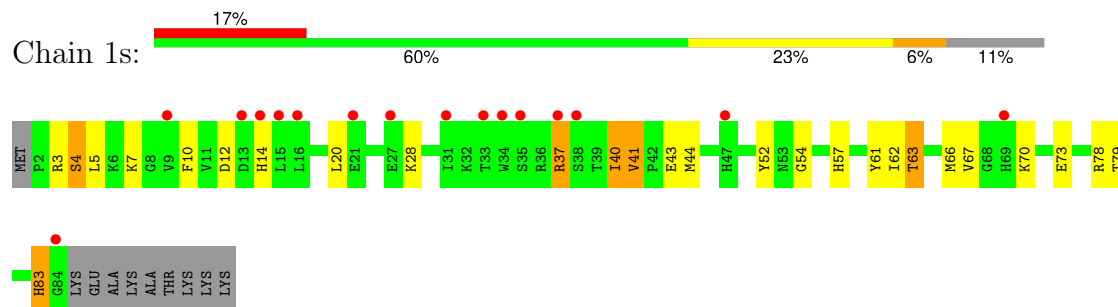
- Molecule 49: 30S ribosomal protein S18



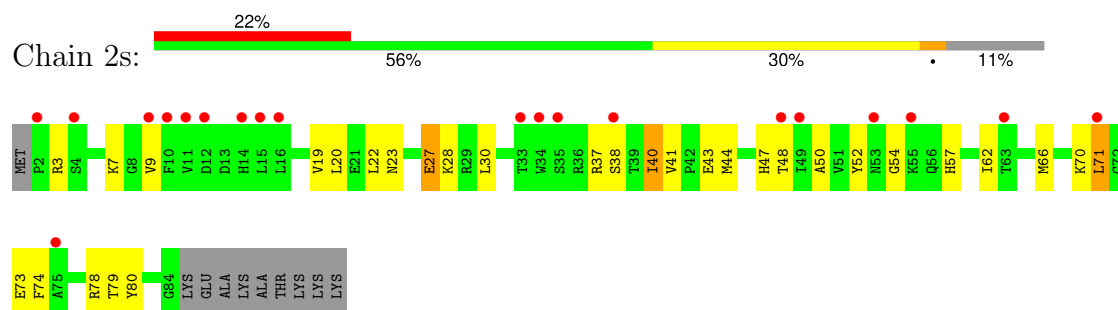
- Molecule 49: 30S ribosomal protein S18



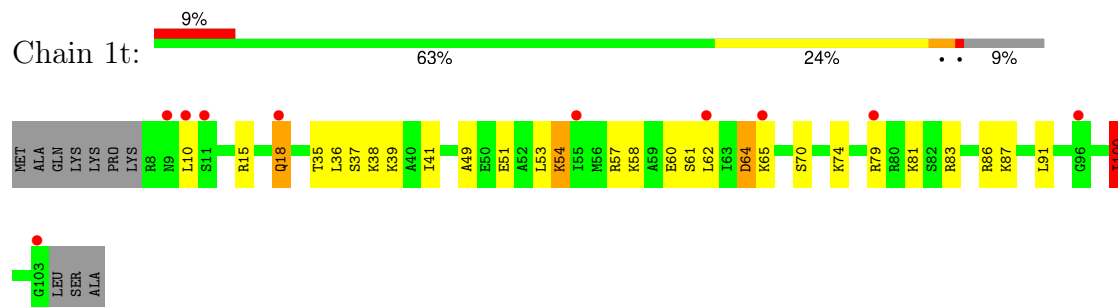
- Molecule 50: 30S ribosomal protein S19



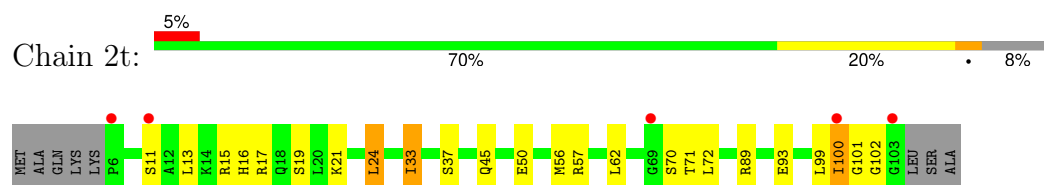
- Molecule 50: 30S ribosomal protein S19



- Molecule 51: 30S ribosomal protein S20

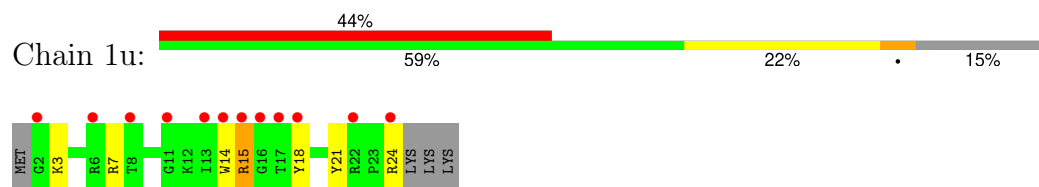


- Molecule 51: 30S ribosomal protein S20

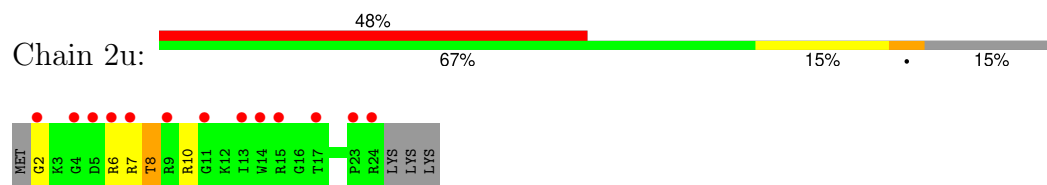




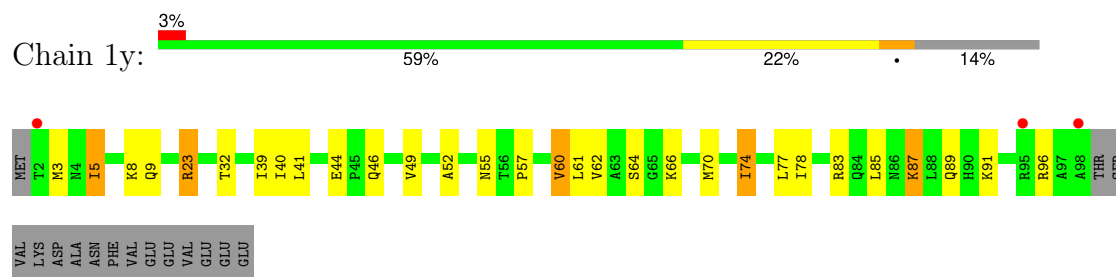
## • Molecule 52: 30S ribosomal protein Thx



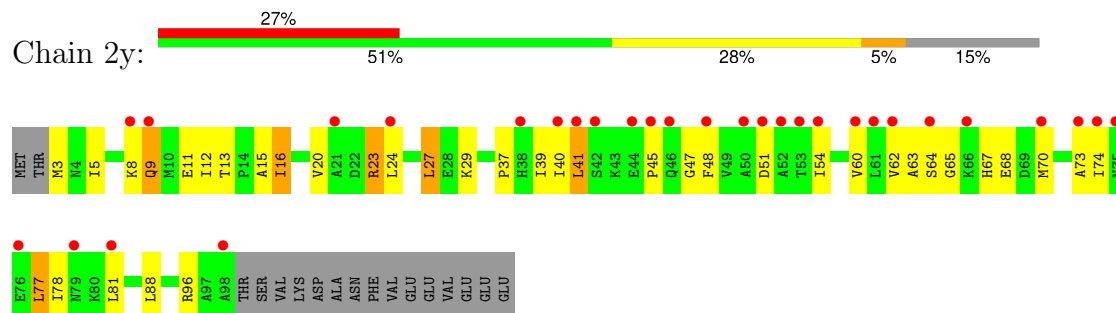
## • Molecule 52: 30S ribosomal protein Thx



## • Molecule 53: Ribosome-associated inhibitor A



## • Molecule 53: Ribosome-associated inhibitor A



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 21 21 21                                                  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 210.10Å 451.17Å 625.72Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 45.39 – 2.85<br>45.39 – 2.85                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.9 (45.39-2.85)<br>99.9 (45.39-2.85)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.38                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.24 (at 2.86Å)                                             | Xtriage          |
| Refinement program                                                      | PHENIX 1.17.1                                               | Depositor        |
| R, $R_{free}$                                                           | 0.209 , 0.260<br>0.208 , 0.258                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 68560 reflections (5.02%)                                   | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 51.0                                                        | Xtriage          |
| Anisotropy                                                              | 0.087                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.28 , 46.9                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.26$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.92                                                        | EDS              |
| Total number of atoms                                                   | 298337                                                      | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 54.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.49% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: 2MG, MG, MPD, OMU, 2MA, MA6, 5MC, ZN, PSU, 5MU, OMC, A1CQ5, 0TD, 4OC, UR3, SF4, OMG, G7M, M2G

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

| Mol | Chain | Bond lengths |         | Bond angles |                 |
|-----|-------|--------------|---------|-------------|-----------------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5         |
| 1   | 1A    | 0.30         | 0/69031 | 0.45        | 0/107754        |
| 1   | 2A    | 0.23         | 0/68903 | 0.41        | 3/107552 (0.0%) |
| 2   | 1B    | 0.22         | 0/2876  | 0.41        | 0/4486          |
| 2   | 2B    | 0.19         | 0/2878  | 0.36        | 0/4490          |
| 3   | 1D    | 0.29         | 0/2181  | 0.53        | 0/2940          |
| 3   | 2D    | 0.24         | 0/2186  | 0.47        | 0/2944          |
| 4   | 1E    | 0.29         | 0/1592  | 0.49        | 0/2149          |
| 4   | 2E    | 0.22         | 0/1592  | 0.47        | 0/2149          |
| 5   | 1F    | 0.29         | 0/1619  | 0.49        | 0/2193          |
| 5   | 2F    | 0.23         | 0/1615  | 0.49        | 2/2188 (0.1%)   |
| 6   | 1G    | 0.20         | 0/1451  | 0.43        | 0/1961          |
| 6   | 2G    | 0.21         | 0/1449  | 0.51        | 0/1957          |
| 7   | 1H    | 0.22         | 0/1356  | 0.42        | 0/1834          |
| 7   | 2H    | 0.20         | 0/1350  | 0.40        | 0/1826          |
| 8   | 1I    | 0.22         | 0/1109  | 0.46        | 0/1512          |
| 8   | 2I    | 0.23         | 0/1091  | 0.49        | 0/1490          |
| 9   | 1N    | 0.27         | 0/1148  | 0.45        | 0/1547          |
| 9   | 2N    | 0.19         | 0/1144  | 0.39        | 0/1543          |
| 10  | 1O    | 0.30         | 0/943   | 0.50        | 0/1269          |
| 10  | 2O    | 0.23         | 0/943   | 0.45        | 0/1269          |
| 11  | 1P    | 0.28         | 0/1152  | 0.53        | 1/1533 (0.1%)   |
| 11  | 2P    | 0.21         | 0/1152  | 0.49        | 0/1533          |
| 12  | 1Q    | 0.26         | 0/1143  | 0.45        | 0/1527          |
| 12  | 2Q    | 0.21         | 0/1143  | 0.44        | 0/1527          |
| 13  | 1R    | 0.29         | 0/982   | 0.53        | 0/1312          |
| 13  | 2R    | 0.22         | 0/982   | 0.47        | 0/1312          |
| 14  | 1S    | 0.22         | 0/887   | 0.47        | 0/1180          |
| 14  | 2S    | 0.22         | 0/880   | 0.44        | 0/1172          |
| 15  | 1T    | 0.27         | 0/1105  | 0.54        | 0/1477          |
| 15  | 2T    | 0.22         | 0/1097  | 0.46        | 0/1468          |
| 16  | 1U    | 0.31         | 0/977   | 0.48        | 0/1301          |

| Mol | Chain | Bond lengths |         | Bond angles |                |
|-----|-------|--------------|---------|-------------|----------------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5        |
| 16  | 2U    | 0.21         | 0/977   | 0.41        | 0/1301         |
| 17  | 1V    | 0.26         | 0/786   | 0.46        | 0/1053         |
| 17  | 2V    | 0.19         | 0/782   | 0.42        | 0/1049         |
| 18  | 1W    | 0.28         | 0/897   | 0.47        | 0/1205         |
| 18  | 2W    | 0.24         | 0/897   | 0.42        | 0/1205         |
| 19  | 1X    | 0.27         | 0/764   | 0.48        | 0/1025         |
| 19  | 2X    | 0.21         | 0/764   | 0.45        | 0/1025         |
| 20  | 1Y    | 0.25         | 0/823   | 0.53        | 0/1099         |
| 20  | 2Y    | 0.22         | 0/823   | 0.47        | 0/1100         |
| 21  | 1Z    | 0.22         | 0/1620  | 0.43        | 0/2200         |
| 21  | 2Z    | 0.21         | 0/1590  | 0.41        | 0/2162         |
| 22  | 10    | 0.28         | 0/616   | 0.53        | 0/821          |
| 22  | 20    | 0.23         | 0/616   | 0.48        | 0/821          |
| 23  | 11    | 0.29         | 0/761   | 0.44        | 0/1013         |
| 23  | 21    | 0.22         | 0/766   | 0.43        | 0/1018         |
| 24  | 12    | 0.25         | 0/590   | 0.46        | 0/781          |
| 24  | 22    | 0.21         | 0/594   | 0.40        | 0/785          |
| 25  | 13    | 0.27         | 0/474   | 0.49        | 0/635          |
| 25  | 23    | 0.20         | 0/469   | 0.43        | 0/630          |
| 26  | 14    | 0.27         | 0/559   | 0.58        | 0/754          |
| 26  | 24    | 0.32         | 0/549   | 0.67        | 3/741 (0.4%)   |
| 27  | 15    | 0.30         | 0/473   | 0.51        | 0/639          |
| 27  | 25    | 0.24         | 0/469   | 0.49        | 0/635          |
| 28  | 16    | 0.26         | 0/460   | 0.46        | 0/613          |
| 28  | 26    | 0.20         | 0/456   | 0.43        | 0/608          |
| 29  | 17    | 0.31         | 0/426   | 0.53        | 0/561          |
| 29  | 27    | 0.25         | 0/426   | 0.48        | 0/561          |
| 30  | 18    | 0.28         | 0/525   | 0.50        | 0/691          |
| 30  | 28    | 0.24         | 0/525   | 0.44        | 0/691          |
| 31  | 19    | 0.25         | 0/310   | 0.47        | 0/407          |
| 31  | 29    | 0.21         | 0/310   | 0.44        | 0/407          |
| 32  | 1a    | 0.21         | 0/35795 | 0.39        | 0/55864        |
| 32  | 2a    | 0.20         | 0/35890 | 0.38        | 1/56012 (0.0%) |
| 33  | 1b    | 0.24         | 0/1876  | 0.51        | 0/2533         |
| 33  | 2b    | 0.24         | 0/1860  | 0.48        | 0/2518         |
| 34  | 1c    | 0.20         | 0/1582  | 0.41        | 0/2137         |
| 34  | 2c    | 0.21         | 0/1566  | 0.40        | 0/2119         |
| 35  | 1d    | 0.22         | 0/1695  | 0.43        | 0/2274         |
| 35  | 2d    | 0.22         | 0/1698  | 0.48        | 0/2277         |
| 36  | 1e    | 0.20         | 0/1149  | 0.45        | 0/1548         |
| 36  | 2e    | 0.20         | 0/1149  | 0.43        | 0/1548         |
| 37  | 1f    | 0.19         | 0/827   | 0.41        | 0/1120         |
| 37  | 2f    | 0.20         | 0/829   | 0.42        | 0/1123         |

| Mol | Chain | Bond lengths |          | Bond angles |                  |
|-----|-------|--------------|----------|-------------|------------------|
|     |       | RMSZ         | # Z  >5  | RMSZ        | # Z  >5          |
| 38  | 1g    | 0.22         | 0/1254   | 0.39        | 0/1683           |
| 38  | 2g    | 0.19         | 0/1248   | 0.41        | 1/1676 (0.1%)    |
| 39  | 1h    | 0.20         | 0/1118   | 0.43        | 0/1506           |
| 39  | 2h    | 0.20         | 0/1108   | 0.41        | 0/1494           |
| 40  | 1i    | 0.21         | 0/1005   | 0.45        | 0/1351           |
| 40  | 2i    | 0.22         | 0/985    | 0.46        | 0/1329           |
| 41  | 1j    | 0.22         | 0/732    | 0.44        | 0/993            |
| 41  | 2j    | 0.22         | 0/723    | 0.47        | 0/984            |
| 42  | 1k    | 0.22         | 0/849    | 0.40        | 0/1150           |
| 42  | 2k    | 0.20         | 0/848    | 0.41        | 0/1149           |
| 43  | 1l    | 0.22         | 0/937    | 0.44        | 0/1260           |
| 43  | 2l    | 0.21         | 0/937    | 0.49        | 0/1260           |
| 44  | 1m    | 0.22         | 0/924    | 0.48        | 0/1242           |
| 44  | 2m    | 0.22         | 0/905    | 0.49        | 0/1217           |
| 45  | 1n    | 0.20         | 0/501    | 0.44        | 0/664            |
| 45  | 2n    | 0.22         | 0/501    | 0.43        | 0/664            |
| 46  | 1o    | 0.20         | 0/739    | 0.39        | 0/985            |
| 46  | 2o    | 0.18         | 0/739    | 0.40        | 0/985            |
| 47  | 1p    | 0.21         | 0/697    | 0.48        | 0/939            |
| 47  | 2p    | 0.20         | 0/693    | 0.44        | 0/935            |
| 48  | 1q    | 0.21         | 0/836    | 0.44        | 0/1117           |
| 48  | 2q    | 0.20         | 0/836    | 0.42        | 0/1117           |
| 49  | 1r    | 0.19         | 0/560    | 0.41        | 0/746            |
| 49  | 2r    | 0.20         | 0/560    | 0.40        | 0/746            |
| 50  | 1s    | 0.21         | 0/663    | 0.45        | 0/895            |
| 50  | 2s    | 0.20         | 0/660    | 0.41        | 0/893            |
| 51  | 1t    | 0.22         | 0/734    | 0.50        | 0/969            |
| 51  | 2t    | 0.20         | 0/736    | 0.43        | 0/976            |
| 52  | 1u    | 0.19         | 0/203    | 0.44        | 0/266            |
| 52  | 2u    | 0.22         | 0/203    | 0.52        | 0/266            |
| 53  | 1y    | 0.25         | 0/776    | 0.36        | 0/1048           |
| 53  | 2y    | 0.20         | 0/761    | 0.36        | 0/1030           |
| All | All   | 0.24         | 0/309941 | 0.43        | 11/463239 (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 |
|-----|-------|---------------------|---------------------|
| 3   | 1D    | 0                   | 1                   |
| 8   | 2I    | 0                   | 1                   |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 11  | 1P    | 0                   | 1                   |
| 14  | 1S    | 0                   | 1                   |
| 19  | 1X    | 0                   | 1                   |
| 26  | 24    | 0                   | 1                   |
| 33  | 1b    | 0                   | 1                   |
| 33  | 2b    | 0                   | 1                   |
| 43  | 2l    | 0                   | 1                   |
| All | All   | 0                   | 9                   |

There are no bond length outliers.

All (11) bond angle outliers are listed below:

| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 32  | 2a    | 266    | G    | P-O3'-C3'   | 5.91  | 129.06      | 120.20   |
| 1   | 2A    | 1992   | G    | C2'-C3'-O3' | 5.79  | 118.18      | 109.50   |
| 11  | 1P    | 116    | GLY  | N-CA-C      | 5.68  | 119.36      | 112.49   |
| 38  | 2g    | 69     | VAL  | N-CA-C      | -5.65 | 108.34      | 113.71   |
| 1   | 2A    | 271(M) | G    | OP1-P-O3'   | 5.52  | 117.34      | 105.20   |
| 26  | 24    | 60     | GLN  | N-CA-C      | 5.48  | 126.35      | 111.00   |
| 1   | 2A    | 271(M) | G    | P-O3'-C3'   | 5.43  | 126.22      | 119.70   |
| 26  | 24    | 59     | PHE  | CA-C-N      | 5.34  | 131.31      | 121.70   |
| 26  | 24    | 59     | PHE  | C-N-CA      | 5.34  | 131.31      | 121.70   |
| 5   | 2F    | 21     | ALA  | CA-C-N      | 5.28  | 131.20      | 121.70   |
| 5   | 2F    | 21     | ALA  | C-N-CA      | 5.28  | 131.20      | 121.70   |

There are no chirality outliers.

All (9) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 3   | 1D    | 141 | VAL  | Peptide |
| 11  | 1P    | 35  | HIS  | Peptide |
| 14  | 1S    | 58  | LEU  | Peptide |
| 19  | 1X    | 93  | GLU  | Peptide |
| 33  | 1b    | 231 | GLU  | Peptide |
| 26  | 24    | 18  | CYS  | Peptide |
| 8   | 2I    | 85  | GLU  | Peptide |
| 33  | 2b    | 199 | TYR  | Peptide |
| 43  | 2l    | 86  | ARG  | 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    | 61869 | 0        | 31202    | 630     | 0            |
| 1   | 2A    | 61758 | 0        | 31153    | 784     | 0            |
| 2   | 1B    | 2572  | 0        | 1304     | 22      | 0            |
| 2   | 2B    | 2573  | 0        | 1306     | 31      | 0            |
| 3   | 1D    | 2131  | 0        | 2207     | 55      | 0            |
| 3   | 2D    | 2136  | 0        | 2218     | 45      | 0            |
| 4   | 1E    | 1559  | 0        | 1618     | 44      | 0            |
| 4   | 2E    | 1559  | 0        | 1618     | 45      | 0            |
| 5   | 1F    | 1584  | 0        | 1625     | 38      | 0            |
| 5   | 2F    | 1580  | 0        | 1619     | 40      | 0            |
| 6   | 1G    | 1426  | 0        | 1445     | 40      | 0            |
| 6   | 2G    | 1424  | 0        | 1441     | 57      | 0            |
| 7   | 1H    | 1330  | 0        | 1407     | 36      | 0            |
| 7   | 2H    | 1324  | 0        | 1402     | 36      | 0            |
| 8   | 1I    | 1094  | 0        | 1127     | 31      | 0            |
| 8   | 2I    | 1076  | 0        | 1094     | 38      | 0            |
| 9   | 1N    | 1121  | 0        | 1195     | 18      | 0            |
| 9   | 2N    | 1117  | 0        | 1184     | 31      | 0            |
| 10  | 1O    | 933   | 0        | 996      | 23      | 0            |
| 10  | 2O    | 933   | 0        | 996      | 23      | 0            |
| 11  | 1P    | 1135  | 0        | 1212     | 33      | 0            |
| 11  | 2P    | 1135  | 0        | 1212     | 31      | 0            |
| 12  | 1Q    | 1122  | 0        | 1179     | 23      | 0            |
| 12  | 2Q    | 1122  | 0        | 1179     | 27      | 0            |
| 13  | 1R    | 968   | 0        | 1033     | 17      | 0            |
| 13  | 2R    | 968   | 0        | 1033     | 25      | 0            |
| 14  | 1S    | 877   | 0        | 938      | 22      | 0            |
| 14  | 2S    | 870   | 0        | 923      | 22      | 0            |
| 15  | 1T    | 1091  | 0        | 1151     | 23      | 0            |
| 15  | 2T    | 1083  | 0        | 1136     | 24      | 0            |
| 16  | 1U    | 959   | 0        | 1019     | 20      | 0            |
| 16  | 2U    | 959   | 0        | 1019     | 23      | 0            |
| 17  | 1V    | 775   | 0        | 841      | 17      | 0            |
| 17  | 2V    | 771   | 0        | 830      | 24      | 0            |
| 18  | 1W    | 886   | 0        | 940      | 21      | 0            |
| 18  | 2W    | 886   | 0        | 940      | 19      | 0            |
| 19  | 1X    | 750   | 0        | 814      | 17      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 19  | 2X    | 750   | 0        | 814      | 16      | 0            |
| 20  | 1Y    | 810   | 0        | 892      | 20      | 0            |
| 20  | 2Y    | 810   | 0        | 887      | 19      | 0            |
| 21  | 1Z    | 1587  | 0        | 1598     | 26      | 0            |
| 21  | 2Z    | 1557  | 0        | 1564     | 51      | 0            |
| 22  | 10    | 608   | 0        | 622      | 21      | 0            |
| 22  | 20    | 608   | 0        | 622      | 18      | 0            |
| 23  | 11    | 754   | 0        | 823      | 14      | 0            |
| 23  | 21    | 759   | 0        | 837      | 23      | 0            |
| 24  | 12    | 588   | 0        | 643      | 13      | 0            |
| 24  | 22    | 592   | 0        | 654      | 13      | 0            |
| 25  | 13    | 469   | 0        | 518      | 5       | 0            |
| 25  | 23    | 464   | 0        | 514      | 11      | 0            |
| 26  | 14    | 546   | 0        | 522      | 22      | 0            |
| 26  | 24    | 536   | 0        | 514      | 26      | 0            |
| 27  | 15    | 459   | 0        | 476      | 12      | 0            |
| 27  | 25    | 455   | 0        | 465      | 16      | 0            |
| 28  | 16    | 453   | 0        | 473      | 8       | 0            |
| 28  | 26    | 449   | 0        | 469      | 10      | 0            |
| 29  | 17    | 418   | 0        | 467      | 9       | 0            |
| 29  | 27    | 418   | 0        | 467      | 6       | 0            |
| 30  | 18    | 517   | 0        | 582      | 21      | 0            |
| 30  | 28    | 517   | 0        | 582      | 15      | 0            |
| 31  | 19    | 307   | 0        | 335      | 4       | 0            |
| 31  | 29    | 307   | 0        | 335      | 10      | 0            |
| 32  | 1a    | 32246 | 0        | 16294    | 503     | 0            |
| 32  | 2a    | 32331 | 0        | 16338    | 473     | 0            |
| 33  | 1b    | 1842  | 0        | 1862     | 75      | 0            |
| 33  | 2b    | 1825  | 0        | 1828     | 72      | 0            |
| 34  | 1c    | 1558  | 0        | 1557     | 36      | 0            |
| 34  | 2c    | 1542  | 0        | 1517     | 38      | 0            |
| 35  | 1d    | 1665  | 0        | 1687     | 65      | 0            |
| 35  | 2d    | 1668  | 0        | 1703     | 57      | 0            |
| 36  | 1e    | 1133  | 0        | 1191     | 38      | 0            |
| 36  | 2e    | 1133  | 0        | 1191     | 37      | 0            |
| 37  | 1f    | 814   | 0        | 808      | 20      | 0            |
| 37  | 2f    | 816   | 0        | 808      | 16      | 0            |
| 38  | 1g    | 1235  | 0        | 1249     | 30      | 0            |
| 38  | 2g    | 1229  | 0        | 1238     | 22      | 0            |
| 39  | 1h    | 1098  | 0        | 1143     | 32      | 0            |
| 39  | 2h    | 1088  | 0        | 1126     | 37      | 0            |
| 40  | 1i    | 986   | 0        | 990      | 36      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 40  | 2i    | 966   | 0        | 953      | 47      | 0            |
| 41  | 1j    | 719   | 0        | 672      | 22      | 0            |
| 41  | 2j    | 710   | 0        | 661      | 26      | 0            |
| 42  | 1k    | 834   | 0        | 838      | 19      | 0            |
| 42  | 2k    | 833   | 0        | 836      | 25      | 0            |
| 43  | 1l    | 932   | 0        | 981      | 14      | 0            |
| 43  | 2l    | 932   | 0        | 981      | 16      | 0            |
| 44  | 1m    | 914   | 0        | 954      | 40      | 0            |
| 44  | 2m    | 895   | 0        | 920      | 41      | 0            |
| 45  | 1n    | 492   | 0        | 529      | 13      | 0            |
| 45  | 2n    | 492   | 0        | 529      | 18      | 0            |
| 46  | 1o    | 728   | 0        | 760      | 18      | 0            |
| 46  | 2o    | 728   | 0        | 760      | 19      | 0            |
| 47  | 1p    | 681   | 0        | 697      | 30      | 0            |
| 47  | 2p    | 677   | 0        | 686      | 26      | 0            |
| 48  | 1q    | 823   | 0        | 891      | 23      | 0            |
| 48  | 2q    | 823   | 0        | 891      | 22      | 0            |
| 49  | 1r    | 555   | 0        | 618      | 12      | 0            |
| 49  | 2r    | 555   | 0        | 618      | 21      | 0            |
| 50  | 1s    | 648   | 0        | 658      | 19      | 0            |
| 50  | 2s    | 645   | 0        | 635      | 21      | 0            |
| 51  | 1t    | 732   | 0        | 809      | 24      | 0            |
| 51  | 2t    | 733   | 0        | 795      | 17      | 0            |
| 52  | 1u    | 199   | 0        | 208      | 5       | 0            |
| 52  | 2u    | 199   | 0        | 208      | 4       | 0            |
| 53  | 1y    | 764   | 0        | 786      | 19      | 0            |
| 53  | 2y    | 749   | 0        | 757      | 16      | 0            |
| 54  | 10    | 7     | 0        | 0        | 0       | 0            |
| 54  | 11    | 5     | 0        | 0        | 0       | 0            |
| 54  | 13    | 3     | 0        | 0        | 0       | 0            |
| 54  | 15    | 8     | 0        | 0        | 0       | 0            |
| 54  | 16    | 1     | 0        | 0        | 0       | 0            |
| 54  | 17    | 5     | 0        | 0        | 0       | 0            |
| 54  | 18    | 3     | 0        | 0        | 0       | 0            |
| 54  | 19    | 3     | 0        | 0        | 0       | 0            |
| 54  | 1A    | 1049  | 0        | 0        | 0       | 0            |
| 54  | 1B    | 30    | 0        | 0        | 0       | 0            |
| 54  | 1D    | 21    | 0        | 0        | 0       | 0            |
| 54  | 1E    | 8     | 0        | 0        | 0       | 0            |
| 54  | 1F    | 18    | 0        | 0        | 0       | 0            |
| 54  | 1G    | 4     | 0        | 0        | 0       | 0            |
| 54  | 1H    | 3     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 54  | 1N    | 2     | 0        | 0        | 0       | 0            |
| 54  | 1O    | 2     | 0        | 0        | 0       | 0            |
| 54  | 1P    | 6     | 0        | 0        | 0       | 0            |
| 54  | 1Q    | 6     | 0        | 0        | 0       | 0            |
| 54  | 1R    | 4     | 0        | 0        | 0       | 0            |
| 54  | 1S    | 2     | 0        | 0        | 0       | 0            |
| 54  | 1T    | 4     | 0        | 0        | 0       | 0            |
| 54  | 1U    | 6     | 0        | 0        | 0       | 0            |
| 54  | 1V    | 6     | 0        | 0        | 0       | 0            |
| 54  | 1W    | 3     | 0        | 0        | 0       | 0            |
| 54  | 1X    | 1     | 0        | 0        | 0       | 0            |
| 54  | 1Y    | 1     | 0        | 0        | 0       | 0            |
| 54  | 1Z    | 1     | 0        | 0        | 0       | 0            |
| 54  | 1a    | 282   | 0        | 0        | 0       | 0            |
| 54  | 1b    | 1     | 0        | 0        | 0       | 0            |
| 54  | 1d    | 5     | 0        | 0        | 0       | 0            |
| 54  | 1e    | 3     | 0        | 0        | 0       | 0            |
| 54  | 1f    | 2     | 0        | 0        | 0       | 0            |
| 54  | 1g    | 2     | 0        | 0        | 0       | 0            |
| 54  | 1h    | 1     | 0        | 0        | 0       | 0            |
| 54  | 1i    | 1     | 0        | 0        | 0       | 0            |
| 54  | 1k    | 1     | 0        | 0        | 0       | 0            |
| 54  | 1l    | 2     | 0        | 0        | 0       | 0            |
| 54  | 1m    | 1     | 0        | 0        | 0       | 0            |
| 54  | 1n    | 1     | 0        | 0        | 0       | 0            |
| 54  | 1o    | 1     | 0        | 0        | 0       | 0            |
| 54  | 1p    | 1     | 0        | 0        | 0       | 0            |
| 54  | 1t    | 2     | 0        | 0        | 0       | 0            |
| 54  | 1y    | 4     | 0        | 0        | 0       | 0            |
| 54  | 20    | 1     | 0        | 0        | 0       | 0            |
| 54  | 21    | 2     | 0        | 0        | 0       | 0            |
| 54  | 23    | 1     | 0        | 0        | 0       | 0            |
| 54  | 25    | 2     | 0        | 0        | 0       | 0            |
| 54  | 27    | 2     | 0        | 0        | 0       | 0            |
| 54  | 28    | 2     | 0        | 0        | 0       | 0            |
| 54  | 2A    | 756   | 0        | 0        | 0       | 0            |
| 54  | 2B    | 19    | 0        | 0        | 0       | 0            |
| 54  | 2D    | 11    | 0        | 0        | 0       | 0            |
| 54  | 2E    | 7     | 0        | 0        | 0       | 0            |
| 54  | 2F    | 5     | 0        | 0        | 0       | 0            |
| 54  | 2G    | 3     | 0        | 0        | 0       | 0            |
| 54  | 2I    | 1     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 54  | 2N    | 1     | 0        | 0        | 0       | 0            |
| 54  | 2O    | 2     | 0        | 0        | 0       | 0            |
| 54  | 2P    | 3     | 0        | 0        | 0       | 0            |
| 54  | 2Q    | 4     | 0        | 0        | 0       | 0            |
| 54  | 2R    | 1     | 0        | 0        | 0       | 0            |
| 54  | 2T    | 4     | 0        | 0        | 0       | 0            |
| 54  | 2V    | 2     | 0        | 0        | 0       | 0            |
| 54  | 2W    | 3     | 0        | 0        | 0       | 0            |
| 54  | 2X    | 1     | 0        | 0        | 0       | 0            |
| 54  | 2Y    | 1     | 0        | 0        | 0       | 0            |
| 54  | 2a    | 193   | 0        | 0        | 0       | 0            |
| 54  | 2e    | 1     | 0        | 0        | 0       | 0            |
| 54  | 2f    | 1     | 0        | 0        | 0       | 0            |
| 54  | 2j    | 1     | 0        | 0        | 0       | 0            |
| 54  | 2k    | 1     | 0        | 0        | 0       | 0            |
| 54  | 2n    | 1     | 0        | 0        | 0       | 0            |
| 54  | 2p    | 1     | 0        | 0        | 0       | 0            |
| 54  | 2q    | 1     | 0        | 0        | 0       | 0            |
| 54  | 2r    | 1     | 0        | 0        | 0       | 0            |
| 54  | 2t    | 1     | 0        | 0        | 0       | 0            |
| 54  | 2y    | 1     | 0        | 0        | 0       | 0            |
| 55  | 1A    | 45    | 0        | 0        | 0       | 0            |
| 55  | 2A    | 45    | 0        | 0        | 0       | 0            |
| 56  | 18    | 8     | 0        | 14       | 4       | 0            |
| 56  | 1A    | 8     | 0        | 14       | 0       | 0            |
| 56  | 1O    | 8     | 0        | 14       | 0       | 0            |
| 56  | 1a    | 8     | 0        | 13       | 5       | 0            |
| 56  | 2A    | 16    | 0        | 28       | 3       | 0            |
| 56  | 2B    | 8     | 0        | 14       | 0       | 0            |
| 57  | 1B    | 12    | 0        | 12       | 3       | 0            |
| 58  | 14    | 1     | 0        | 0        | 0       | 0            |
| 58  | 15    | 1     | 0        | 0        | 0       | 0            |
| 58  | 16    | 1     | 0        | 0        | 0       | 0            |
| 58  | 19    | 1     | 0        | 0        | 0       | 0            |
| 58  | 1Y    | 1     | 0        | 0        | 0       | 0            |
| 58  | 1n    | 1     | 0        | 0        | 0       | 0            |
| 58  | 24    | 1     | 0        | 0        | 0       | 0            |
| 58  | 25    | 1     | 0        | 0        | 0       | 0            |
| 58  | 26    | 1     | 0        | 0        | 0       | 0            |
| 58  | 29    | 1     | 0        | 0        | 0       | 0            |
| 58  | 2Y    | 1     | 0        | 0        | 0       | 0            |
| 58  | 2n    | 1     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 59  | 1d    | 8     | 0        | 0        | 0       | 0            |
| 59  | 2d    | 8     | 0        | 0        | 2       | 0            |
| 60  | 10    | 22    | 0        | 0        | 0       | 0            |
| 60  | 11    | 25    | 0        | 0        | 0       | 0            |
| 60  | 12    | 12    | 0        | 0        | 2       | 0            |
| 60  | 13    | 25    | 0        | 0        | 0       | 0            |
| 60  | 14    | 1     | 0        | 0        | 0       | 0            |
| 60  | 15    | 26    | 0        | 0        | 1       | 0            |
| 60  | 16    | 18    | 0        | 0        | 0       | 0            |
| 60  | 17    | 16    | 0        | 0        | 2       | 0            |
| 60  | 18    | 32    | 0        | 0        | 3       | 0            |
| 60  | 19    | 12    | 0        | 0        | 0       | 0            |
| 60  | 1A    | 4087  | 0        | 0        | 152     | 0            |
| 60  | 1B    | 107   | 0        | 0        | 6       | 0            |
| 60  | 1D    | 109   | 0        | 0        | 6       | 0            |
| 60  | 1E    | 73    | 0        | 0        | 4       | 0            |
| 60  | 1F    | 66    | 0        | 0        | 5       | 0            |
| 60  | 1G    | 19    | 0        | 0        | 2       | 0            |
| 60  | 1H    | 15    | 0        | 0        | 1       | 0            |
| 60  | 1I    | 7     | 0        | 0        | 0       | 0            |
| 60  | 1N    | 53    | 0        | 0        | 2       | 0            |
| 60  | 1O    | 26    | 0        | 0        | 0       | 0            |
| 60  | 1P    | 58    | 0        | 0        | 3       | 0            |
| 60  | 1Q    | 42    | 0        | 0        | 0       | 0            |
| 60  | 1R    | 31    | 0        | 0        | 3       | 0            |
| 60  | 1S    | 8     | 0        | 0        | 0       | 0            |
| 60  | 1T    | 28    | 0        | 0        | 2       | 0            |
| 60  | 1U    | 49    | 0        | 0        | 4       | 0            |
| 60  | 1V    | 42    | 0        | 0        | 2       | 0            |
| 60  | 1W    | 32    | 0        | 0        | 3       | 0            |
| 60  | 1X    | 27    | 0        | 0        | 2       | 0            |
| 60  | 1Y    | 20    | 0        | 0        | 3       | 0            |
| 60  | 1Z    | 10    | 0        | 0        | 0       | 0            |
| 60  | 1a    | 596   | 0        | 0        | 39      | 0            |
| 60  | 1b    | 2     | 0        | 0        | 0       | 0            |
| 60  | 1d    | 7     | 0        | 0        | 2       | 0            |
| 60  | 1e    | 6     | 0        | 0        | 0       | 0            |
| 60  | 1f    | 2     | 0        | 0        | 0       | 0            |
| 60  | 1h    | 1     | 0        | 0        | 0       | 0            |
| 60  | 1j    | 1     | 0        | 0        | 0       | 0            |
| 60  | 1l    | 6     | 0        | 0        | 1       | 0            |
| 60  | 1m    | 2     | 0        | 0        | 1       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 60  | 1n    | 1     | 0        | 0        | 0       | 0            |
| 60  | 1o    | 3     | 0        | 0        | 0       | 0            |
| 60  | 1p    | 3     | 0        | 0        | 0       | 0            |
| 60  | 1q    | 1     | 0        | 0        | 0       | 0            |
| 60  | 1t    | 1     | 0        | 0        | 0       | 0            |
| 60  | 1u    | 2     | 0        | 0        | 0       | 0            |
| 60  | 1y    | 9     | 0        | 0        | 0       | 0            |
| 60  | 20    | 16    | 0        | 0        | 2       | 0            |
| 60  | 21    | 22    | 0        | 0        | 1       | 0            |
| 60  | 22    | 2     | 0        | 0        | 0       | 0            |
| 60  | 23    | 3     | 0        | 0        | 0       | 0            |
| 60  | 24    | 1     | 0        | 0        | 0       | 0            |
| 60  | 25    | 7     | 0        | 0        | 0       | 0            |
| 60  | 26    | 7     | 0        | 0        | 1       | 0            |
| 60  | 27    | 13    | 0        | 0        | 0       | 0            |
| 60  | 28    | 15    | 0        | 0        | 2       | 0            |
| 60  | 29    | 1     | 0        | 0        | 0       | 0            |
| 60  | 2A    | 2546  | 0        | 0        | 161     | 0            |
| 60  | 2B    | 60    | 0        | 0        | 5       | 0            |
| 60  | 2D    | 50    | 0        | 0        | 1       | 0            |
| 60  | 2E    | 36    | 0        | 0        | 5       | 0            |
| 60  | 2F    | 25    | 0        | 0        | 0       | 0            |
| 60  | 2G    | 8     | 0        | 0        | 0       | 0            |
| 60  | 2H    | 2     | 0        | 0        | 0       | 0            |
| 60  | 2I    | 4     | 0        | 0        | 1       | 0            |
| 60  | 2N    | 8     | 0        | 0        | 1       | 0            |
| 60  | 2O    | 20    | 0        | 0        | 0       | 0            |
| 60  | 2P    | 30    | 0        | 0        | 4       | 0            |
| 60  | 2Q    | 18    | 0        | 0        | 1       | 0            |
| 60  | 2R    | 19    | 0        | 0        | 1       | 0            |
| 60  | 2S    | 5     | 0        | 0        | 0       | 0            |
| 60  | 2T    | 10    | 0        | 0        | 0       | 0            |
| 60  | 2U    | 12    | 0        | 0        | 0       | 0            |
| 60  | 2V    | 9     | 0        | 0        | 1       | 0            |
| 60  | 2W    | 25    | 0        | 0        | 3       | 0            |
| 60  | 2X    | 9     | 0        | 0        | 0       | 0            |
| 60  | 2Y    | 7     | 0        | 0        | 1       | 0            |
| 60  | 2Z    | 11    | 0        | 0        | 1       | 0            |
| 60  | 2a    | 461   | 0        | 0        | 32      | 0            |
| 60  | 2d    | 4     | 0        | 0        | 0       | 0            |
| 60  | 2e    | 2     | 0        | 0        | 0       | 0            |
| 60  | 2f    | 1     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 60  | 2j    | 2      | 0        | 0        | 0       | 0            |
| 60  | 2l    | 3      | 0        | 0        | 0       | 0            |
| 60  | 2o    | 3      | 0        | 0        | 0       | 0            |
| 60  | 2p    | 2      | 0        | 0        | 0       | 0            |
| 60  | 2q    | 1      | 0        | 0        | 0       | 0            |
| 60  | 2r    | 4      | 0        | 0        | 0       | 0            |
| 60  | 2t    | 2      | 0        | 0        | 0       | 0            |
| 60  | 2y    | 4      | 0        | 0        | 0       | 0            |
| All | All   | 298337 | 0        | 194501   | 4419    | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (4419) 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    | 1.25                     | 1.35              |
| 32:2a:1003:G:H2'  | 32:2a:1004:A:H4'  | 1.28                     | 1.10              |
| 1:1A:1082:U:O4    | 1:1A:1086:A:N1    | 1.96                     | 0.99              |
| 32:1a:255:G:H1'   | 48:1q:16:GLN:HE21 | 1.26                     | 0.97              |
| 15:1T:55:ASN:H    | 15:1T:59:THR:HG22 | 1.28                     | 0.97              |
| 32:1a:201:C:H42   | 32:1a:216:G:H1    | 1.15                     | 0.92              |
| 1:2A:2602:A:H1'   | 1:2A:2603:G:H5''  | 1.51                     | 0.92              |
| 32:1a:1500:A:OP1  | 60:1a:1905:HOH:O  | 1.88                     | 0.91              |
| 1:1A:1798:U:H5'   | 3:1D:259:THR:HG22 | 1.54                     | 0.89              |
| 1:1A:2127:G:H21   | 1:1A:2173:A:H1'   | 1.36                     | 0.89              |
| 32:2a:1500:A:OP1  | 60:2a:3205:HOH:O  | 1.91                     | 0.89              |
| 1:2A:1065:U:H3    | 1:2A:1073:A:H61   | 1.21                     | 0.88              |
| 20:1Y:92:ASN:HB2  | 20:1Y:94:LYS:H    | 1.37                     | 0.88              |
| 29:17:24:THR:HG22 | 29:17:27:GLY:H    | 1.38                     | 0.88              |
| 32:1a:1158:C:H5   | 32:1a:1181:G:H1   | 1.22                     | 0.88              |
| 1:2A:2499:C:OP1   | 60:2A:3814:HOH:O  | 1.91                     | 0.88              |
| 32:2a:134:A:H61   | 47:2p:25:ARG:HH22 | 1.23                     | 0.86              |
| 1:1A:2304:G:H22   | 1:1A:2312:U:H3    | 1.19                     | 0.86              |
| 6:1G:161:THR:HG22 | 6:1G:163:ALA:H    | 1.40                     | 0.86              |
| 1:2A:2130:U:H2'   | 1:2A:2158:A:H61   | 1.39                     | 0.85              |
| 4:1E:110:GLY:O    | 60:1R:301:HOH:O   | 1.94                     | 0.85              |
| 4:2E:110:GLY:O    | 60:2R:301:HOH:O   | 1.95                     | 0.84              |
| 40:2i:3:GLN:HG2   | 40:2i:20:ARG:HE   | 1.41                     | 0.84              |
| 1:2A:1041:C:H42   | 1:2A:1114:G:H1    | 1.25                     | 0.84              |
| 12:2Q:135:ASP:OD2 | 21:2Z:49:ARG:NH1  | 2.11                     | 0.83              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 10:2O:48:PRO:HB3    | 32:2a:1422:G:H5''   | 1.59                     | 0.83              |
| 41:1j:35:SER:HB3    | 41:1j:73:ASP:HB2    | 1.59                     | 0.83              |
| 27:15:15:ARG:NH1    | 60:15:201:HOH:O     | 2.06                     | 0.83              |
| 48:1q:6:LEU:HD23    | 48:1q:23:VAL:HG11   | 1.60                     | 0.83              |
| 1:2A:805:G:OP1      | 60:2A:3816:HOH:O    | 1.97                     | 0.83              |
| 32:2a:1182:G:H5'    | 32:2a:1184:G:H5''   | 1.59                     | 0.83              |
| 32:1a:664:G:H22     | 32:1a:741:G:H1      | 1.26                     | 0.83              |
| 32:2a:1086:U:H3     | 32:2a:1099:G:H22    | 1.27                     | 0.82              |
| 33:2b:16:HIS:HB2    | 33:2b:204:ASN:HB3   | 1.59                     | 0.82              |
| 32:1a:437:U:H5'     | 35:1d:155:LEU:HD21  | 1.60                     | 0.82              |
| 1:1A:1082:U:N3      | 1:1A:1086:A:N6      | 2.09                     | 0.81              |
| 1:2A:685:A:OP1      | 60:2A:3815:HOH:O    | 1.97                     | 0.81              |
| 1:2A:1007:C:OP1     | 9:2N:35:ARG:NH1     | 2.13                     | 0.81              |
| 32:1a:1212:U:H5''   | 32:1a:1213:A:H5'    | 1.63                     | 0.81              |
| 20:1Y:15:VAL:HG21   | 20:1Y:42:VAL:HG11   | 1.63                     | 0.81              |
| 10:1O:48:PRO:HB3    | 32:1a:1422:G:H5''   | 1.64                     | 0.80              |
| 1:1A:2819:G:OP1     | 60:1A:4110:HOH:O    | 2.00                     | 0.80              |
| 1:2A:2849:U:O4      | 15:2T:23:ARG:NH2    | 2.13                     | 0.80              |
| 27:25:16:ARG:NH1    | 27:25:17:ASP:OD1    | 2.15                     | 0.80              |
| 1:2A:585:G:OP2      | 60:2A:3817:HOH:O    | 1.99                     | 0.79              |
| 1:2A:1365:A:O2'     | 23:21:11:ARG:NH1    | 2.15                     | 0.79              |
| 32:2a:768:A:OP2     | 60:2a:3206:HOH:O    | 2.01                     | 0.79              |
| 1:2A:1335:U:O4      | 60:2A:3818:HOH:O    | 2.00                     | 0.79              |
| 1:1A:1669:A:OP2     | 60:1A:4109:HOH:O    | 1.99                     | 0.79              |
| 1:2A:2427:C:OP1     | 60:2A:3819:HOH:O    | 2.01                     | 0.79              |
| 32:2a:401:C:OP2     | 35:2d:73:ARG:NH2    | 2.13                     | 0.79              |
| 44:2m:16:ASP:HB3    | 44:2m:34:LEU:HD11   | 1.63                     | 0.79              |
| 1:1A:1772:G:O6      | 60:1A:4112:HOH:O    | 2.01                     | 0.79              |
| 32:2a:442:C:H42     | 32:2a:492:G:H1      | 1.27                     | 0.79              |
| 1:2A:731:C:OP2      | 60:2A:3820:HOH:O    | 2.02                     | 0.78              |
| 40:2i:51:ARG:HG2    | 40:2i:56:LEU:HD21   | 1.63                     | 0.78              |
| 1:1A:631:A:OP1      | 11:1P:65:ARG:NH1    | 2.16                     | 0.78              |
| 32:1a:964:A:OP2     | 53:1y:9:GLN:NE2     | 2.17                     | 0.78              |
| 1:2A:2584:U:H2'     | 1:2A:2585:U:H2'     | 1.63                     | 0.78              |
| 8:2I:85:GLU:HB3     | 8:2I:87:LYS:H       | 1.48                     | 0.78              |
| 34:2c:70:VAL:HG22   | 34:2c:72:LYS:H      | 1.46                     | 0.78              |
| 1:1A:1648:C:OP1     | 60:1A:4111:HOH:O    | 2.00                     | 0.78              |
| 32:1a:1224:G:OP2    | 60:1a:1907:HOH:O    | 2.03                     | 0.77              |
| 33:1b:69:LEU:HB3    | 33:1b:162:ILE:HG22  | 1.66                     | 0.77              |
| 32:2a:1030(B):C:H41 | 32:2a:1030(C):G:H21 | 1.33                     | 0.77              |
| 1:1A:1023:U:OP2     | 60:1A:4113:HOH:O    | 2.03                     | 0.77              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 21:2Z:28:MET:HE3  | 21:2Z:37:VAL:HG11  | 1.65                     | 0.77              |
| 18:2W:2:GLU:OE2   | 18:2W:72:LYS:NZ    | 2.18                     | 0.77              |
| 32:2a:533:A:OP2   | 60:2a:3207:HOH:O   | 2.03                     | 0.77              |
| 1:1A:517:C:OP1    | 27:15:16:ARG:NH2   | 2.16                     | 0.77              |
| 5:1F:195:ASP:HB2  | 5:1F:198:ALA:H     | 1.49                     | 0.77              |
| 17:2V:72:VAL:HG13 | 17:2V:85:LYS:HB3   | 1.64                     | 0.77              |
| 24:12:31:GLU:HB3  | 24:12:53:LEU:HD11  | 1.67                     | 0.76              |
| 1:1A:2134:A:H1'   | 1:1A:2159:G:H1'    | 1.66                     | 0.76              |
| 35:2d:13:ARG:HB3  | 35:2d:40:PRO:HD3   | 1.67                     | 0.76              |
| 32:1a:812:C:N3    | 60:1a:1930:HOH:O   | 2.18                     | 0.76              |
| 32:1a:1505:G:OP2  | 60:1a:1906:HOH:O   | 2.03                     | 0.76              |
| 39:2h:86:ILE:HG21 | 39:2h:133:LEU:HD13 | 1.68                     | 0.76              |
| 32:1a:1003:G:N2   | 32:1a:1004:A:N3    | 2.34                     | 0.76              |
| 1:2A:962:G:OP1    | 60:2A:3821:HOH:O   | 2.02                     | 0.76              |
| 40:2i:53:VAL:O    | 40:2i:55:ALA:N     | 2.19                     | 0.76              |
| 4:2E:11:MET:HG2   | 4:2E:24:THR:HG22   | 1.68                     | 0.76              |
| 1:2A:1264:G:OP1   | 27:25:19:ARG:NH2   | 2.15                     | 0.76              |
| 32:1a:608:A:OP2   | 60:1a:1909:HOH:O   | 2.04                     | 0.76              |
| 32:1a:673:G:H2'   | 32:1a:674:G:C8     | 2.21                     | 0.75              |
| 32:1a:965:A:OP2   | 53:1y:8:LYS:NZ     | 2.19                     | 0.75              |
| 32:1a:1291:G:OP1  | 38:1g:37:ASN:ND2   | 2.18                     | 0.75              |
| 39:2h:64:LYS:HG2  | 39:2h:79:VAL:HG21  | 1.69                     | 0.75              |
| 38:1g:78:ARG:NH1  | 38:1g:154:TYR:O    | 2.18                     | 0.75              |
| 41:2j:38:ILE:HG13 | 41:2j:71:LEU:HB3   | 1.67                     | 0.75              |
| 34:2c:179:ARG:NH1 | 34:2c:206:GLU:OE1  | 2.18                     | 0.75              |
| 1:2A:1031:G:H5''  | 31:29:8:LYS:HE3    | 1.68                     | 0.75              |
| 3:1D:69:ARG:NH2   | 3:1D:128:GLY:O     | 2.20                     | 0.75              |
| 14:1S:59:LYS:HD2  | 14:1S:60:GLY:H     | 1.51                     | 0.75              |
| 1:2A:2640:G:O3'   | 9:2N:74:ARG:NH2    | 2.17                     | 0.75              |
| 5:2F:53:THR:HG23  | 5:2F:55:GLY:H      | 1.50                     | 0.74              |
| 32:1a:572:A:OP2   | 60:1a:1908:HOH:O   | 2.04                     | 0.74              |
| 32:2a:1278:U:H5'' | 32:2a:1279:A:H5'   | 1.69                     | 0.74              |
| 32:1a:1182:G:H4'  | 32:1a:1183:A:H5'   | 1.68                     | 0.74              |
| 1:2A:31:C:OP1     | 60:2A:3822:HOH:O   | 2.04                     | 0.74              |
| 1:2A:2298:A:H62   | 1:2A:2318:G:H8     | 1.35                     | 0.74              |
| 1:2A:2839:G:H5'   | 13:2R:46:GLY:HA2   | 1.68                     | 0.74              |
| 32:2a:426:G:OP1   | 35:2d:38:TYR:OH    | 2.05                     | 0.74              |
| 1:1A:1085:A:HO2'  | 1:1A:1104:C:HO2'   | 1.24                     | 0.74              |
| 22:10:10:THR:HG22 | 22:10:12:ASN:H     | 1.51                     | 0.74              |
| 23:21:50:ARG:HG2  | 23:21:59:THR:HG22  | 1.70                     | 0.74              |
| 32:2a:677:U:H3    | 32:2a:713:G:H22    | 1.35                     | 0.74              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:2A:1315:C:OP2   | 60:2A:3825:HOH:O   | 2.06                     | 0.74              |
| 1:2A:2573:C:OP2   | 60:2A:3823:HOH:O   | 2.05                     | 0.74              |
| 39:2h:51:VAL:HG11 | 39:2h:60:ARG:HD2   | 1.70                     | 0.74              |
| 1:2A:2296:U:OP2   | 14:2S:9:ARG:NH2    | 2.20                     | 0.74              |
| 1:1A:218:A:OP2    | 60:1A:4114:HOH:O   | 2.06                     | 0.74              |
| 32:2a:975:A:H4'   | 32:2a:976:G:H5''   | 1.68                     | 0.74              |
| 42:2k:99:GLN:HE21 | 42:2k:105:VAL:HG21 | 1.53                     | 0.73              |
| 14:1S:25:ARG:NH1  | 14:1S:42:ASP:OD1   | 2.21                     | 0.73              |
| 32:2a:770:C:OP1   | 60:2a:3208:HOH:O   | 2.06                     | 0.73              |
| 1:2A:956:G:H5''   | 12:2Q:77:LYS:HD2   | 1.68                     | 0.73              |
| 1:2A:2748:A:H5'   | 7:2H:4:ILE:HD12    | 1.69                     | 0.73              |
| 21:2Z:69:THR:HG22 | 21:2Z:90:VAL:HA    | 1.68                     | 0.73              |
| 11:1P:64:LYS:NZ   | 60:1P:302:HOH:O    | 2.22                     | 0.73              |
| 1:1A:1064:C:H3'   | 1:1A:1065:U:H5''   | 1.68                     | 0.73              |
| 3:2D:69:ARG:NH2   | 3:2D:128:GLY:O     | 2.21                     | 0.73              |
| 12:2Q:111:GLU:OE2 | 12:2Q:133:ARG:NH2  | 2.22                     | 0.73              |
| 1:1A:131:G:OP1    | 60:1A:4121:HOH:O   | 2.07                     | 0.73              |
| 32:1a:289:G:OP2   | 60:1a:1912:HOH:O   | 2.06                     | 0.73              |
| 32:1a:803:G:OP1   | 60:1a:1910:HOH:O   | 2.05                     | 0.73              |
| 32:2a:547:A:OP1   | 60:2a:3209:HOH:O   | 2.06                     | 0.73              |
| 1:1A:2319:G:H22   | 14:1S:3:ARG:HD2    | 1.53                     | 0.73              |
| 1:2A:1995:U:OP1   | 60:2A:3824:HOH:O   | 2.05                     | 0.73              |
| 1:1A:601:C:OP1    | 5:1F:108:LYS:NZ    | 2.22                     | 0.73              |
| 32:1a:975:A:H4'   | 32:1a:976:G:H5''   | 1.70                     | 0.73              |
| 26:24:16:CYS:SG   | 26:24:17:GLY:N     | 2.59                     | 0.72              |
| 1:2A:1239:G:OP1   | 60:2A:3822:HOH:O   | 2.06                     | 0.72              |
| 1:1A:370:G:OP2    | 60:1A:4120:HOH:O   | 2.07                     | 0.72              |
| 1:1A:762:U:OP1    | 60:1A:4115:HOH:O   | 2.06                     | 0.72              |
| 1:1A:2134:A:H62   | 1:1A:2157:G:H4'    | 1.53                     | 0.72              |
| 26:14:40:HIS:HB3  | 26:14:43:TYR:HD2   | 1.54                     | 0.72              |
| 32:1a:394:G:O6    | 60:1a:1911:HOH:O   | 2.05                     | 0.72              |
| 32:2a:572:A:OP2   | 60:2a:3210:HOH:O   | 2.06                     | 0.72              |
| 41:2j:49:VAL:HG23 | 45:2n:41:ARG:HB2   | 1.71                     | 0.72              |
| 8:1I:77:LEU:HB3   | 8:1I:142:VAL:HG22  | 1.71                     | 0.72              |
| 1:2A:615:G:OP1    | 5:2F:40:GLN:NE2    | 2.22                     | 0.72              |
| 32:2a:656:C:O2'   | 46:2o:28:GLN:NE2   | 2.17                     | 0.72              |
| 32:2a:962:C:O2'   | 60:2a:3211:HOH:O   | 2.07                     | 0.72              |
| 1:2A:1332:G:OP1   | 60:2A:3825:HOH:O   | 2.07                     | 0.72              |
| 1:1A:2242:G:OP1   | 60:1A:4117:HOH:O   | 2.06                     | 0.72              |
| 1:1A:2337:G:OP1   | 60:1A:4119:HOH:O   | 2.07                     | 0.72              |
| 1:2A:888:C:OP1    | 44:2m:93:ARG:NH1   | 2.23                     | 0.72              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:2A:2407:G:OP1    | 60:2A:3828:HOH:O   | 2.08                     | 0.72              |
| 1:1A:1647:G:OP1    | 60:1A:4111:HOH:O   | 2.06                     | 0.72              |
| 15:2T:109:GLU:HG2  | 15:2T:112:ARG:HH22 | 1.54                     | 0.72              |
| 1:2A:1023:U:OP2    | 60:2A:3826:HOH:O   | 2.07                     | 0.72              |
| 1:1A:2822:G:OP2    | 60:1A:4122:HOH:O   | 2.07                     | 0.72              |
| 5:2F:132:VAL:HG21  | 5:2F:163:VAL:HG22  | 1.71                     | 0.72              |
| 32:2a:1129:C:H2'   | 32:2a:1139:G:N7    | 2.05                     | 0.72              |
| 1:1A:1143:A:OP1    | 9:1N:25:ARG:NH2    | 2.23                     | 0.71              |
| 1:2A:761:A:OP1     | 60:2A:3820:HOH:O   | 2.07                     | 0.71              |
| 1:2A:875:G:H5''    | 21:2Z:149:SER:HB3  | 1.72                     | 0.71              |
| 16:2U:104:GLN:HE21 | 16:2U:105:VAL:HG23 | 1.53                     | 0.71              |
| 1:1A:530:G:N1      | 1:1A:2023:G:OP1    | 2.21                     | 0.71              |
| 1:2A:1266:G:O5'    | 18:2W:15:ARG:NH2   | 2.23                     | 0.71              |
| 32:2a:673:G:H2'    | 32:2a:674:G:C8     | 2.25                     | 0.71              |
| 8:1I:92:VAL:HG13   | 8:1I:120:ILE:HB    | 1.72                     | 0.71              |
| 1:1A:995:C:OP1     | 60:1A:4118:HOH:O   | 2.06                     | 0.71              |
| 35:1d:83:SER:O     | 60:1d:401:HOH:O    | 2.08                     | 0.71              |
| 22:10:11:ARG:O     | 22:10:14:ARG:NH2   | 2.21                     | 0.71              |
| 21:2Z:19:ARG:NH1   | 21:2Z:84:GLU:O     | 2.24                     | 0.71              |
| 44:2m:58:GLU:O     | 44:2m:62:ASN:ND2   | 2.24                     | 0.71              |
| 48:2q:3:LYS:HD2    | 48:2q:60:ILE:HD11  | 1.71                     | 0.71              |
| 32:1a:258:G:H2'    | 32:1a:259:G:H8     | 1.56                     | 0.71              |
| 1:2A:477:A:OP2     | 60:2A:3829:HOH:O   | 2.08                     | 0.71              |
| 32:2a:1285:A:H4'   | 32:2a:1286:A:H5'   | 1.72                     | 0.71              |
| 1:2A:399:G:OP2     | 60:2A:3827:HOH:O   | 2.07                     | 0.71              |
| 5:2F:21:ALA:HB3    | 5:2F:22:ALA:HA     | 1.71                     | 0.71              |
| 1:1A:1185:C:OP2    | 60:1A:4124:HOH:O   | 2.08                     | 0.71              |
| 12:1Q:34:LEU:HD11  | 12:1Q:129:THR:HB   | 1.72                     | 0.71              |
| 1:1A:749:C:OP2     | 60:1A:4123:HOH:O   | 2.08                     | 0.70              |
| 1:2A:495:G:OP2     | 60:2A:3834:HOH:O   | 2.10                     | 0.70              |
| 1:2A:749:C:OP2     | 60:2A:3835:HOH:O   | 2.10                     | 0.70              |
| 1:2A:1670:C:OP1    | 60:2A:3832:HOH:O   | 2.09                     | 0.70              |
| 32:2a:390:C:O3'    | 47:2p:28:ARG:NH2   | 2.25                     | 0.70              |
| 33:2b:63:MET:HG3   | 33:2b:225:ALA:HB1  | 1.72                     | 0.70              |
| 1:1A:11:G:H2'      | 1:1A:12:U:H5''     | 1.73                     | 0.70              |
| 32:1a:407:G:H5''   | 35:1d:115:ARG:HB3  | 1.73                     | 0.70              |
| 1:1A:945:A:N7      | 60:1A:4239:HOH:O   | 2.24                     | 0.70              |
| 19:1X:31:HIS:HD2   | 19:1X:33:LYS:H     | 1.39                     | 0.70              |
| 3:2D:222:ARG:NH2   | 60:2D:401:HOH:O    | 2.22                     | 0.70              |
| 41:2j:7:LYS:HB3    | 41:2j:97:GLU:HB2   | 1.73                     | 0.70              |
| 1:1A:1352:U:OP2    | 60:1A:4125:HOH:O   | 2.09                     | 0.70              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:1A:1509(A):A:H2' | 1:1A:1509(B):A:O4' | 1.90                     | 0.70              |
| 32:1a:450:G:OP1    | 47:1p:43:LYS:NZ    | 2.24                     | 0.70              |
| 32:1a:758:G:OP1    | 60:1a:1915:HOH:O   | 2.10                     | 0.70              |
| 32:1a:1441:G:H5''  | 32:1a:1442:G:H5'   | 1.71                     | 0.70              |
| 1:2A:2589:A:N3     | 60:2A:3961:HOH:O   | 2.24                     | 0.70              |
| 4:2E:28:ALA:HB3    | 4:2E:93:VAL:HG12   | 1.74                     | 0.70              |
| 21:2Z:180:VAL:HG13 | 21:2Z:183:LEU:HD12 | 1.71                     | 0.70              |
| 26:24:46:GLN:HE21  | 26:24:48:ARG:HH22  | 1.38                     | 0.70              |
| 1:1A:1022:G:OP1    | 60:1A:4126:HOH:O   | 2.09                     | 0.70              |
| 1:1A:2431:U:OP1    | 60:1A:4127:HOH:O   | 2.09                     | 0.70              |
| 1:2A:1701:A:OP2    | 60:2A:3830:HOH:O   | 2.09                     | 0.70              |
| 6:2G:131:TYR:HE2   | 6:2G:133:LEU:HD23  | 1.57                     | 0.70              |
| 32:2a:406:G:H5'    | 35:2d:5:ILE:HD11   | 1.73                     | 0.70              |
| 1:1A:1176:G:H1'    | 1:1A:1177:A:H5'    | 1.74                     | 0.70              |
| 32:2a:617:G:OP2    | 60:2a:3212:HOH:O   | 2.09                     | 0.70              |
| 1:1A:1359:A:H61    | 1:1A:1372:U:H3     | 1.38                     | 0.70              |
| 32:1a:1356:G:H2'   | 32:1a:1357:A:C8    | 2.27                     | 0.70              |
| 32:1a:1518:MA6:H93 | 32:1a:1519:MA6:H92 | 1.74                     | 0.70              |
| 17:2V:40:LEU:HB2   | 17:2V:46:VAL:HG13  | 1.74                     | 0.70              |
| 33:2b:7:VAL:O      | 33:2b:217:ARG:NH1  | 2.25                     | 0.70              |
| 32:1a:547:A:OP1    | 60:1a:1913:HOH:O   | 2.09                     | 0.69              |
| 1:2A:1216:G:OP1    | 60:2A:3838:HOH:O   | 2.11                     | 0.69              |
| 1:2A:1199:U:OP1    | 60:2A:3833:HOH:O   | 2.09                     | 0.69              |
| 1:1A:990:A:OP2     | 60:1A:4131:HOH:O   | 2.11                     | 0.69              |
| 1:1A:1017:G:N7     | 60:1A:4254:HOH:O   | 2.25                     | 0.69              |
| 1:2A:1053:C:H2'    | 1:2A:1054:A:H8     | 1.57                     | 0.69              |
| 1:2A:2541:A:N7     | 60:2A:3977:HOH:O   | 2.25                     | 0.69              |
| 40:2i:9:ARG:HG2    | 40:2i:14:VAL:HG12  | 1.74                     | 0.69              |
| 1:1A:1082:U:H3     | 1:1A:1086:A:H61    | 0.70                     | 0.69              |
| 1:1A:2779:U:OP1    | 60:1A:4129:HOH:O   | 2.10                     | 0.69              |
| 33:1b:8:LYS:O      | 33:1b:217:ARG:NH2  | 2.25                     | 0.69              |
| 1:2A:135:G:N7      | 60:2A:3969:HOH:O   | 2.25                     | 0.69              |
| 33:2b:101:MET:HA   | 33:2b:108:ILE:HG13 | 1.74                     | 0.69              |
| 33:1b:185:ILE:HG23 | 33:1b:199:TYR:HB2  | 1.74                     | 0.69              |
| 1:2A:1349:A:OP1    | 60:2A:3839:HOH:O   | 2.11                     | 0.69              |
| 1:2A:1648:C:OP1    | 60:2A:3831:HOH:O   | 2.09                     | 0.69              |
| 13:1R:96:ARG:NH2   | 13:1R:118:GLU:OE2  | 2.20                     | 0.69              |
| 4:2E:47:VAL:HG11   | 4:2E:86:PRO:HD2    | 1.74                     | 0.69              |
| 1:2A:743:G:N7      | 60:2A:3971:HOH:O   | 2.25                     | 0.69              |
| 1:2A:1334:G:OP2    | 60:2A:3836:HOH:O   | 2.10                     | 0.69              |
| 1:2A:1843:C:H5'    | 3:2D:253:GLN:NE2   | 2.06                     | 0.69              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 5:2F:20:LEU:HD23   | 5:2F:21:ALA:H      | 1.57                     | 0.69              |
| 8:2I:78:THR:HA     | 8:2I:143:SER:HB2   | 1.75                     | 0.69              |
| 60:2A:3948:HOH:O   | 11:2P:55:ARG:NH2   | 2.26                     | 0.69              |
| 36:2e:12:LEU:HD12  | 36:2e:128:PRO:HB2  | 1.75                     | 0.69              |
| 50:2s:40:ILE:HG21  | 50:2s:62:ILE:HG21  | 1.74                     | 0.69              |
| 34:1c:116:VAL:HG21 | 34:1c:202:ILE:HD11 | 1.75                     | 0.69              |
| 40:1i:50:LEU:HD13  | 40:1i:56:LEU:HA    | 1.75                     | 0.69              |
| 1:1A:942:G:O6      | 60:1A:4128:HOH:O   | 2.10                     | 0.68              |
| 1:1A:2526:G:N2     | 60:1A:4252:HOH:O   | 2.25                     | 0.68              |
| 19:1X:35:THR:HG22  | 19:1X:38:GLU:H     | 1.57                     | 0.68              |
| 1:2A:1314:C:OP1    | 60:2A:3825:HOH:O   | 2.09                     | 0.68              |
| 32:1a:100:C:H2'    | 32:1a:101:A:C8     | 2.28                     | 0.68              |
| 32:1a:1286:A:H2'   | 32:1a:1287:A:H4'   | 1.74                     | 0.68              |
| 1:2A:1455:G:OP2    | 60:2A:3845:HOH:O   | 2.12                     | 0.68              |
| 32:2a:59:A:N1      | 60:2a:3236:HOH:O   | 2.24                     | 0.68              |
| 32:2a:532:A:H61    | 34:2c:193:TYR:HB3  | 1.59                     | 0.68              |
| 32:2a:1238:A:OP2   | 60:2a:3214:HOH:O   | 2.11                     | 0.68              |
| 32:1a:330:C:OP2    | 60:1a:1914:HOH:O   | 2.10                     | 0.68              |
| 39:1h:51:VAL:HG12  | 39:1h:52:ASP:H     | 1.58                     | 0.68              |
| 1:2A:53:A:OP2      | 60:2A:3837:HOH:O   | 2.10                     | 0.68              |
| 1:1A:1707:G:O6     | 60:1A:4116:HOH:O   | 2.06                     | 0.68              |
| 1:2A:2032:G:OP1    | 60:2A:3842:HOH:O   | 2.11                     | 0.68              |
| 5:2F:154:VAL:HG22  | 5:2F:191:ARG:HB2   | 1.75                     | 0.68              |
| 1:1A:1642:G:N7     | 60:1A:4279:HOH:O   | 2.26                     | 0.68              |
| 1:2A:2006:C:OP2    | 60:2A:3844:HOH:O   | 2.12                     | 0.68              |
| 1:2A:2364:C:OP1    | 22:20:55:ARG:NH1   | 2.26                     | 0.68              |
| 1:2A:2366:A:OP1    | 60:2A:3849:HOH:O   | 2.12                     | 0.68              |
| 1:1A:1775:U:OP1    | 60:1A:4130:HOH:O   | 2.10                     | 0.68              |
| 17:1V:23:GLU:OE2   | 60:1V:301:HOH:O    | 2.10                     | 0.68              |
| 1:2A:1843:C:H5'    | 3:2D:253:GLN:HE22  | 1.58                     | 0.68              |
| 2:2B:8:U:O3'       | 14:2S:25:ARG:NH2   | 2.26                     | 0.68              |
| 33:2b:21:ARG:HA    | 33:2b:39:ILE:HA    | 1.76                     | 0.68              |
| 39:2h:49:GLU:OE2   | 39:2h:62:TYR:OH    | 2.10                     | 0.68              |
| 3:1D:242:ARG:HG3   | 3:1D:242:ARG:HH11  | 1.58                     | 0.68              |
| 21:1Z:157:LEU:HD11 | 21:1Z:163:LEU:HD13 | 1.76                     | 0.68              |
| 42:2k:99:GLN:HG2   | 42:2k:105:VAL:HG11 | 1.75                     | 0.68              |
| 2:1B:84:C:N4       | 60:1B:306:HOH:O    | 2.27                     | 0.68              |
| 1:2A:14:A:OP2      | 60:2A:3840:HOH:O   | 2.11                     | 0.68              |
| 1:2A:994:C:OP1     | 16:2U:53:ARG:NH2   | 2.27                     | 0.68              |
| 4:2E:199:ARG:NH1   | 60:2E:404:HOH:O    | 2.27                     | 0.68              |
| 1:1A:2258:C:OP1    | 60:1A:4135:HOH:O   | 2.12                     | 0.68              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 5:1F:86:GLY:O      | 60:1F:401:HOH:O    | 2.11                     | 0.68              |
| 8:1I:109:ILE:HG13  | 8:1I:130:TYR:CZ    | 2.29                     | 0.68              |
| 20:1Y:50:ARG:NH1   | 60:1Y:301:HOH:O    | 2.26                     | 0.68              |
| 17:2V:60:GLU:HB2   | 17:2V:97:LYS:HE2   | 1.76                     | 0.68              |
| 21:2Z:45:ASP:OD1   | 21:2Z:49:ARG:NH2   | 2.26                     | 0.68              |
| 35:2d:98:GLU:OE1   | 35:2d:103:ASN:ND2  | 2.27                     | 0.68              |
| 1:1A:1024:G:OP2    | 60:1A:4113:HOH:O   | 2.11                     | 0.67              |
| 32:1a:78:G:H1      | 32:1a:91:C:H42     | 1.40                     | 0.67              |
| 45:1n:48:ALA:HB2   | 45:1n:53:LEU:HD12  | 1.76                     | 0.67              |
| 51:1t:51:GLU:HA    | 51:1t:54:LYS:HE3   | 1.75                     | 0.67              |
| 1:1A:1140:C:OP2    | 60:1A:4136:HOH:O   | 2.12                     | 0.67              |
| 1:1A:1315:C:OP2    | 60:1A:4134:HOH:O   | 2.12                     | 0.67              |
| 1:2A:881:G:H1      | 1:2A:895:U:H3      | 1.41                     | 0.67              |
| 17:2V:12:TYR:OH    | 60:2V:301:HOH:O    | 2.13                     | 0.67              |
| 21:2Z:10:ARG:NH1   | 21:2Z:26:GLY:O     | 2.26                     | 0.67              |
| 32:2a:53:A:OP2     | 60:2a:3213:HOH:O   | 2.10                     | 0.67              |
| 1:1A:2427:C:OP1    | 60:1A:4132:HOH:O   | 2.11                     | 0.67              |
| 11:1P:59:LEU:HD11  | 30:18:10:ALA:HB2   | 1.77                     | 0.67              |
| 1:2A:2066:C:OP1    | 60:2A:3841:HOH:O   | 2.11                     | 0.67              |
| 32:2a:773:G:OP1    | 60:2a:3216:HOH:O   | 2.13                     | 0.67              |
| 34:1c:131:ARG:HH11 | 34:1c:166:GLU:HG3  | 1.60                     | 0.67              |
| 1:2A:2788:C:OP1    | 4:2E:61:ARG:NH2    | 2.26                     | 0.67              |
| 4:2E:127:ASP:OD2   | 60:2E:401:HOH:O    | 2.13                     | 0.67              |
| 13:2R:51:LEU:HD22  | 13:2R:66:VAL:HG13  | 1.75                     | 0.67              |
| 1:1A:364:C:OP2     | 60:1A:4133:HOH:O   | 2.12                     | 0.67              |
| 12:1Q:116:GLU:OE2  | 12:1Q:119:ARG:NH2  | 2.27                     | 0.67              |
| 1:2A:641:C:O2'     | 1:2A:2350:C:OP1    | 2.12                     | 0.67              |
| 1:2A:2062:A:OP1    | 60:2A:3853:HOH:O   | 2.13                     | 0.67              |
| 32:2a:7:G:O2'      | 36:2e:120:THR:O    | 2.12                     | 0.67              |
| 1:1A:1671:U:O4     | 60:1A:4109:HOH:O   | 2.09                     | 0.67              |
| 32:1a:1069:C:OP2   | 60:1a:1916:HOH:O   | 2.12                     | 0.67              |
| 42:1k:34:ASP:HB3   | 42:1k:40:ILE:HD11  | 1.75                     | 0.67              |
| 34:2c:78:GLY:HA3   | 34:2c:83:ARG:H     | 1.60                     | 0.67              |
| 1:1A:2319:G:N2     | 14:1S:3:ARG:HD2    | 2.08                     | 0.67              |
| 36:1e:102:ALA:HB1  | 36:1e:106:PRO:HG2  | 1.75                     | 0.67              |
| 1:2A:2270:G:OP2    | 60:2A:3846:HOH:O   | 2.12                     | 0.67              |
| 1:1A:2447:G:OP2    | 60:1A:4140:HOH:O   | 2.13                     | 0.67              |
| 32:1a:1124:G:N2    | 32:1a:1125:U:O4    | 2.27                     | 0.67              |
| 33:1b:54:THR:HG21  | 33:1b:201:ILE:HD11 | 1.74                     | 0.67              |
| 1:2A:2051:A:OP2    | 60:2A:3854:HOH:O   | 2.13                     | 0.67              |
| 32:2a:421:U:H3     | 34:2c:127:ARG:HE   | 1.43                     | 0.67              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 32:1a:116:A:OP1     | 60:1a:1912:HOH:O   | 2.12                     | 0.67              |
| 34:2c:150:LYS:HG3   | 34:2c:169:ALA:HB2  | 1.77                     | 0.67              |
| 38:2g:50:ILE:HD11   | 38:2g:58:PRO:HA    | 1.76                     | 0.67              |
| 47:2p:42:ARG:HB3    | 47:2p:44:THR:HG23  | 1.76                     | 0.67              |
| 1:1A:2458:G:OP2     | 60:1A:4138:HOH:O   | 2.13                     | 0.67              |
| 20:1Y:92:ASN:N      | 20:1Y:93:GLY:HA2   | 2.09                     | 0.67              |
| 50:1s:3:ARG:HH21    | 50:1s:7:LYS:HE2    | 1.60                     | 0.67              |
| 1:2A:1783:A:OP1     | 60:2A:3855:HOH:O   | 2.13                     | 0.67              |
| 1:1A:771:G:OP1      | 29:17:10:ARG:NH1   | 2.28                     | 0.66              |
| 1:1A:1224:C:OP2     | 60:1A:4143:HOH:O   | 2.14                     | 0.66              |
| 4:2E:185:LYS:O      | 60:2E:402:HOH:O    | 2.13                     | 0.66              |
| 9:2N:123:TYR:OH     | 9:2N:130:HIS:NE2   | 2.22                     | 0.66              |
| 38:2g:77:SER:OG     | 38:2g:86:GLN:NE2   | 2.29                     | 0.66              |
| 1:1A:2550:G:OP1     | 60:1A:4109:HOH:O   | 2.14                     | 0.66              |
| 32:2a:1500:A:OP2    | 60:2a:3215:HOH:O   | 2.11                     | 0.66              |
| 40:2i:19:LEU:HD23   | 40:2i:61:ALA:HB2   | 1.77                     | 0.66              |
| 1:2A:785:G:OP2      | 60:2A:3852:HOH:O   | 2.12                     | 0.66              |
| 11:2P:54:GLY:O      | 60:2P:303:HOH:O    | 2.12                     | 0.66              |
| 32:1a:1003:G:H2'    | 32:1a:1004:A:H4'   | 1.76                     | 0.66              |
| 34:1c:78:GLY:HA3    | 34:1c:83:ARG:H     | 1.60                     | 0.66              |
| 1:2A:1026:U:OP1     | 60:2A:3826:HOH:O   | 2.14                     | 0.66              |
| 32:2a:811:C:N4      | 60:2a:3249:HOH:O   | 2.28                     | 0.66              |
| 1:1A:679:C:OP1      | 60:1A:4117:HOH:O   | 2.14                     | 0.66              |
| 1:2A:1840:G:OP2     | 60:2A:3857:HOH:O   | 2.13                     | 0.66              |
| 23:21:54:ALA:HB1    | 23:21:83:GLU:HG3   | 1.77                     | 0.66              |
| 30:28:33:ASN:HA     | 30:28:36:LYS:HD2   | 1.77                     | 0.66              |
| 32:2a:1402:4OC:HM22 | 32:2a:1403:C:H5'   | 1.76                     | 0.66              |
| 32:2a:1505:G:OP1    | 60:2a:3205:HOH:O   | 2.12                     | 0.66              |
| 42:2k:18:ARG:HA     | 42:2k:81:ASP:H     | 1.61                     | 0.66              |
| 51:2t:57:ARG:HH22   | 51:2t:100:ILE:HD12 | 1.60                     | 0.66              |
| 1:2A:1105:U:H2'     | 1:2A:1106:G:H8     | 1.61                     | 0.66              |
| 1:1A:2133:G:H3'     | 1:1A:2157:G:H21    | 1.58                     | 0.66              |
| 1:2A:321:G:OP1      | 5:2F:135:LYS:NZ    | 2.27                     | 0.66              |
| 1:2A:1199:U:O2'     | 60:2A:3860:HOH:O   | 2.13                     | 0.66              |
| 2:2B:66:A:H61       | 2:2B:109:C:H5'     | 1.59                     | 0.66              |
| 14:2S:27:SER:HA     | 14:2S:88:ASP:HB3   | 1.77                     | 0.66              |
| 1:1A:1173:G:OP2     | 60:1A:4141:HOH:O   | 2.13                     | 0.66              |
| 1:1A:1381:G:N7      | 60:1A:4286:HOH:O   | 2.27                     | 0.66              |
| 1:1A:2238:G:OP2     | 60:1A:4139:HOH:O   | 2.13                     | 0.66              |
| 32:1a:780:A:OP2     | 60:1a:1918:HOH:O   | 2.13                     | 0.66              |
| 32:1a:976:G:H5'     | 32:1a:1358:U:O2'   | 1.95                     | 0.66              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 47:1p:60:LEU:HD11  | 47:1p:66:PRO:HD3    | 1.78                     | 0.66              |
| 26:24:48:ARG:O     | 26:24:50:VAL:N      | 2.27                     | 0.66              |
| 32:2a:1518:MA6:H93 | 32:2a:1519:MA6:H102 | 1.76                     | 0.66              |
| 33:2b:78:GLN:O     | 33:2b:94:ASN:ND2    | 2.29                     | 0.66              |
| 33:2b:119:GLU:HG3  | 33:2b:153:ARG:HH22  | 1.59                     | 0.66              |
| 36:2e:102:ALA:HB1  | 36:2e:106:PRO:HG2   | 1.78                     | 0.66              |
| 8:1I:93:THR:HG22   | 8:1I:119:PRO:HB3    | 1.78                     | 0.66              |
| 32:1a:1373:G:H5'   | 38:1g:36:LYS:HE2    | 1.78                     | 0.66              |
| 2:2B:15:A:OP1      | 60:2B:304:HOH:O     | 2.14                     | 0.66              |
| 32:2a:536:C:OP2    | 60:2a:3217:HOH:O    | 2.14                     | 0.66              |
| 42:2k:21:ILE:HB    | 42:2k:84:VAL:HG22   | 1.78                     | 0.66              |
| 2:1B:8:U:O3'       | 14:1S:25:ARG:NH2    | 2.29                     | 0.65              |
| 38:1g:153:HIS:CE1  | 42:1k:58:PRO:HD2    | 2.31                     | 0.65              |
| 1:2A:2111:C:H42    | 1:2A:2147:G:H22     | 1.42                     | 0.65              |
| 1:2A:2579:C:OP1    | 60:2A:3866:HOH:O    | 2.14                     | 0.65              |
| 22:20:10:THR:HG22  | 22:20:12:ASN:H      | 1.62                     | 0.65              |
| 22:20:53:MET:HG3   | 22:20:59:LEU:HD23   | 1.78                     | 0.65              |
| 32:2a:999:C:H42    | 32:2a:1042:G:H1     | 1.42                     | 0.65              |
| 32:2a:1118:C:H1'   | 32:2a:1179:A:C4     | 2.31                     | 0.65              |
| 1:1A:1968:G:OP1    | 60:1A:4137:HOH:O    | 2.13                     | 0.65              |
| 34:1c:15:THR:HG21  | 34:1c:181:ASN:HA    | 1.78                     | 0.65              |
| 23:21:76:ARG:NH1   | 23:21:97:LEU:O      | 2.29                     | 0.65              |
| 1:1A:1271:G:OP2    | 60:1A:4111:HOH:O    | 2.13                     | 0.65              |
| 1:1A:1784:A:OP1    | 60:1A:4146:HOH:O    | 2.14                     | 0.65              |
| 1:1A:2375:G:N7     | 60:1A:4306:HOH:O    | 2.29                     | 0.65              |
| 18:2W:53:SER:OG    | 60:2W:301:HOH:O     | 2.13                     | 0.65              |
| 19:2X:5:TYR:HD1    | 24:22:33:MET:HE2    | 1.62                     | 0.65              |
| 1:1A:1267:U:OP1    | 60:1A:4144:HOH:O    | 2.14                     | 0.65              |
| 31:29:2:LYS:NZ     | 31:29:31:LYS:O      | 2.29                     | 0.65              |
| 44:2m:19:LEU:HD21  | 44:2m:56:LEU:HD21   | 1.79                     | 0.65              |
| 1:1A:639:U:H2'     | 1:1A:640:C:C6       | 2.32                     | 0.65              |
| 1:1A:2683:C:O2     | 10:1O:70:LYS:NZ     | 2.26                     | 0.65              |
| 32:1a:1103:C:OP1   | 33:1b:96:ARG:NH2    | 2.30                     | 0.65              |
| 39:1h:14:ARG:NH1   | 39:1h:83:ILE:O      | 2.30                     | 0.65              |
| 1:2A:198:C:OP2     | 60:2A:3806:HOH:O    | 2.12                     | 0.65              |
| 1:2A:1332:G:OP2    | 60:2A:3864:HOH:O    | 2.14                     | 0.65              |
| 1:2A:1798:U:H5'    | 3:2D:259:THR:HG22   | 1.79                     | 0.65              |
| 1:2A:2602:A:H4'    | 1:2A:2603:G:OP1     | 1.94                     | 0.65              |
| 32:2a:1187:G:H5'   | 40:2i:113:LYS:HE2   | 1.78                     | 0.65              |
| 51:2t:33:ILE:O     | 51:2t:37:SER:OG     | 2.14                     | 0.65              |
| 1:1A:217:G:OP2     | 60:1A:4142:HOH:O    | 2.14                     | 0.65              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 32:1a:473:G:H2'    | 32:1a:474:G:H8     | 1.62                     | 0.65              |
| 1:2A:740:U:OP2     | 60:2A:3869:HOH:O   | 2.15                     | 0.65              |
| 1:2A:2519:U:OP2    | 60:2A:3868:HOH:O   | 2.15                     | 0.65              |
| 1:2A:2722:G:O6     | 60:2A:3851:HOH:O   | 2.12                     | 0.65              |
| 2:2B:58:A:OP2      | 60:2B:306:HOH:O    | 2.15                     | 0.65              |
| 1:1A:321:G:OP2     | 60:1A:4148:HOH:O   | 2.15                     | 0.65              |
| 1:1A:1427:A:OP1    | 60:1A:4151:HOH:O   | 2.15                     | 0.65              |
| 4:1E:127:ASP:OD2   | 60:1E:402:HOH:O    | 2.15                     | 0.65              |
| 7:1H:173:PRO:O     | 60:1H:301:HOH:O    | 2.14                     | 0.65              |
| 32:1a:757:U:O2'    | 32:1a:879:C:O2     | 2.14                     | 0.65              |
| 33:1b:158:LEU:HG   | 33:1b:182:ILE:HD11 | 1.79                     | 0.65              |
| 1:2A:2074:U:OP2    | 60:2A:3870:HOH:O   | 2.15                     | 0.65              |
| 1:2A:2536:G:O6     | 60:2A:3858:HOH:O   | 2.13                     | 0.65              |
| 26:24:50:VAL:HG21  | 44:2m:65:LYS:HB3   | 1.77                     | 0.65              |
| 44:2m:22:ILE:HG21  | 44:2m:66:LEU:HD13  | 1.79                     | 0.65              |
| 1:1A:2079:U:OP1    | 23:11:21:ARG:NH2   | 2.29                     | 0.65              |
| 33:1b:87:ARG:NH2   | 33:1b:220:ASP:OD1  | 2.24                     | 0.65              |
| 1:2A:2719:G:OP2    | 60:2A:3862:HOH:O   | 2.14                     | 0.65              |
| 32:1a:1295:G:O2'   | 44:1m:14:ARG:NH1   | 2.30                     | 0.65              |
| 7:2H:20:ALA:HB3    | 7:2H:23:ARG:HB3    | 1.77                     | 0.65              |
| 32:2a:564:C:O2'    | 39:2h:91:ARG:NH2   | 2.28                     | 0.65              |
| 32:2a:582:U:OP1    | 46:2o:68:ARG:NH2   | 2.29                     | 0.65              |
| 44:2m:10:PRO:HG2   | 44:2m:13:LYS:HD2   | 1.76                     | 0.65              |
| 1:1A:379:G:N7      | 60:1A:4305:HOH:O   | 2.29                     | 0.65              |
| 21:1Z:128:VAL:HG23 | 21:1Z:161:VAL:HB   | 1.79                     | 0.65              |
| 33:1b:231:GLU:HB3  | 33:1b:232:PRO:HD3  | 1.79                     | 0.65              |
| 1:2A:670:A:O2'     | 60:2A:3865:HOH:O   | 2.14                     | 0.65              |
| 6:2G:170:ARG:NH2   | 6:2G:174:GLU:OE2   | 2.30                     | 0.65              |
| 14:2S:10:ARG:NE    | 14:2S:91:PRO:O     | 2.30                     | 0.65              |
| 32:2a:1028:C:C2    | 32:2a:1033:G:N2    | 2.65                     | 0.65              |
| 32:2a:1305:G:OP1   | 52:2u:2:GLY:N      | 2.30                     | 0.65              |
| 3:1D:148:GLU:HB2   | 3:1D:151:LYS:HD2   | 1.78                     | 0.64              |
| 1:2A:1001:A:OP2    | 60:2A:3867:HOH:O   | 2.14                     | 0.64              |
| 2:2B:102:A:OP2     | 60:2B:305:HOH:O    | 2.14                     | 0.64              |
| 1:1A:888:C:N3      | 44:1m:93:ARG:NH1   | 2.45                     | 0.64              |
| 1:1A:1622:G:OP2    | 60:1A:4155:HOH:O   | 2.15                     | 0.64              |
| 1:1A:1784:A:OP2    | 60:1A:4147:HOH:O   | 2.15                     | 0.64              |
| 1:1A:2499:C:OP1    | 60:1A:4149:HOH:O   | 2.15                     | 0.64              |
| 16:1U:33:ARG:NH2   | 60:1U:302:HOH:O    | 2.30                     | 0.64              |
| 35:2d:12:CYS:CB    | 59:2d:501:SF4:S2   | 2.85                     | 0.64              |
| 39:2h:17:THR:HG22  | 39:2h:63:LEU:HG    | 1.80                     | 0.64              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:1A:2009:G:N7     | 60:1A:4311:HOH:O   | 2.29                     | 0.64              |
| 1:1A:2056:G:OP1    | 60:1A:4154:HOH:O   | 2.15                     | 0.64              |
| 20:1Y:102:CYS:SG   | 20:1Y:103:GLY:N    | 2.70                     | 0.64              |
| 32:1a:102:G:O6     | 60:1a:1917:HOH:O   | 2.12                     | 0.64              |
| 32:1a:328:C:OP1    | 60:1a:1920:HOH:O   | 2.14                     | 0.64              |
| 32:1a:562:C:OP1    | 60:1a:1923:HOH:O   | 2.15                     | 0.64              |
| 32:1a:757:U:H2'    | 32:1a:758:G:O4'    | 1.98                     | 0.64              |
| 1:1A:330:A:H2      | 1:1A:1210:A:O2'    | 1.80                     | 0.64              |
| 1:1A:1021:A:OP1    | 60:1A:4145:HOH:O   | 2.14                     | 0.64              |
| 32:1a:1340:A:OP2   | 60:1a:1921:HOH:O   | 2.14                     | 0.64              |
| 1:2A:1057:A:H2'    | 1:2A:1058:G:H8     | 1.61                     | 0.64              |
| 6:2G:60:LEU:HA     | 6:2G:63:ILE:HD12   | 1.79                     | 0.64              |
| 34:2c:155:GLY:HA3  | 34:2c:196:LEU:HD22 | 1.80                     | 0.64              |
| 1:1A:1817:G:OP1    | 3:1D:88:ARG:NH2    | 2.29                     | 0.64              |
| 26:14:16:CYS:SG    | 26:14:17:GLY:N     | 2.71                     | 0.64              |
| 33:1b:9:GLU:OE2    | 33:1b:217:ARG:NH1  | 2.30                     | 0.64              |
| 1:2A:826:U:OP1     | 60:2A:3819:HOH:O   | 2.14                     | 0.64              |
| 1:2A:1316:U:H2'    | 1:2A:1317:A:H8     | 1.62                     | 0.64              |
| 12:2Q:60:ARG:NH2   | 21:2Z:181:GLU:OE2  | 2.29                     | 0.64              |
| 36:2e:88:LYS:HB3   | 36:2e:123:LEU:HB2  | 1.79                     | 0.64              |
| 38:2g:113:GLU:HG3  | 38:2g:119:ARG:HG2  | 1.80                     | 0.64              |
| 1:1A:668:G:H5'     | 1:1A:669:G:OP2     | 1.97                     | 0.64              |
| 1:1A:1779:U:OP2    | 60:1A:4156:HOH:O   | 2.15                     | 0.64              |
| 5:1F:93:LYS:O      | 60:1F:402:HOH:O    | 2.14                     | 0.64              |
| 32:1a:108:G:N1     | 51:1t:15:ARG:HG2   | 2.12                     | 0.64              |
| 1:2A:1090:U:H2'    | 1:2A:1091:G:H8     | 1.63                     | 0.64              |
| 32:2a:398:C:OP2    | 60:2a:3219:HOH:O   | 2.15                     | 0.64              |
| 32:2a:1411:C:H2'   | 32:2a:1412:C:H6    | 1.61                     | 0.64              |
| 33:2b:189:ASP:OD1  | 33:2b:189:ASP:N    | 2.29                     | 0.64              |
| 42:2k:98:LEU:O     | 42:2k:101:SER:OG   | 2.10                     | 0.64              |
| 1:1A:975:C:OP1     | 60:1A:4152:HOH:O   | 2.15                     | 0.64              |
| 32:1a:444:C:H2'    | 32:1a:445:G:C8     | 2.33                     | 0.64              |
| 48:1q:66:SER:O     | 48:1q:70:ARG:NH1   | 2.30                     | 0.64              |
| 1:2A:2313:C:H5''   | 6:2G:91:ARG:HD3    | 1.79                     | 0.64              |
| 21:2Z:144:LEU:HD21 | 21:2Z:150:LEU:HD13 | 1.80                     | 0.64              |
| 32:2a:43:C:OP2     | 60:2a:3218:HOH:O   | 2.15                     | 0.64              |
| 51:2t:57:ARG:NH1   | 51:2t:101:GLY:O    | 2.30                     | 0.64              |
| 1:1A:1243:G:O2'    | 11:1P:7:ARG:NH2    | 2.31                     | 0.64              |
| 1:2A:2206:G:H3'    | 1:2A:2207:G:C8     | 2.33                     | 0.64              |
| 49:2r:32:ARG:HA    | 49:2r:69:THR:HG21  | 1.79                     | 0.64              |
| 49:2r:54:ARG:HB2   | 49:2r:54:ARG:HH11  | 1.62                     | 0.64              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 11:1P:42:SER:O     | 60:1P:301:HOH:O   | 2.15                     | 0.64              |
| 32:1a:198:G:H2'    | 32:1a:199:G:H8    | 1.63                     | 0.64              |
| 32:1a:444:C:H2'    | 32:1a:445:G:H8    | 1.62                     | 0.64              |
| 40:1i:4:TYR:HB2    | 40:1i:19:LEU:HB2  | 1.79                     | 0.64              |
| 1:2A:1276:A:O5'    | 60:2A:3872:HOH:O  | 2.15                     | 0.64              |
| 35:2d:10:ARG:HB2   | 35:2d:40:PRO:HG3  | 1.80                     | 0.64              |
| 4:1E:105:THR:OG1   | 4:1E:199:ARG:NH2  | 2.31                     | 0.64              |
| 38:1g:152:ALA:O    | 38:1g:155:ARG:NH1 | 2.29                     | 0.64              |
| 1:2A:2805:G:H2'    | 1:2A:2807:G:C8    | 2.33                     | 0.64              |
| 21:2Z:157:LEU:HD11 | 21:2Z:163:LEU:HB2 | 1.79                     | 0.64              |
| 26:24:59:PHE:HA    | 26:24:60:GLN:C    | 2.23                     | 0.63              |
| 33:2b:98:LEU:HG    | 33:2b:101:MET:HE3 | 1.79                     | 0.63              |
| 26:14:61:ARG:HG3   | 26:14:62:ARG:H    | 1.62                     | 0.63              |
| 27:15:33:CYS:HB2   | 27:15:40:LYS:HD3  | 1.81                     | 0.63              |
| 32:1a:96:U:H2'     | 32:1a:97:G:H8     | 1.63                     | 0.63              |
| 15:1T:56:GLY:O     | 15:1T:59:THR:HG23 | 1.99                     | 0.63              |
| 1:2A:1090:U:H2'    | 1:2A:1091:G:C8    | 2.31                     | 0.63              |
| 1:2A:2206:G:H8     | 1:2A:2207:G:N7    | 1.97                     | 0.63              |
| 16:1U:33:ARG:NH1   | 60:1U:303:HOH:O   | 2.31                     | 0.63              |
| 32:1a:737:A:H2'    | 32:1a:738:C:C6    | 2.34                     | 0.63              |
| 34:1c:70:VAL:HG22  | 34:1c:72:LYS:H    | 1.63                     | 0.63              |
| 1:2A:143:G:H4'     | 19:2X:35:THR:HG21 | 1.78                     | 0.63              |
| 1:2A:1053:C:H2'    | 1:2A:1054:A:C8    | 2.33                     | 0.63              |
| 1:2A:1075:C:H2'    | 1:2A:1076:C:H5'   | 1.79                     | 0.63              |
| 1:2A:1241:A:OP2    | 60:2A:3874:HOH:O  | 2.15                     | 0.63              |
| 1:2A:1631(A):A:N6  | 60:2A:4037:HOH:O  | 2.31                     | 0.63              |
| 1:2A:2353:G:N7     | 60:2A:4029:HOH:O  | 2.30                     | 0.63              |
| 7:2H:24:VAL:HG13   | 7:2H:37:VAL:HG21  | 1.79                     | 0.63              |
| 32:2a:662:G:H2'    | 32:2a:663:A:C8    | 2.33                     | 0.63              |
| 32:2a:1226:C:OP2   | 44:2m:91:ARG:NH1  | 2.31                     | 0.63              |
| 35:2d:163:GLU:HA   | 35:2d:166:LYS:HD3 | 1.80                     | 0.63              |
| 32:1a:964:A:OP1    | 60:1a:1924:HOH:O  | 2.15                     | 0.63              |
| 32:1a:1442:G:H2'   | 32:1a:1442:G:N3   | 2.14                     | 0.63              |
| 44:1m:87:TYR:HA    | 44:1m:90:LEU:HD12 | 1.79                     | 0.63              |
| 32:2a:1004:A:H5''  | 32:2a:1025:U:C5   | 2.34                     | 0.63              |
| 1:1A:773:U:OP1     | 60:1A:4158:HOH:O  | 2.15                     | 0.63              |
| 1:1A:1047:G:H2'    | 1:1A:1110:G:H22   | 1.64                     | 0.63              |
| 1:1A:1456:G:OP2    | 60:1A:4162:HOH:O  | 2.16                     | 0.63              |
| 1:1A:1721:G:H8     | 1:1A:1741:A:H62   | 1.46                     | 0.63              |
| 17:1V:72:VAL:HG13  | 17:1V:85:LYS:HB3  | 1.80                     | 0.63              |
| 38:1g:59:LEU:HD11  | 38:1g:63:LYS:HE2  | 1.81                     | 0.63              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 44:1m:58:GLU:O     | 44:1m:62:ASN:ND2   | 2.31                     | 0.63              |
| 16:2U:49:HIS:HA    | 16:2U:52:ARG:HB3   | 1.80                     | 0.63              |
| 32:2a:1191:A:OP2   | 34:2c:3:ASN:ND2    | 2.31                     | 0.63              |
| 32:2a:1348:U:H4'   | 40:2i:120:ARG:HD2  | 1.79                     | 0.63              |
| 1:1A:1970:A:OP1    | 60:1A:4161:HOH:O   | 2.16                     | 0.63              |
| 19:1X:76:ARG:NH1   | 60:1X:202:HOH:O    | 2.31                     | 0.63              |
| 32:1a:472:A:H5''   | 47:1p:80:PHE:HB3   | 1.79                     | 0.63              |
| 1:2A:2327:A:H2'    | 1:2A:2328:A:C8     | 2.33                     | 0.63              |
| 17:2V:98:GLU:OE2   | 17:2V:100:ARG:NH1  | 2.32                     | 0.63              |
| 6:1G:43:LEU:HD11   | 6:1G:153:ARG:HD3   | 1.80                     | 0.63              |
| 1:2A:2439:A:OP1    | 60:2A:3875:HOH:O   | 2.16                     | 0.63              |
| 14:2S:43:GLU:OE2   | 22:20:49:LYS:NZ    | 2.31                     | 0.63              |
| 26:14:50:VAL:HG11  | 44:1m:65:LYS:HA    | 1.81                     | 0.63              |
| 41:1j:26:ALA:HB1   | 41:1j:84:GLN:HE22  | 1.64                     | 0.63              |
| 1:2A:2104:G:O6     | 1:2A:2185:C:N3     | 2.31                     | 0.63              |
| 17:2V:43:GLU:OE1   | 17:2V:43:GLU:N     | 2.32                     | 0.63              |
| 33:2b:77:ALA:HB2   | 33:2b:211:ILE:HD13 | 1.81                     | 0.63              |
| 1:1A:1174:A:H4'    | 1:1A:1175:U:OP1    | 1.99                     | 0.62              |
| 40:1i:27:THR:HG22  | 40:1i:62:TYR:HA    | 1.81                     | 0.62              |
| 1:2A:451:C:H5'     | 60:2A:3965:HOH:O   | 1.97                     | 0.62              |
| 1:2A:958:U:OP2     | 12:2Q:14:ARG:NH1   | 2.32                     | 0.62              |
| 21:2Z:129:SER:HB3  | 21:2Z:132:ASN:HD22 | 1.64                     | 0.62              |
| 1:1A:588:U:H2'     | 1:1A:589:C:C6      | 2.34                     | 0.62              |
| 11:1P:63:PRO:HG2   | 30:18:25:MET:HB2   | 1.81                     | 0.62              |
| 32:1a:911:U:OP2    | 43:1l:97:ARG:NH2   | 2.32                     | 0.62              |
| 32:1a:1077:G:N2    | 32:1a:1080:A:OP2   | 2.32                     | 0.62              |
| 21:2Z:152:ALA:HB1  | 21:2Z:163:LEU:HD21 | 1.81                     | 0.62              |
| 32:1a:1329:A:N7    | 52:1u:7:ARG:NH2    | 2.48                     | 0.62              |
| 1:2A:1057:A:H2'    | 1:2A:1058:G:C8     | 2.34                     | 0.62              |
| 1:2A:2105:C:N4     | 1:2A:2106:G:O6     | 2.33                     | 0.62              |
| 32:2a:189(K):U:H2' | 32:2a:189(L):G:C8  | 2.34                     | 0.62              |
| 34:2c:63:ASN:HB2   | 34:2c:98:ASN:HB2   | 1.81                     | 0.62              |
| 5:2F:185:ASP:HA    | 5:2F:188:ARG:HD3   | 1.81                     | 0.62              |
| 36:2e:77:PRO:HD2   | 36:2e:142:LEU:HD22 | 1.82                     | 0.62              |
| 1:1A:1665:A:N7     | 60:1A:4105:HOH:O   | 2.29                     | 0.62              |
| 7:1H:52:VAL:O      | 7:1H:65:HIS:NE2    | 2.26                     | 0.62              |
| 8:1I:104:GLN:HB2   | 8:1I:105:HIS:HD2   | 1.63                     | 0.62              |
| 32:1a:96:U:H2'     | 32:1a:97:G:C8      | 2.35                     | 0.62              |
| 40:1i:3:GLN:HE21   | 40:1i:20:ARG:HE    | 1.48                     | 0.62              |
| 1:2A:2206:G:H5''   | 1:2A:2207:G:C5     | 2.35                     | 0.62              |
| 32:2a:1103:C:OP1   | 33:2b:96:ARG:NH2   | 2.32                     | 0.62              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 41:2j:6:ILE:HB    | 41:2j:72:VAL:HG23  | 1.81                     | 0.62              |
| 42:2k:87:THR:HA   | 42:2k:91:ARG:HH11  | 1.65                     | 0.62              |
| 32:1a:269:C:H2'   | 32:1a:270:A:C8     | 2.35                     | 0.62              |
| 32:1a:1007:C:N3   | 32:1a:1022:G:O6    | 2.32                     | 0.62              |
| 35:1d:53:ASP:HB3  | 35:1d:57:ARG:HH12  | 1.64                     | 0.62              |
| 28:26:18:ARG:HH21 | 28:26:42:TRP:HB3   | 1.64                     | 0.62              |
| 33:1b:16:HIS:HB3  | 33:1b:210:SER:HB2  | 1.81                     | 0.62              |
| 41:1j:61:GLU:OE2  | 45:1n:58:LYS:NZ    | 2.25                     | 0.62              |
| 1:2A:1377:G:O6    | 60:2A:3843:HOH:O   | 2.11                     | 0.62              |
| 1:2A:2685:G:OP2   | 15:2T:51:ARG:NH2   | 2.32                     | 0.62              |
| 10:2O:24:VAL:HG13 | 10:2O:33:ALA:HB2   | 1.81                     | 0.62              |
| 32:2a:266:G:O2'   | 32:2a:267:C:OP2    | 2.10                     | 0.62              |
| 47:2p:53:VAL:HG13 | 47:2p:79:VAL:HG22  | 1.80                     | 0.62              |
| 40:1i:26:VAL:HG13 | 40:1i:61:ALA:HB3   | 1.82                     | 0.62              |
| 48:1q:22:LEU:HD11 | 48:1q:39:SER:HB2   | 1.81                     | 0.62              |
| 1:2A:97:C:OP1     | 24:22:2:LYS:NZ     | 2.30                     | 0.62              |
| 1:2A:1316:U:H2'   | 1:2A:1317:A:C8     | 2.34                     | 0.62              |
| 1:2A:2272:U:O4    | 60:2A:3850:HOH:O   | 2.12                     | 0.62              |
| 11:2P:50:ARG:HD3  | 30:28:7:HIS:CD2    | 2.35                     | 0.62              |
| 32:2a:1192:C:OP2  | 34:2c:4:LYS:NZ     | 2.32                     | 0.62              |
| 1:1A:1842:G:O2'   | 3:1D:253:GLN:NE2   | 2.32                     | 0.62              |
| 2:1B:58:A:OP2     | 60:1B:303:HOH:O    | 2.16                     | 0.62              |
| 13:1R:12:ARG:O    | 13:1R:17:ARG:NH1   | 2.32                     | 0.62              |
| 51:1t:57:ARG:HH22 | 51:1t:100:ILE:HD12 | 1.64                     | 0.62              |
| 6:2G:46:ALA:HB1   | 6:2G:51:ARG:HA     | 1.81                     | 0.62              |
| 3:1D:13:ARG:NH1   | 3:1D:16:MET:SD     | 2.73                     | 0.62              |
| 33:1b:187:LEU:HA  | 33:1b:201:ILE:HB   | 1.82                     | 0.62              |
| 32:1a:486:U:H2'   | 32:1a:487:A:H8     | 1.64                     | 0.61              |
| 1:2A:2115:G:N2    | 1:2A:2119:A:H5'    | 2.14                     | 0.61              |
| 1:2A:2141:G:H1    | 1:2A:2150:U:H3     | 1.48                     | 0.61              |
| 1:2A:2646:C:OP2   | 1:2A:2732:G:O2'    | 2.16                     | 0.61              |
| 32:2a:864:A:OP2   | 60:2a:3221:HOH:O   | 2.16                     | 0.61              |
| 1:1A:1013:C:OP2   | 60:1A:4159:HOH:O   | 2.15                     | 0.61              |
| 1:1A:1537:G:H2'   | 1:1A:1538:G:H8     | 1.65                     | 0.61              |
| 44:1m:17:VAL:O    | 44:1m:20:THR:OG1   | 2.15                     | 0.61              |
| 1:2A:1102:C:H2'   | 1:2A:1103:A:H8     | 1.63                     | 0.61              |
| 1:2A:2572:A:OP1   | 1:2A:2574:G:O2'    | 2.18                     | 0.61              |
| 33:1b:17:PHE:HA   | 33:1b:44:LEU:HD11  | 1.81                     | 0.61              |
| 51:1t:64:ASP:OD1  | 51:1t:64:ASP:N     | 2.31                     | 0.61              |
| 1:2A:2431:U:O4    | 60:2A:3848:HOH:O   | 2.12                     | 0.61              |
| 1:2A:2591:C:OP1   | 60:2A:3881:HOH:O   | 2.16                     | 0.61              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 3:2D:108:PRO:HD2  | 3:2D:111:LEU:HD12  | 1.82                     | 0.61              |
| 6:2G:98:ARG:CZ    | 26:24:1:MET:HE3    | 2.30                     | 0.61              |
| 15:2T:85:LYS:NZ   | 15:2T:87:ASP:OD2   | 2.33                     | 0.61              |
| 33:2b:8:LYS:HD2   | 33:2b:48:MET:HG2   | 1.82                     | 0.61              |
| 33:2b:15:VAL:O    | 33:2b:17:PHE:N     | 2.32                     | 0.61              |
| 33:2b:166:ASP:HB3 | 33:2b:169:LYS:HB3  | 1.82                     | 0.61              |
| 37:2f:35:ALA:HA   | 37:2f:67:MET:HB3   | 1.80                     | 0.61              |
| 1:1A:1300:U:H4'   | 1:1A:1301:A:H5''   | 1.81                     | 0.61              |
| 11:1P:87:ASP:O    | 11:1P:90:ARG:NH1   | 2.33                     | 0.61              |
| 23:11:80:LEU:HB3  | 23:11:82:LEU:HG    | 1.83                     | 0.61              |
| 1:2A:1890:A:OP2   | 60:2A:3877:HOH:O   | 2.16                     | 0.61              |
| 32:2a:1372:U:H5'' | 40:2i:71:SER:HB3   | 1.81                     | 0.61              |
| 44:2m:34:LEU:HD13 | 44:2m:41:PRO:HB3   | 1.81                     | 0.61              |
| 1:2A:1419:A:H5'   | 1:2A:1579:A:H61    | 1.65                     | 0.61              |
| 1:2A:2637:U:OP1   | 4:2E:82:ARG:NH1    | 2.34                     | 0.61              |
| 20:2Y:55:TYR:CZ   | 20:2Y:61:ILE:HG21  | 2.36                     | 0.61              |
| 32:2a:1000:U:H3   | 32:2a:1041:A:H61   | 1.47                     | 0.61              |
| 32:2a:1151:A:N3   | 41:2j:39:PRO:HG3   | 2.15                     | 0.61              |
| 1:1A:1048:A:OP2   | 1:1A:1109:C:N4     | 2.34                     | 0.61              |
| 18:1W:83:LYS:NZ   | 60:1W:305:HOH:O    | 2.33                     | 0.61              |
| 32:1a:180:U:O2    | 32:1a:196:A:N6     | 2.33                     | 0.61              |
| 40:1i:21:PRO:HA   | 40:1i:59:PHE:HA    | 1.82                     | 0.61              |
| 1:2A:2396:G:OP2   | 60:2A:3883:HOH:O   | 2.16                     | 0.61              |
| 1:1A:2126:A:H4'   | 1:1A:2127:G:O5'    | 1.99                     | 0.61              |
| 32:1a:1108:G:O6   | 60:1a:1925:HOH:O   | 2.15                     | 0.61              |
| 44:1m:3:ARG:HG2   | 44:1m:8:GLU:HG3    | 1.82                     | 0.61              |
| 1:2A:1420:U:O2'   | 1:2A:1421:G:OP1    | 2.18                     | 0.61              |
| 1:1A:2448:A:OP1   | 60:1A:4149:HOH:O   | 2.16                     | 0.61              |
| 40:1i:46:ALA:HB2  | 40:1i:74:ILE:HG23  | 1.81                     | 0.61              |
| 18:2W:97:LYS:O    | 60:2W:302:HOH:O    | 2.16                     | 0.61              |
| 32:2a:1256:A:H61  | 32:2a:1278:U:H1'   | 1.66                     | 0.61              |
| 39:2h:112:LEU:HA  | 39:2h:134:ILE:HG12 | 1.82                     | 0.61              |
| 48:2q:66:SER:O    | 48:2q:70:ARG:NH1   | 2.33                     | 0.61              |
| 53:2y:12:ILE:HD12 | 53:2y:16:ILE:HG12  | 1.82                     | 0.61              |
| 1:1A:1175:U:H3'   | 1:1A:1176:G:H4'    | 1.83                     | 0.61              |
| 1:1A:2319:G:H22   | 14:1S:3:ARG:HH11   | 1.47                     | 0.61              |
| 10:1O:64:ARG:HG2  | 10:1O:83:ALA:HB3   | 1.83                     | 0.61              |
| 30:18:33:ASN:HA   | 30:18:36:LYS:HD2   | 1.83                     | 0.61              |
| 1:2A:2126:A:H4'   | 1:2A:2127:G:O5'    | 2.01                     | 0.61              |
| 4:2E:144:ARG:NH2  | 60:2E:406:HOH:O    | 2.34                     | 0.61              |
| 26:24:59:PHE:HA   | 26:24:61:ARG:N     | 2.16                     | 0.61              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 32:2a:1005:A:H5''  | 32:2a:1006:C:C5    | 2.36                     | 0.61              |
| 20:1Y:28:LYS:HG3   | 20:1Y:40:GLU:HG2   | 1.83                     | 0.61              |
| 1:2A:2136:C:C2     | 1:2A:2155:G:N2     | 2.68                     | 0.61              |
| 32:2a:1274:G:N2    | 32:2a:1275:A:N7    | 2.48                     | 0.61              |
| 1:1A:1093:G:O2'    | 1:1A:1098:A:N6     | 2.34                     | 0.60              |
| 26:14:57:GLU:HB2   | 26:14:58:ARG:HA    | 1.83                     | 0.60              |
| 33:1b:67:THR:HA    | 33:1b:90:MET:HE2   | 1.83                     | 0.60              |
| 41:1j:11:PHE:HE1   | 41:1j:67:THR:HG22  | 1.65                     | 0.60              |
| 46:1o:39:LEU:HD13  | 46:1o:56:LEU:HB2   | 1.83                     | 0.60              |
| 1:2A:11:G:H2'      | 1:2A:12:U:H5'      | 1.83                     | 0.60              |
| 20:2Y:57:GLN:NE2   | 60:2Y:301:HOH:O    | 2.33                     | 0.60              |
| 1:1A:2314:C:H2'    | 1:1A:2315:G:H8     | 1.65                     | 0.60              |
| 1:1A:2763:G:OP2    | 60:1A:4157:HOH:O   | 2.15                     | 0.60              |
| 32:1a:67:C:H2'     | 32:1a:68:G:C8      | 2.35                     | 0.60              |
| 1:2A:886:C:O2'     | 1:2A:889:C:N4      | 2.34                     | 0.60              |
| 9:2N:12:ARG:NH1    | 9:2N:50:ASP:OD2    | 2.34                     | 0.60              |
| 32:2a:1002:G:C2    | 32:2a:1003:G:H8    | 2.20                     | 0.60              |
| 3:1D:236:GLY:O     | 60:1D:401:HOH:O    | 2.17                     | 0.60              |
| 21:1Z:144:LEU:HD11 | 21:1Z:150:LEU:HD22 | 1.83                     | 0.60              |
| 1:2A:1816:G:O6     | 3:2D:35:LYS:NZ     | 2.19                     | 0.60              |
| 1:2A:2741:A:H5''   | 31:29:22:ARG:HH12  | 1.66                     | 0.60              |
| 35:2d:153:ARG:NH1  | 35:2d:180:GLY:O    | 2.31                     | 0.60              |
| 1:1A:1105:U:H2'    | 1:1A:1106:G:H8     | 1.67                     | 0.60              |
| 1:1A:1173:G:O2'    | 1:1A:1174:A:O4'    | 2.19                     | 0.60              |
| 7:1H:164:TYR:HB2   | 7:1H:167:GLU:HB2   | 1.82                     | 0.60              |
| 10:1O:68:GLU:OE1   | 10:1O:78:ARG:NH1   | 2.34                     | 0.60              |
| 34:1c:56:ASP:HB2   | 34:1c:67:THR:HB    | 1.83                     | 0.60              |
| 39:2h:29:SER:HB3   | 39:2h:32:LYS:HE3   | 1.84                     | 0.60              |
| 32:1a:659:U:H2'    | 32:1a:660:G:C8     | 2.37                     | 0.60              |
| 1:2A:209:C:OP1     | 60:2A:3871:HOH:O   | 2.15                     | 0.60              |
| 1:2A:2382:G:N7     | 60:2A:4042:HOH:O   | 2.31                     | 0.60              |
| 8:2I:26:ALA:HA     | 8:2I:30:LEU:HB2    | 1.82                     | 0.60              |
| 1:1A:2025:C:N4     | 60:1A:4360:HOH:O   | 2.35                     | 0.60              |
| 1:2A:981:A:OP1     | 60:2A:3880:HOH:O   | 2.16                     | 0.60              |
| 1:2A:1062:G:H2'    | 1:2A:1063:G:H8     | 1.65                     | 0.60              |
| 1:2A:2242:G:OP2    | 60:2A:3887:HOH:O   | 2.17                     | 0.60              |
| 31:29:25:VAL:HB    | 31:29:34:GLN:HB2   | 1.83                     | 0.60              |
| 2:1B:79:C:OP2      | 60:1B:304:HOH:O    | 2.16                     | 0.60              |
| 32:1a:142:G:H2'    | 32:1a:143:A:C8     | 2.37                     | 0.60              |
| 32:1a:393:A:OP1    | 60:1a:1926:HOH:O   | 2.17                     | 0.60              |
| 37:1f:4:TYR:HD2    | 37:1f:67:MET:HE3   | 1.65                     | 0.60              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 47:1p:74:LEU:HD23  | 47:1p:79:VAL:HG11  | 1.83                     | 0.60              |
| 1:2A:2023:G:OP2    | 60:2A:3873:HOH:O   | 2.15                     | 0.60              |
| 32:2a:1279:A:H2'   | 32:2a:1279:A:N3    | 2.16                     | 0.60              |
| 1:1A:793:A:OP1     | 60:1A:4163:HOH:O   | 2.16                     | 0.60              |
| 6:1G:64:THR:HB     | 6:1G:94:LEU:HD21   | 1.82                     | 0.60              |
| 1:2A:84:A:H5''     | 20:2Y:8:LYS:HD2    | 1.84                     | 0.60              |
| 8:2I:4:ILE:HG12    | 8:2I:18:VAL:HG22   | 1.84                     | 0.60              |
| 32:2a:560:U:H5'    | 32:2a:566:G:N2     | 2.17                     | 0.60              |
| 41:2j:8:LEU:HB2    | 41:2j:70:ARG:HB2   | 1.84                     | 0.60              |
| 47:2p:75:ARG:HG3   | 47:2p:80:PHE:HD2   | 1.67                     | 0.60              |
| 1:1A:1027:A:N3     | 60:1A:4341:HOH:O   | 2.32                     | 0.60              |
| 1:1A:1173:G:O2'    | 1:1A:1174:A:O5'    | 2.20                     | 0.60              |
| 11:1P:126:VAL:HG12 | 11:1P:148:LEU:HG   | 1.84                     | 0.60              |
| 32:1a:560:U:O2'    | 32:1a:561:U:OP2    | 2.19                     | 0.60              |
| 1:2A:2144:U:O2'    | 1:2A:2147:G:N1     | 2.34                     | 0.60              |
| 6:2G:29:TRP:O      | 6:2G:33:ARG:NH1    | 2.33                     | 0.60              |
| 9:2N:30:ILE:HG23   | 9:2N:52:VAL:HG11   | 1.82                     | 0.60              |
| 18:2W:65:LEU:HD12  | 18:2W:68:ARG:HE    | 1.67                     | 0.60              |
| 25:23:6:VAL:HG13   | 25:23:56:VAL:HG13  | 1.82                     | 0.60              |
| 34:2c:6:HIS:HB3    | 45:2n:49:HIS:ND1   | 2.17                     | 0.60              |
| 1:1A:251:A:OP2     | 60:1A:4160:HOH:O   | 2.16                     | 0.60              |
| 1:1A:748:G:O6      | 18:1W:90:ARG:NH1   | 2.35                     | 0.60              |
| 1:1A:1359:A:N6     | 1:1A:1372:U:H3     | 2.00                     | 0.60              |
| 14:1S:27:SER:HA    | 14:1S:88:ASP:HB3   | 1.84                     | 0.60              |
| 29:17:35:ARG:NH1   | 60:17:201:HOH:O    | 2.35                     | 0.60              |
| 37:1f:37:VAL:HA    | 37:1f:65:VAL:HG12  | 1.82                     | 0.60              |
| 41:1j:64:GLU:HB3   | 45:1n:59:ALA:HB2   | 1.84                     | 0.60              |
| 43:1l:70:ILE:HG12  | 43:1l:100:ILE:HD12 | 1.84                     | 0.60              |
| 1:2A:2112:G:H2'    | 1:2A:2113:U:C6     | 2.37                     | 0.60              |
| 40:2i:4:TYR:O      | 40:2i:19:LEU:N     | 2.33                     | 0.60              |
| 1:1A:1188:U:H4'    | 17:1V:79:VAL:HG22  | 1.83                     | 0.59              |
| 28:16:13:CYS:SG    | 28:16:47:THR:HG21  | 2.42                     | 0.59              |
| 32:1a:1412:C:H2'   | 32:1a:1413:A:C8    | 2.37                     | 0.59              |
| 37:1f:1:MET:HE3    | 37:1f:66:GLU:HG2   | 1.83                     | 0.59              |
| 1:1A:1756:G:OP2    | 60:1A:4165:HOH:O   | 2.17                     | 0.59              |
| 1:1A:1816:G:O6     | 3:1D:35:LYS:NZ     | 2.28                     | 0.59              |
| 1:1A:2623:G:OP1    | 60:1A:4164:HOH:O   | 2.16                     | 0.59              |
| 32:1a:811:C:O2'    | 32:1a:901:A:N1     | 2.35                     | 0.59              |
| 33:1b:21:ARG:HB3   | 33:1b:39:ILE:HD13  | 1.82                     | 0.59              |
| 34:1c:182:ILE:HG12 | 34:1c:203:PHE:HD1  | 1.67                     | 0.59              |
| 42:1k:33:THR:HA    | 42:1k:39:PRO:HA    | 1.84                     | 0.59              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:2A:855:G:O2'    | 22:20:27:GLU:OE2   | 2.16                     | 0.59              |
| 1:2A:2010:G:H5''  | 18:2W:42:ARG:HB2   | 1.83                     | 0.59              |
| 7:2H:150:ALA:HA   | 7:2H:153:LYS:HG3   | 1.84                     | 0.59              |
| 30:28:49:VAL:O    | 60:28:201:HOH:O    | 2.17                     | 0.59              |
| 1:1A:2483:C:N3    | 12:1Q:124:LYS:NZ   | 2.50                     | 0.59              |
| 8:1I:75:LEU:HD22  | 8:1I:105:HIS:ND1   | 2.17                     | 0.59              |
| 19:1X:80:ILE:O    | 60:1X:201:HOH:O    | 2.16                     | 0.59              |
| 22:10:24:LYS:O    | 22:10:25:ARG:NH1   | 2.32                     | 0.59              |
| 32:1a:1158:C:H5   | 32:1a:1181:G:N1    | 1.98                     | 0.59              |
| 39:1h:91:ARG:HE   | 48:1q:33:GLY:HA3   | 1.68                     | 0.59              |
| 1:2A:652(T):C:H2' | 1:2A:652(U):G:C8   | 2.35                     | 0.59              |
| 1:2A:2103:C:H42   | 1:2A:2185:C:H42    | 1.49                     | 0.59              |
| 1:2A:2104:G:O6    | 1:2A:2185:C:C4     | 2.55                     | 0.59              |
| 56:2A:3758:MPD:O2 | 60:2A:3878:HOH:O   | 2.16                     | 0.59              |
| 8:2I:91:SER:OG    | 8:2I:92:VAL:N      | 2.27                     | 0.59              |
| 36:2e:74:GLY:HA3  | 36:2e:116:THR:HG22 | 1.82                     | 0.59              |
| 15:1T:91:ARG:NE   | 15:1T:124:ASP:OD2  | 2.35                     | 0.59              |
| 40:1i:127:LYS:HB3 | 40:1i:127:LYS:HZ3  | 1.68                     | 0.59              |
| 33:2b:88:ALA:HB2  | 33:2b:219:VAL:HG13 | 1.84                     | 0.59              |
| 1:1A:1264:G:OP1   | 27:15:19:ARG:NH2   | 2.22                     | 0.59              |
| 14:1S:14:VAL:O    | 14:1S:18:ILE:HG12  | 2.02                     | 0.59              |
| 1:2A:531:C:OP2    | 60:2A:3888:HOH:O   | 2.17                     | 0.59              |
| 1:2A:1064:C:N4    | 1:2A:1074:G:O6     | 2.34                     | 0.59              |
| 1:2A:1069:A:H5'   | 1:2A:1096:A:H5'    | 1.84                     | 0.59              |
| 3:2D:221:VAL:HG22 | 3:2D:226:MET:HE3   | 1.84                     | 0.59              |
| 12:2Q:63:LYS:HD2  | 21:2Z:175:VAL:HG21 | 1.85                     | 0.59              |
| 1:1A:123:G:OP2    | 60:1A:4167:HOH:O   | 2.17                     | 0.59              |
| 1:1A:307:G:H21    | 1:1A:330:A:H62     | 1.49                     | 0.59              |
| 1:1A:2327:A:H2'   | 1:1A:2328:A:C8     | 2.37                     | 0.59              |
| 8:1I:72:LEU:C     | 8:1I:74:ASN:H      | 2.11                     | 0.59              |
| 42:1k:84:VAL:HG21 | 42:1k:95:ILE:HD11  | 1.84                     | 0.59              |
| 44:1m:60:VAL:HG12 | 44:1m:66:LEU:HD11  | 1.84                     | 0.59              |
| 32:2a:737:A:H2'   | 32:2a:738:C:C6     | 2.37                     | 0.59              |
| 32:2a:1505:G:OP2  | 60:2a:3220:HOH:O   | 2.15                     | 0.59              |
| 38:2g:42:ILE:HD13 | 38:2g:116:ALA:HB3  | 1.85                     | 0.59              |
| 1:1A:2584:U:H2'   | 1:1A:2585:U:H2'    | 1.83                     | 0.59              |
| 18:1W:71:VAL:HA   | 18:1W:107:LEU:HD12 | 1.85                     | 0.59              |
| 32:1a:258:G:H2'   | 32:1a:259:G:C8     | 2.38                     | 0.59              |
| 32:1a:659:U:H2'   | 32:1a:660:G:H8     | 1.66                     | 0.59              |
| 53:1y:39:ILE:HD13 | 53:1y:52:ALA:HB2   | 1.85                     | 0.59              |
| 32:2a:501:C:H2'   | 32:2a:502:G:C8     | 2.37                     | 0.59              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 32:2a:1003:G:H3'  | 32:2a:1003:G:N3    | 2.17                     | 0.59              |
| 32:2a:1289:A:OP1  | 52:2u:10:ARG:NH2   | 2.35                     | 0.59              |
| 32:2a:1376:U:H2'  | 32:2a:1377:A:C8    | 2.38                     | 0.59              |
| 34:2c:180:ALA:HB1 | 34:2c:203:PHE:HE1  | 1.67                     | 0.59              |
| 47:2p:5:ARG:HH21  | 47:2p:28:ARG:HA    | 1.68                     | 0.59              |
| 48:2q:62:SER:OG   | 48:2q:72:ARG:NH1   | 2.34                     | 0.59              |
| 51:2t:50:GLU:HB2  | 51:2t:99:LEU:HD22  | 1.84                     | 0.59              |
| 11:1P:50:ARG:HD3  | 30:18:7:HIS:CD2    | 2.37                     | 0.59              |
| 34:1c:69:HIS:HA   | 34:1c:104:GLN:HB3  | 1.84                     | 0.59              |
| 35:1d:173:TRP:HE1 | 35:1d:193:ASP:HB3  | 1.68                     | 0.59              |
| 36:1e:33:VAL:HG21 | 36:1e:109:ILE:HA   | 1.85                     | 0.59              |
| 8:2I:63:ALA:HA    | 8:2I:66:GLU:HB3    | 1.83                     | 0.59              |
| 19:2X:35:THR:HG22 | 19:2X:37:THR:H     | 1.67                     | 0.59              |
| 32:2a:438:G:H4'   | 35:2d:123:HIS:HD2  | 1.68                     | 0.59              |
| 32:2a:624:C:H2'   | 32:2a:625:G:H8     | 1.66                     | 0.59              |
| 34:2c:36:ASP:O    | 34:2c:40:ARG:HG2   | 2.03                     | 0.59              |
| 1:1A:576:U:H2'    | 1:1A:577:G:C8      | 2.38                     | 0.59              |
| 1:1A:2328:A:H2'   | 1:1A:2329:G:C8     | 2.38                     | 0.59              |
| 1:1A:2751:G:C2    | 7:1H:2:SER:HB3     | 2.38                     | 0.59              |
| 1:1A:2788:C:OP1   | 4:1E:61:ARG:NH2    | 2.36                     | 0.59              |
| 32:1a:373:A:H2'   | 32:1a:374:A:H8     | 1.68                     | 0.59              |
| 38:1g:23:VAL:O    | 38:1g:27:ILE:HG12  | 2.03                     | 0.59              |
| 1:2A:688:U:O4     | 60:2A:3879:HOH:O   | 2.16                     | 0.59              |
| 2:2B:114:C:H4'    | 14:2S:46:VAL:HG13  | 1.85                     | 0.59              |
| 4:2E:192:ASN:ND2  | 60:2E:405:HOH:O    | 2.30                     | 0.59              |
| 8:2I:81:VAL:HG23  | 8:2I:145:VAL:O     | 2.03                     | 0.59              |
| 9:2N:14:VAL:HG11  | 9:2N:138:LEU:HD12  | 1.85                     | 0.59              |
| 32:2a:64:G:H4'    | 32:2a:65:U:H3'     | 1.83                     | 0.59              |
| 40:2i:89:ASN:O    | 40:2i:92:TYR:HB2   | 2.03                     | 0.59              |
| 32:1a:316:G:OP2   | 32:1a:351:G:O2'    | 2.20                     | 0.58              |
| 32:1a:411:A:OP2   | 35:1d:25:ARG:NH2   | 2.35                     | 0.58              |
| 32:1a:1031:G:H2'  | 32:1a:1032:G:H8    | 1.67                     | 0.58              |
| 47:1p:43:LYS:HG2  | 47:1p:48:TRP:CE2   | 2.38                     | 0.58              |
| 1:2A:956:G:OP1    | 60:2A:3890:HOH:O   | 2.17                     | 0.58              |
| 1:2A:1338:G:O2'   | 1:2A:1393:A:N1     | 2.35                     | 0.58              |
| 9:2N:4:TYR:CD2    | 16:2U:100:VAL:HG11 | 2.38                     | 0.58              |
| 16:2U:88:ILE:HG22 | 16:2U:90:VAL:HG23  | 1.85                     | 0.58              |
| 32:2a:79:G:H1     | 32:2a:90:U:H3      | 1.51                     | 0.58              |
| 42:2k:62:GLN:HG3  | 42:2k:97:ALA:HB2   | 1.84                     | 0.58              |
| 42:2k:81:ASP:OD1  | 42:2k:107:SER:OG   | 2.20                     | 0.58              |
| 9:1N:58:ASP:OD1   | 9:1N:58:ASP:N      | 2.29                     | 0.58              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:1P:63:PRO:HD3   | 30:18:27:THR:HG22  | 1.85                     | 0.58              |
| 32:1a:410:G:OP1    | 35:1d:30:LYS:NZ    | 2.36                     | 0.58              |
| 36:1e:100:VAL:O    | 36:1e:107:ARG:NH2  | 2.36                     | 0.58              |
| 47:1p:22:THR:HA    | 47:1p:33:ILE:HG13  | 1.85                     | 0.58              |
| 49:1r:32:ARG:HA    | 49:1r:69:THR:HG21  | 1.85                     | 0.58              |
| 1:2A:800:A:H8      | 1:2A:800:A:OP1     | 1.86                     | 0.58              |
| 1:2A:2029:G:OP2    | 60:2A:3882:HOH:O   | 2.16                     | 0.58              |
| 41:2j:30:SER:OG    | 41:2j:84:GLN:OE1   | 2.14                     | 0.58              |
| 32:1a:21:G:H2'     | 32:1a:22:G:C8      | 2.37                     | 0.58              |
| 1:2A:1184:G:OP1    | 25:23:30:ARG:NH1   | 2.36                     | 0.58              |
| 15:2T:27:THR:HB    | 15:2T:89:VAL:HG22  | 1.84                     | 0.58              |
| 21:2Z:144:LEU:HD11 | 21:2Z:150:LEU:HD22 | 1.84                     | 0.58              |
| 32:2a:976:G:H5'    | 32:2a:1358:U:O2'   | 2.03                     | 0.58              |
| 33:2b:124:SER:HB2  | 33:2b:125:PRO:HD3  | 1.85                     | 0.58              |
| 38:2g:37:ASN:HD21  | 40:2i:40:LEU:HA    | 1.68                     | 0.58              |
| 40:2i:7:THR:OG1    | 40:2i:83:ARG:NH1   | 2.37                     | 0.58              |
| 1:1A:1331:A:OP2    | 60:1A:4171:HOH:O   | 2.17                     | 0.58              |
| 3:1D:71:ASP:CB     | 3:1D:103:ARG:HH22  | 2.16                     | 0.58              |
| 32:1a:142:G:H2'    | 32:1a:143:A:H8     | 1.67                     | 0.58              |
| 32:1a:1183:A:O2'   | 32:1a:1184:G:OP1   | 2.18                     | 0.58              |
| 40:1i:10:ARG:HG3   | 40:1i:11:LYS:HG3   | 1.85                     | 0.58              |
| 1:2A:597:U:H2'     | 1:2A:598:G:C8      | 2.38                     | 0.58              |
| 1:2A:2159:G:H2'    | 1:2A:2160:G:H8     | 1.68                     | 0.58              |
| 8:2I:55:ALA:HA     | 8:2I:58:LEU:HD23   | 1.85                     | 0.58              |
| 23:21:23:LYS:HB3   | 23:21:29:GLY:HA3   | 1.85                     | 0.58              |
| 34:2c:131:ARG:HD3  | 34:2c:166:GLU:HG2  | 1.85                     | 0.58              |
| 1:1A:2114:A:H1'    | 1:1A:2168:G:H5'    | 1.86                     | 0.58              |
| 3:1D:119:ALA:N     | 60:1D:411:HOH:O    | 2.35                     | 0.58              |
| 32:1a:198:G:H2'    | 32:1a:199:G:C8     | 2.38                     | 0.58              |
| 35:1d:89:THR:OG1   | 60:1d:402:HOH:O    | 2.17                     | 0.58              |
| 1:2A:686:G:H1      | 29:27:16:HIS:CD2   | 2.22                     | 0.58              |
| 32:2a:407:G:H5''   | 35:2d:115:ARG:HG2  | 1.84                     | 0.58              |
| 32:2a:1286:A:H2'   | 32:2a:1287:A:H4'   | 1.84                     | 0.58              |
| 41:1j:6:ILE:HA     | 41:1j:98:ILE:HG12  | 1.85                     | 0.58              |
| 1:2A:468:G:N7      | 29:27:39:ARG:NH2   | 2.48                     | 0.58              |
| 1:2A:1105:U:H2'    | 1:2A:1106:G:C8     | 2.39                     | 0.58              |
| 4:2E:36:ARG:HG2    | 4:2E:47:VAL:HG12   | 1.86                     | 0.58              |
| 4:2E:54:GLN:HB2    | 4:2E:76:ARG:HG2    | 1.83                     | 0.58              |
| 32:2a:1126:U:O4'   | 32:2a:1281:U:H1'   | 2.03                     | 0.58              |
| 15:1T:91:ARG:HD2   | 15:1T:120:ARG:HB3  | 1.86                     | 0.58              |
| 21:1Z:128:VAL:HG22 | 21:1Z:132:ASN:HB3  | 1.86                     | 0.58              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:29:29:ASN:HD22  | 31:29:32:HIS:CE1   | 2.22                     | 0.58              |
| 32:2a:662:G:O2'    | 32:2a:836:G:OP1    | 2.21                     | 0.58              |
| 32:2a:1411:C:H2'   | 32:2a:1412:C:C6    | 2.39                     | 0.58              |
| 32:1a:473:G:H2'    | 32:1a:474:G:C8     | 2.39                     | 0.58              |
| 39:1h:6:ILE:HB     | 39:1h:85:ARG:NH1   | 2.18                     | 0.58              |
| 1:2A:2285:C:OP2    | 28:26:6:ARG:NH1    | 2.37                     | 0.58              |
| 1:2A:2659:G:P      | 7:2H:158:HIS:HE2   | 2.27                     | 0.58              |
| 9:2N:96:GLU:HB2    | 9:2N:122:VAL:HG12  | 1.86                     | 0.58              |
| 1:1A:1815:A:OP2    | 3:1D:54:ARG:NH2    | 2.37                     | 0.58              |
| 1:1A:2079:U:O3'    | 23:11:35:THR:OG1   | 2.22                     | 0.58              |
| 32:1a:946:A:H2'    | 32:1a:947:G:C8     | 2.39                     | 0.58              |
| 32:1a:1067:A:O3'   | 60:1a:1927:HOH:O   | 2.17                     | 0.58              |
| 23:21:2:SER:HB3    | 23:21:46:LEU:HD12  | 1.85                     | 0.58              |
| 33:2b:102:LEU:HD23 | 33:2b:182:ILE:HD12 | 1.86                     | 0.58              |
| 60:1A:7439:HOH:O   | 18:1W:92:ARG:HD2   | 2.04                     | 0.58              |
| 32:1a:1391:U:H2'   | 32:1a:1392:G:C8    | 2.39                     | 0.58              |
| 7:2H:95:ARG:HB2    | 7:2H:128:PRO:HB3   | 1.84                     | 0.58              |
| 15:2T:29:ARG:HB3   | 15:2T:87:ASP:HB2   | 1.86                     | 0.58              |
| 28:26:35:GLU:HG2   | 28:26:50:ARG:HG3   | 1.86                     | 0.58              |
| 32:2a:448:A:OP2    | 32:2a:485:G:N2     | 2.26                     | 0.58              |
| 32:2a:624:C:H2'    | 32:2a:625:G:C8     | 2.39                     | 0.58              |
| 32:2a:1147:C:O2    | 40:2i:16:ARG:NH2   | 2.36                     | 0.58              |
| 1:1A:447:A:OP2     | 60:1A:4168:HOH:O   | 2.17                     | 0.57              |
| 1:1A:1919:A:N1     | 32:1a:1495:U:O2'   | 2.36                     | 0.57              |
| 32:1a:903:G:OP1    | 60:1a:1928:HOH:O   | 2.17                     | 0.57              |
| 40:1i:9:ARG:HB2    | 40:1i:104:ARG:HE   | 1.68                     | 0.57              |
| 1:2A:2641:G:P      | 9:2N:74:ARG:HH22   | 2.27                     | 0.57              |
| 2:2B:75:G:O3'      | 21:2Z:10:ARG:NH2   | 2.35                     | 0.57              |
| 6:2G:145:THR:HG22  | 6:2G:148:MET:H     | 1.69                     | 0.57              |
| 32:2a:501:C:OP1    | 43:2l:117:ARG:NH2  | 2.37                     | 0.57              |
| 32:2a:646:U:H2'    | 32:2a:647:C:C6     | 2.39                     | 0.57              |
| 32:2a:960:U:H5     | 50:2s:78:ARG:HD3   | 1.68                     | 0.57              |
| 51:2t:89:ARG:O     | 51:2t:93:GLU:HG2   | 2.04                     | 0.57              |
| 1:1A:826:U:OP1     | 60:1A:4132:HOH:O   | 2.17                     | 0.57              |
| 10:1O:2:ILE:HD12   | 10:1O:6:THR:HG21   | 1.85                     | 0.57              |
| 32:1a:419:C:OP1    | 32:1a:513:C:O2'    | 2.19                     | 0.57              |
| 44:1m:23:TYR:HB3   | 44:1m:67:GLU:HA    | 1.85                     | 0.57              |
| 46:1o:55:GLY:HA2   | 46:1o:58:MET:HE2   | 1.87                     | 0.57              |
| 1:2A:1639:U:H2'    | 1:2A:1640:C:H5''   | 1.86                     | 0.57              |
| 32:2a:134:A:N6     | 47:2p:25:ARG:HH22  | 1.97                     | 0.57              |
| 50:2s:41:VAL:HG13  | 50:2s:43:GLU:H     | 1.68                     | 0.57              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 2:1B:81:G:N7        | 57:1B:231:ARG:NH2  | 2.48                     | 0.57              |
| 35:1d:60:GLU:HG3    | 35:1d:202:LEU:HD12 | 1.86                     | 0.57              |
| 1:2A:271(H):G:H2'   | 1:2A:271(I):G:H8   | 1.68                     | 0.57              |
| 32:2a:890:G:O2'     | 32:2a:906:G:O6     | 2.22                     | 0.57              |
| 32:2a:1149:C:O2'    | 32:2a:1280:A:N1    | 2.32                     | 0.57              |
| 44:2m:39:ILE:HD12   | 44:2m:56:LEU:HD13  | 1.85                     | 0.57              |
| 1:1A:920:G:OP1      | 60:1A:4169:HOH:O   | 2.17                     | 0.57              |
| 2:1B:66:A:H61       | 2:1B:108:U:H2'     | 1.69                     | 0.57              |
| 11:1P:82:GLY:HA2    | 11:1P:113:LYS:O    | 2.04                     | 0.57              |
| 12:1Q:55:VAL:HG12   | 12:1Q:64:ILE:HD12  | 1.86                     | 0.57              |
| 32:1a:186:C:H2'     | 32:1a:187:C:C6     | 2.40                     | 0.57              |
| 32:1a:1505:G:O6     | 60:1a:1922:HOH:O   | 2.14                     | 0.57              |
| 40:1i:69:GLY:O      | 40:1i:73:GLN:HG3   | 2.04                     | 0.57              |
| 1:2A:775:G:OP1      | 60:2A:3893:HOH:O   | 2.17                     | 0.57              |
| 1:2A:2317:C:H2'     | 1:2A:2318:G:H5'    | 1.86                     | 0.57              |
| 15:2T:60:THR:HG22   | 15:2T:77:PRO:HA    | 1.85                     | 0.57              |
| 32:2a:1030(A):G:H1' | 32:2a:1030(C):G:C5 | 2.39                     | 0.57              |
| 32:2a:1151:A:O2'    | 32:2a:1152:A:H8    | 1.87                     | 0.57              |
| 21:1Z:158:PRO:HG2   | 21:1Z:161:VAL:HG11 | 1.86                     | 0.57              |
| 32:1a:1009:G:O6     | 32:1a:1020:U:O2    | 2.22                     | 0.57              |
| 32:1a:1212:U:H4'    | 32:1a:1213:A:C8    | 2.39                     | 0.57              |
| 32:1a:1499:A:OP2    | 60:1a:1906:HOH:O   | 2.17                     | 0.57              |
| 1:2A:995:C:O2       | 9:2N:3:THR:OG1     | 2.23                     | 0.57              |
| 1:2A:2134:A:N6      | 1:2A:2156:G:O2'    | 2.35                     | 0.57              |
| 8:2I:126:TYR:HE2    | 8:2I:144:VAL:HG21  | 1.69                     | 0.57              |
| 23:11:4:VAL:HG22    | 23:11:11:ARG:HG3   | 1.87                     | 0.57              |
| 32:1a:539:A:H2'     | 32:1a:540:G:C8     | 2.39                     | 0.57              |
| 32:1a:598:U:O4      | 60:1a:1919:HOH:O   | 2.14                     | 0.57              |
| 40:2i:85:LEU:HB3    | 40:2i:92:TYR:HD2   | 1.68                     | 0.57              |
| 2:1B:13:A:N1        | 2:1B:69:G:O2'      | 2.35                     | 0.57              |
| 32:1a:1003:G:C2'    | 32:1a:1004:A:H4'   | 2.34                     | 0.57              |
| 1:2A:517:C:OP1      | 27:25:16:ARG:NH2   | 2.37                     | 0.57              |
| 3:2D:101:GLU:OE2    | 3:2D:103:ARG:NH1   | 2.37                     | 0.57              |
| 15:2T:64:ARG:HB2    | 15:2T:73:GLU:HG2   | 1.87                     | 0.57              |
| 32:2a:558:G:OP1     | 60:2a:3223:HOH:O   | 2.17                     | 0.57              |
| 35:2d:119:GLN:O     | 35:2d:123:HIS:ND1  | 2.32                     | 0.57              |
| 1:1A:217:G:OP2      | 60:1A:4173:HOH:O   | 2.17                     | 0.57              |
| 1:1A:2336:A:H61     | 22:10:43:THR:HG22  | 1.70                     | 0.57              |
| 1:1A:2753:A:O2'     | 31:19:15:LYS:NZ    | 2.37                     | 0.57              |
| 33:1b:78:GLN:NE2    | 33:1b:94:ASN:O     | 2.38                     | 0.57              |
| 1:2A:9:U:H3         | 1:2A:2629:A:H2     | 1.52                     | 0.57              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:2A:2244:U:O2'    | 60:2A:3847:HOH:O  | 2.12                     | 0.57              |
| 23:21:21:ARG:HD3   | 23:21:35:THR:HG21 | 1.87                     | 0.57              |
| 36:2e:12:LEU:HB3   | 36:2e:31:LEU:HB2  | 1.87                     | 0.57              |
| 1:1A:994:C:OP1     | 16:1U:53:ARG:NH2  | 2.38                     | 0.57              |
| 2:1B:23:G:O6       | 60:1B:302:HOH:O   | 2.16                     | 0.57              |
| 3:1D:85:ASP:OD2    | 3:1D:88:ARG:NH1   | 2.35                     | 0.57              |
| 32:1a:1280:A:H5'   | 41:1j:40:LEU:HD22 | 1.86                     | 0.57              |
| 32:1a:1320:C:H2'   | 32:1a:1321:C:O4'  | 2.05                     | 0.57              |
| 32:1a:1414:U:H3    | 32:1a:1486:G:H1   | 1.52                     | 0.57              |
| 38:1g:48:LYS:O     | 38:1g:52:GLU:HG2  | 2.04                     | 0.57              |
| 38:1g:76:ARG:HH21  | 38:1g:89:MET:HE2  | 1.70                     | 0.57              |
| 1:2A:1721:G:H8     | 1:2A:1741:A:H62   | 1.53                     | 0.57              |
| 26:24:40:HIS:HB3   | 26:24:43:TYR:CD2  | 2.40                     | 0.57              |
| 32:2a:108:G:C6     | 51:2t:15:ARG:HG2  | 2.40                     | 0.57              |
| 32:2a:839:U:H5''   | 32:2a:840:C:H5    | 1.69                     | 0.57              |
| 36:2e:9:LYS:NZ     | 36:2e:111:GLU:OE1 | 2.38                     | 0.57              |
| 1:1A:400:G:O6      | 60:1A:4150:HOH:O  | 2.15                     | 0.57              |
| 1:1A:1379:A:H4'    | 1:1A:1380:G:OP2   | 2.05                     | 0.57              |
| 15:1T:54:ARG:HA    | 15:1T:59:THR:HB   | 1.86                     | 0.57              |
| 32:1a:332:G:O6     | 60:1a:1929:HOH:O  | 2.18                     | 0.57              |
| 44:1m:60:VAL:HG22  | 44:1m:64:TRP:HZ3  | 1.70                     | 0.57              |
| 46:1o:74:ASP:HB3   | 46:1o:77:ARG:HB2  | 1.87                     | 0.57              |
| 1:2A:2574:G:OP1    | 60:2A:3884:HOH:O  | 2.16                     | 0.57              |
| 2:2B:43:C:H5''     | 26:24:1:MET:HE2   | 1.86                     | 0.57              |
| 32:2a:130:A:H5'    | 48:2q:63:ARG:HE   | 1.70                     | 0.57              |
| 32:2a:1366:C:O2'   | 41:2j:60:ARG:NH2  | 2.27                     | 0.57              |
| 32:2a:1391:U:H2'   | 32:2a:1392:G:C8   | 2.40                     | 0.57              |
| 35:2d:57:ARG:HB3   | 35:2d:206:PHE:HB2 | 1.86                     | 0.57              |
| 1:1A:1229:G:N7     | 60:1A:4353:HOH:O  | 2.33                     | 0.56              |
| 17:1V:21:ARG:HD3   | 17:1V:91:TYR:CD1  | 2.39                     | 0.56              |
| 21:1Z:154:ASP:OD1  | 21:1Z:154:ASP:N   | 2.34                     | 0.56              |
| 32:1a:411:A:OP1    | 35:1d:30:LYS:NZ   | 2.35                     | 0.56              |
| 32:1a:1118:C:H1'   | 32:1a:1179:A:C4   | 2.40                     | 0.56              |
| 1:2A:576:U:H2'     | 1:2A:577:G:C8     | 2.40                     | 0.56              |
| 1:2A:2125:G:H22    | 1:2A:2172:U:H3'   | 1.70                     | 0.56              |
| 19:2X:11:PRO:HB3   | 19:2X:92:LEU:HD11 | 1.87                     | 0.56              |
| 32:2a:1203:C:H2'   | 32:2a:1204:A:H8   | 1.69                     | 0.56              |
| 33:2b:71:VAL:HG23  | 33:2b:164:VAL:HA  | 1.86                     | 0.56              |
| 33:2b:178:ARG:HH22 | 39:2h:74:PRO:HB3  | 1.69                     | 0.56              |
| 34:2c:40:ARG:NH1   | 34:2c:55:VAL:O    | 2.37                     | 0.56              |
| 17:1V:95:LEU:HD23  | 17:1V:97:LYS:HE3  | 1.87                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 32:1a:600:C:H2'   | 32:1a:601:C:H6    | 1.70                     | 0.56              |
| 40:1i:105:ASP:HB2 | 40:1i:107:ARG:HG3 | 1.87                     | 0.56              |
| 1:2A:805:G:N2     | 1:2A:829:A:OP1    | 2.36                     | 0.56              |
| 1:2A:1250:G:H5''  | 60:2A:5437:HOH:O  | 2.04                     | 0.56              |
| 36:2e:52:PRO:HA   | 36:2e:55:VAL:HG23 | 1.87                     | 0.56              |
| 1:1A:184:C:H2'    | 1:1A:185:U:C6     | 2.40                     | 0.56              |
| 1:1A:825:C:O2     | 11:1P:55:ARG:NH1  | 2.38                     | 0.56              |
| 1:1A:1105:U:H2'   | 1:1A:1106:G:C8    | 2.39                     | 0.56              |
| 4:1E:47:VAL:HG21  | 4:1E:86:PRO:HD2   | 1.87                     | 0.56              |
| 7:1H:149:ARG:NH1  | 7:1H:167:GLU:OE2  | 2.37                     | 0.56              |
| 12:1Q:58:PHE:O    | 12:1Q:60:ARG:N    | 2.37                     | 0.56              |
| 32:1a:517:G:N2    | 32:1a:533:A:OP2   | 2.35                     | 0.56              |
| 32:1a:1202:G:O4'  | 45:1n:29:ARG:NH1  | 2.38                     | 0.56              |
| 34:1c:150:LYS:HG3 | 34:1c:169:ALA:HB2 | 1.86                     | 0.56              |
| 51:1t:87:LYS:O    | 51:1t:91:LEU:HG   | 2.05                     | 0.56              |
| 11:2P:95:VAL:HG13 | 11:2P:125:VAL:HA  | 1.87                     | 0.56              |
| 32:2a:922:G:H4'   | 36:2e:20:GLN:HA   | 1.86                     | 0.56              |
| 1:1A:2150:U:H2'   | 1:1A:2151:G:C8    | 2.41                     | 0.56              |
| 32:1a:1409:C:H2'  | 32:1a:1410:G:C8   | 2.41                     | 0.56              |
| 1:2A:212:G:H2'    | 1:2A:213:A:O4'    | 2.05                     | 0.56              |
| 1:2A:2698:U:H2'   | 1:2A:2699:C:C6    | 2.41                     | 0.56              |
| 18:2W:78:GLU:OE2  | 18:2W:99:ARG:HD3  | 2.06                     | 0.56              |
| 1:1A:500:G:O6     | 60:1A:4174:HOH:O  | 2.17                     | 0.56              |
| 1:1A:2852:G:OP1   | 60:1A:4176:HOH:O  | 2.18                     | 0.56              |
| 22:10:37:LEU:HD21 | 22:10:61:ALA:HB2  | 1.87                     | 0.56              |
| 24:12:59:ARG:NH2  | 60:12:101:HOH:O   | 2.38                     | 0.56              |
| 37:1f:89:MET:HE1  | 49:1r:72:ARG:HG2  | 1.88                     | 0.56              |
| 38:1g:111:ARG:NH1 | 38:1g:113:GLU:OE2 | 2.29                     | 0.56              |
| 1:2A:1633:G:OP2   | 60:2A:3896:HOH:O  | 2.18                     | 0.56              |
| 17:2V:24:LYS:HG3  | 17:2V:64:HIS:HD2  | 1.71                     | 0.56              |
| 32:2a:1166:G:N2   | 32:2a:1170:A:OP2  | 2.33                     | 0.56              |
| 40:2i:23:ASN:ND2  | 40:2i:25:LYS:HE2  | 2.20                     | 0.56              |
| 50:2s:20:LEU:HA   | 50:2s:23:ASN:HD22 | 1.71                     | 0.56              |
| 1:1A:365:C:OP2    | 60:1A:4133:HOH:O  | 2.18                     | 0.56              |
| 5:1F:116:ASP:OD2  | 11:1P:1:MET:HB3   | 2.05                     | 0.56              |
| 6:1G:39:ILE:HB    | 6:1G:92:VAL:HG12  | 1.86                     | 0.56              |
| 32:1a:184:G:H2'   | 32:1a:185:A:H8    | 1.71                     | 0.56              |
| 32:1a:1048:G:OP1  | 45:1n:3:ARG:HB3   | 2.05                     | 0.56              |
| 32:1a:1346:A:H5'' | 40:1i:120:ARG:NH1 | 2.21                     | 0.56              |
| 51:1t:64:ASP:OD1  | 51:1t:81:LYS:HD2  | 2.06                     | 0.56              |
| 2:2B:106:G:H5'    | 21:2Z:31:ARG:HB3  | 1.87                     | 0.56              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 18:2W:18:ARG:HG2 | 18:2W:76:VAL:HB    | 1.88                     | 0.56              |
| 1:1A:2099:U:H3   | 1:1A:2190:G:H1     | 1.53                     | 0.56              |
| 1:1A:2406:U:H2'  | 1:1A:2406:U:OP2    | 2.05                     | 0.56              |
| 32:1a:815:A:N7   | 32:1a:1509:C:O2'   | 2.34                     | 0.56              |
| 32:1a:1244:C:H42 | 32:1a:1293:G:H1    | 1.54                     | 0.56              |
| 32:1a:1435:G:H2' | 32:1a:1436:U:C6    | 2.41                     | 0.56              |
| 51:1t:37:SER:O   | 51:1t:41:ILE:HG13  | 2.06                     | 0.56              |
| 1:2A:227:A:OP1   | 11:2P:76:LYS:NZ    | 2.37                     | 0.56              |
| 1:2A:1087:G:H1   | 1:2A:1102:C:H42    | 1.53                     | 0.56              |
| 30:28:56:GLU:HA  | 30:28:59:LYS:HE3   | 1.87                     | 0.56              |
| 2:1B:57:A:H1'    | 6:1G:29:TRP:HB2    | 1.87                     | 0.56              |
| 6:1G:15:VAL:HG22 | 6:1G:175:LEU:HB3   | 1.86                     | 0.56              |
| 21:1Z:19:ARG:NH1 | 21:1Z:84:GLU:O     | 2.39                     | 0.56              |
| 32:1a:532:A:H2   | 32:1a:1206:G:H21   | 1.53                     | 0.56              |
| 4:2E:52:LEU:H    | 4:2E:76:ARG:HB2    | 1.71                     | 0.56              |
| 18:2W:71:VAL:HA  | 18:2W:107:LEU:HD12 | 1.86                     | 0.56              |
| 32:2a:563:A:N6   | 60:2a:3267:HOH:O   | 2.37                     | 0.56              |
| 32:2a:1301:U:O2' | 32:2a:1302:U:H5'   | 2.06                     | 0.56              |
| 50:2s:38:SER:HB2 | 50:2s:71:LEU:HD22  | 1.87                     | 0.56              |
| 1:1A:1292:U:H2'  | 1:1A:1293:C:C6     | 2.41                     | 0.56              |
| 1:1A:1796:U:H2'  | 1:1A:1797:C:C6     | 2.40                     | 0.56              |
| 5:1F:64:ILE:HG21 | 5:1F:78:ILE:HG23   | 1.88                     | 0.56              |
| 6:2G:66:GLN:HG2  | 26:24:1:MET:HE1    | 1.88                     | 0.56              |
| 32:2a:999:C:N4   | 32:2a:1042:G:H1    | 2.04                     | 0.56              |
| 32:2a:1497:G:H1' | 32:2a:1518:MA6:H2  | 1.88                     | 0.56              |
| 1:1A:389:G:OP2   | 60:1A:4177:HOH:O   | 2.18                     | 0.56              |
| 1:1A:1155:A:OP1  | 16:1U:55:ARG:HD3   | 2.06                     | 0.56              |
| 1:1A:1582:C:O2'  | 1:1A:1586:A:N3     | 2.37                     | 0.56              |
| 9:1N:73:THR:HG23 | 9:1N:82:LEU:HD11   | 1.88                     | 0.56              |
| 10:1O:16:ALA:HB2 | 10:1O:52:VAL:HG21  | 1.88                     | 0.56              |
| 32:1a:73:G:H1    | 32:1a:96:U:H3      | 1.54                     | 0.56              |
| 32:1a:1062:U:H2' | 32:1a:1063:C:C6    | 2.41                     | 0.56              |
| 1:2A:1155:A:H5'' | 16:2U:55:ARG:HD3   | 1.88                     | 0.56              |
| 25:23:11:SER:HA  | 25:23:31:LEU:HD21  | 1.87                     | 0.56              |
| 1:1A:2474:C:OP1  | 60:1A:4180:HOH:O   | 2.18                     | 0.55              |
| 32:1a:1503:A:H5' | 32:1a:1531:A:H1'   | 1.88                     | 0.55              |
| 48:1q:67:LYS:O   | 48:1q:69:LYS:N     | 2.37                     | 0.55              |
| 5:2F:11:VAL:HG22 | 5:2F:125:LEU:HB2   | 1.87                     | 0.55              |
| 13:2R:13:HIS:CE1 | 13:2R:16:HIS:HB2   | 2.40                     | 0.55              |
| 43:2L:28:LYS:N   | 43:2L:29:GLY:HA2   | 2.20                     | 0.55              |
| 1:1A:1278:A:OP1  | 13:1R:36:THR:HG23  | 2.06                     | 0.55              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 32:1a:376:G:H5''   | 47:1p:5:ARG:HD3   | 1.88                     | 0.55              |
| 32:1a:1148:U:H2'   | 32:1a:1149:C:O4'  | 2.05                     | 0.55              |
| 53:1y:55:ASN:HA    | 53:1y:60:VAL:HA   | 1.88                     | 0.55              |
| 1:2A:857:C:H4'     | 22:20:23:VAL:HG21 | 1.86                     | 0.55              |
| 1:2A:1073:A:H2'    | 1:2A:1074:G:C8    | 2.41                     | 0.55              |
| 1:2A:2815:C:H5'    | 27:25:29:THR:HG21 | 1.88                     | 0.55              |
| 32:2a:1255:G:HO2'  | 32:2a:1258:G:HO2' | 1.52                     | 0.55              |
| 1:1A:2232:U:P      | 23:11:40:ARG:HH12 | 2.29                     | 0.55              |
| 17:1V:98:GLU:OE2   | 17:1V:100:ARG:NH1 | 2.39                     | 0.55              |
| 32:1a:148:G:H2'    | 32:1a:149:A:H8    | 1.72                     | 0.55              |
| 32:1a:177:C:OP1    | 51:1t:65:LYS:NZ   | 2.21                     | 0.55              |
| 39:1h:112:LEU:HD22 | 39:1h:133:LEU:HA  | 1.87                     | 0.55              |
| 46:1o:25:THR:HG21  | 46:1o:70:LEU:HB2  | 1.88                     | 0.55              |
| 1:2A:1062:G:N7     | 1:2A:1070:A:H1'   | 2.21                     | 0.55              |
| 1:2A:1187:G:H5'    | 17:2V:81:TYR:CE1  | 2.41                     | 0.55              |
| 32:2a:573:A:N3     | 32:2a:883:C:O2'   | 2.37                     | 0.55              |
| 32:2a:1286:A:C8    | 32:2a:1287:A:H4'  | 2.42                     | 0.55              |
| 1:1A:1583:A:H5'    | 1:1A:1584:C:OP1   | 2.06                     | 0.55              |
| 1:1A:2100:G:H1     | 1:1A:2189:U:H3    | 1.53                     | 0.55              |
| 3:1D:242:ARG:HD2   | 3:1D:246:PRO:HG3  | 1.89                     | 0.55              |
| 32:1a:1305:G:N2    | 32:1a:1331:G:H1'  | 2.20                     | 0.55              |
| 1:2A:1815:A:OP2    | 3:2D:54:ARG:NH2   | 2.39                     | 0.55              |
| 32:2a:111:G:OP2    | 60:2a:3222:HOH:O  | 2.17                     | 0.55              |
| 28:16:11:LEU:HB3   | 28:16:49:HIS:HB3  | 1.88                     | 0.55              |
| 32:1a:166:G:H2'    | 32:1a:167:G:H8    | 1.71                     | 0.55              |
| 1:2A:446:G:OP1     | 16:2U:3:ARG:NH1   | 2.34                     | 0.55              |
| 1:2A:528:A:O2'     | 1:2A:529:A:H5'    | 2.06                     | 0.55              |
| 1:2A:2273:A:H2'    | 1:2A:2274:A:C8    | 2.41                     | 0.55              |
| 19:2X:31:HIS:HB3   | 19:2X:34:ALA:HB2  | 1.89                     | 0.55              |
| 32:2a:1117:G:N2    | 32:2a:1180:A:O2'  | 2.39                     | 0.55              |
| 32:1a:984:C:H42    | 32:1a:1221:G:H1   | 1.53                     | 0.55              |
| 39:1h:39:LEU:HB3   | 39:1h:45:ILE:HG12 | 1.88                     | 0.55              |
| 1:2A:271(H):G:H2'  | 1:2A:271(I):G:C8  | 2.41                     | 0.55              |
| 1:2A:1602:U:O4     | 60:2A:3859:HOH:O  | 2.13                     | 0.55              |
| 6:2G:75:LYS:HA     | 6:2G:84:LYS:HD2   | 1.89                     | 0.55              |
| 6:2G:97:ASP:HA     | 6:2G:100:TRP:HD1  | 1.70                     | 0.55              |
| 12:2Q:1:MET:HG3    | 12:2Q:44:ALA:HB1  | 1.88                     | 0.55              |
| 32:2a:21:G:H2'     | 32:2a:22:G:C8     | 2.41                     | 0.55              |
| 35:2d:127:THR:HG23 | 35:2d:147:ALA:HB3 | 1.88                     | 0.55              |
| 39:2h:87:SER:HB2   | 39:2h:93:VAL:HB   | 1.87                     | 0.55              |
| 1:1A:1138:G:N3     | 9:1N:106:MET:HE2  | 2.21                     | 0.55              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 39:1h:10:LEU:HD22  | 39:1h:83:ILE:HD11  | 1.87                     | 0.55              |
| 1:2A:310:A:O2'     | 60:2A:3900:HOH:O   | 2.18                     | 0.55              |
| 1:2A:1012:U:C5     | 9:2N:28:THR:HG21   | 2.41                     | 0.55              |
| 6:2G:12:TYR:HA     | 6:2G:16:ARG:HG3    | 1.87                     | 0.55              |
| 23:21:3:LYS:HB2    | 23:21:61:ARG:HH22  | 1.71                     | 0.55              |
| 32:2a:975:A:N1     | 41:2j:48:THR:HB    | 2.20                     | 0.55              |
| 32:2a:1435:G:H2'   | 32:2a:1436:U:C6    | 2.42                     | 0.55              |
| 44:2m:15:VAL:HG12  | 44:2m:48:LEU:HD11  | 1.89                     | 0.55              |
| 1:1A:694:U:OP1     | 3:1D:59:LYS:NZ     | 2.39                     | 0.55              |
| 5:1F:11:VAL:HB     | 5:1F:18:ARG:HG3    | 1.88                     | 0.55              |
| 32:1a:201:C:N4     | 32:1a:216:G:H1     | 1.95                     | 0.55              |
| 33:1b:76:GLN:HG2   | 33:1b:206:ASP:O    | 2.06                     | 0.55              |
| 36:1e:110:LEU:HD13 | 36:1e:118:ILE:HG21 | 1.89                     | 0.55              |
| 43:1l:38:THR:OG1   | 43:1l:39:VAL:N     | 2.40                     | 0.55              |
| 44:1m:11:ARG:HA    | 44:1m:45:VAL:HB    | 1.87                     | 0.55              |
| 3:2D:75:ILE:HG21   | 3:2D:99:ASP:HB2    | 1.87                     | 0.55              |
| 32:2a:718:G:C8     | 42:2k:116:HIS:HB3  | 2.41                     | 0.55              |
| 32:2a:742:G:OP2    | 46:2o:35:ARG:NH2   | 2.38                     | 0.55              |
| 51:2t:33:ILE:HG13  | 51:2t:62:LEU:HB3   | 1.88                     | 0.55              |
| 1:1A:760:G:OP1     | 60:1A:4178:HOH:O   | 2.18                     | 0.55              |
| 1:1A:1518:U:H2'    | 1:1A:1519:G:O4'    | 2.07                     | 0.55              |
| 3:1D:175:LEU:HD12  | 3:1D:185:VAL:HG21  | 1.88                     | 0.55              |
| 32:1a:1183:A:H3'   | 32:1a:1184:G:H5''  | 1.88                     | 0.55              |
| 34:1c:182:ILE:HG12 | 34:1c:203:PHE:CD1  | 2.42                     | 0.55              |
| 42:1k:86:GLY:H     | 42:1k:112:THR:HG1  | 1.53                     | 0.55              |
| 44:1m:3:ARG:HD2    | 44:1m:9:ILE:HG12   | 1.89                     | 0.55              |
| 1:2A:948:G:OP2     | 60:2A:3898:HOH:O   | 2.18                     | 0.55              |
| 1:2A:1012:U:H5     | 9:2N:28:THR:HG21   | 1.71                     | 0.55              |
| 1:2A:1032:A:H2     | 1:2A:1122:G:H22    | 1.53                     | 0.55              |
| 1:2A:1503:U:H2'    | 1:2A:1504:C:C6     | 2.41                     | 0.55              |
| 1:2A:2134:A:O2'    | 1:2A:2159:G:N3     | 2.40                     | 0.55              |
| 7:2H:3:ARG:HG2     | 7:2H:6:ARG:NH1     | 2.22                     | 0.55              |
| 27:25:41:PRO:O     | 27:25:44:THR:OG1   | 2.24                     | 0.55              |
| 32:2a:920:U:H2'    | 32:2a:921:U:C6     | 2.41                     | 0.55              |
| 32:2a:977:A:O2'    | 32:2a:980:C:N4     | 2.39                     | 0.55              |
| 35:2d:79:PHE:CE1   | 35:2d:204:ILE:HD13 | 2.42                     | 0.55              |
| 1:1A:404:C:OP1     | 60:1A:4182:HOH:O   | 2.18                     | 0.55              |
| 4:1E:29:GLY:H      | 4:1E:180:ASN:HB3   | 1.71                     | 0.55              |
| 26:14:18:CYS:SG    | 26:14:20:ASN:HB2   | 2.47                     | 0.55              |
| 26:14:59:PHE:HE1   | 50:1s:67:VAL:HG21  | 1.72                     | 0.55              |
| 32:1a:840:C:H4'    | 32:1a:841:U:OP2    | 2.06                     | 0.55              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 33:1b:77:ALA:HB2  | 33:1b:211:ILE:HD13 | 1.89                     | 0.55              |
| 26:24:46:GLN:O    | 26:24:48:ARG:N     | 2.37                     | 0.55              |
| 32:2a:433:C:H2'   | 32:2a:434:U:C6     | 2.42                     | 0.55              |
| 40:2i:3:GLN:NE2   | 40:2i:20:ARG:HH21  | 2.05                     | 0.55              |
| 32:1a:474:G:H2'   | 32:1a:475:G:C8     | 2.42                     | 0.54              |
| 32:1a:826:C:H2'   | 32:1a:827:U:C6     | 2.42                     | 0.54              |
| 35:1d:108:LEU:HB3 | 35:1d:110:PHE:CE1  | 2.42                     | 0.54              |
| 1:2A:1005:C:H2'   | 1:2A:1006:C:C6     | 2.42                     | 0.54              |
| 1:2A:1527:G:OP1   | 60:2A:3902:HOH:O   | 2.18                     | 0.54              |
| 1:2A:1945:G:OP1   | 60:2A:3891:HOH:O   | 2.17                     | 0.54              |
| 1:2A:2103:C:N4    | 1:2A:2185:C:H42    | 2.05                     | 0.54              |
| 1:2A:2379:G:O2'   | 14:2S:17:ARG:NH1   | 2.37                     | 0.54              |
| 1:2A:2601:C:H3'   | 60:2A:5698:HOH:O   | 2.06                     | 0.54              |
| 6:2G:44:GLY:HA2   | 6:2G:88:ILE:HG22   | 1.87                     | 0.54              |
| 13:2R:98:LEU:HD12 | 13:2R:113:LEU:HD11 | 1.89                     | 0.54              |
| 32:2a:619:U:N3    | 35:2d:134:ASP:OD1  | 2.29                     | 0.54              |
| 1:1A:2364:C:H2'   | 1:1A:2365:G:O4'    | 2.06                     | 0.54              |
| 1:1A:2815:C:H5'   | 27:15:29:THR:HG21  | 1.89                     | 0.54              |
| 4:1E:60:ASN:OD1   | 4:1E:63:LEU:HB2    | 2.06                     | 0.54              |
| 14:1S:20:ARG:NH2  | 22:10:51:VAL:O     | 2.31                     | 0.54              |
| 18:1W:65:LEU:HB2  | 18:1W:68:ARG:HD2   | 1.87                     | 0.54              |
| 32:1a:1002:G:H1   | 32:1a:1038:C:H42   | 1.54                     | 0.54              |
| 1:2A:588:U:H2'    | 1:2A:589:C:C6      | 2.43                     | 0.54              |
| 23:21:50:ARG:NH1  | 23:21:57:GLU:OE2   | 2.37                     | 0.54              |
| 42:2k:92:GLU:HA   | 42:2k:95:ILE:HD12  | 1.89                     | 0.54              |
| 20:1Y:99:CYS:HB2  | 20:1Y:106:LEU:HD21 | 1.88                     | 0.54              |
| 33:1b:162:ILE:O   | 33:1b:185:ILE:HG13 | 2.06                     | 0.54              |
| 35:1d:119:GLN:HG3 | 35:1d:123:HIS:CE1  | 2.43                     | 0.54              |
| 38:1g:74:GLU:HG2  | 38:1g:91:VAL:HG22  | 1.89                     | 0.54              |
| 41:1j:49:VAL:HG23 | 45:1n:41:ARG:HG3   | 1.89                     | 0.54              |
| 1:2A:365:C:OP2    | 60:2A:3901:HOH:O   | 2.18                     | 0.54              |
| 1:2A:888:C:H2'    | 1:2A:889:C:C2      | 2.42                     | 0.54              |
| 1:2A:1507:A:O2'   | 1:2A:1508:A:O5'    | 2.26                     | 0.54              |
| 28:26:8:LYS:NZ    | 60:26:601:HOH:O    | 2.38                     | 0.54              |
| 32:2a:149:A:H2'   | 32:2a:150:C:H6     | 1.72                     | 0.54              |
| 32:2a:859:A:H2'   | 32:2a:860:A:O4'    | 2.08                     | 0.54              |
| 1:1A:1060:U:H4'   | 1:1A:1061:U:H5'    | 1.90                     | 0.54              |
| 60:1A:4227:HOH:O  | 5:1F:52:LYS:NZ     | 2.38                     | 0.54              |
| 5:1F:155:LEU:HD11 | 5:1F:176:LEU:HD12  | 1.88                     | 0.54              |
| 32:1a:1376:U:H2'  | 32:1a:1377:A:C8    | 2.42                     | 0.54              |
| 1:2A:2111:C:N3    | 1:2A:2145:C:O2'    | 2.38                     | 0.54              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:2A:2142:C:H2'   | 1:2A:2143:C:C6     | 2.43                     | 0.54              |
| 6:2G:115:ARG:NH1  | 44:2m:6:GLY:O      | 2.33                     | 0.54              |
| 32:2a:45:U:H2'    | 32:2a:46:G:C8      | 2.42                     | 0.54              |
| 32:2a:1309:G:N7   | 44:2m:99:ARG:NH2   | 2.55                     | 0.54              |
| 1:1A:1113:U:H2'   | 1:1A:1114:G:C8     | 2.43                     | 0.54              |
| 32:1a:13:U:OP1    | 60:1a:1931:HOH:O   | 2.18                     | 0.54              |
| 32:1a:1412:C:H2'  | 32:1a:1413:A:H8    | 1.71                     | 0.54              |
| 44:1m:49:THR:HG22 | 44:1m:51:ALA:H     | 1.72                     | 0.54              |
| 1:2A:2168:G:O2'   | 1:2A:2170:A:N7     | 2.38                     | 0.54              |
| 10:2O:23:ARG:HD3  | 10:2O:24:VAL:N     | 2.23                     | 0.54              |
| 25:23:18:ASP:OD1  | 25:23:18:ASP:N     | 2.39                     | 0.54              |
| 44:2m:3:ARG:HG3   | 44:2m:9:ILE:H      | 1.72                     | 0.54              |
| 51:2t:50:GLU:HG3  | 51:2t:100:ILE:HD11 | 1.89                     | 0.54              |
| 1:1A:2267:A:H5''  | 1:1A:2268:A:H5'    | 1.90                     | 0.54              |
| 10:1O:64:ARG:HB2  | 10:1O:79:PHE:CG    | 2.43                     | 0.54              |
| 32:1a:1070:U:OP1  | 36:1e:25:ARG:NH1   | 2.40                     | 0.54              |
| 49:1r:56:THR:HB   | 49:1r:58:LEU:HD13  | 1.88                     | 0.54              |
| 50:1s:3:ARG:HH11  | 50:1s:10:PHE:HB2   | 1.72                     | 0.54              |
| 1:2A:154(A):C:H42 | 1:2A:171:G:H1      | 1.55                     | 0.54              |
| 6:2G:80:PHE:O     | 6:2G:82:LEU:N      | 2.40                     | 0.54              |
| 24:22:65:ASN:OD1  | 24:22:69:ARG:NH1   | 2.41                     | 0.54              |
| 32:2a:306:G:OP2   | 60:2a:3225:HOH:O   | 2.18                     | 0.54              |
| 32:2a:562:C:H1'   | 43:2l:15:ARG:HB3   | 1.89                     | 0.54              |
| 32:2a:685:G:N1    | 32:2a:704:A:OP2    | 2.38                     | 0.54              |
| 6:1G:103:LEU:HD23 | 6:1G:106:LEU:HD23  | 1.88                     | 0.54              |
| 1:2A:2081:C:OP2   | 60:2A:3894:HOH:O   | 2.18                     | 0.54              |
| 5:2F:64:ILE:HD11  | 5:2F:75:HIS:HB2    | 1.88                     | 0.54              |
| 29:27:5:TRP:NE1   | 29:27:7:PRO:HG3    | 2.23                     | 0.54              |
| 33:2b:97:TRP:CH2  | 33:2b:173:ALA:HA   | 2.42                     | 0.54              |
| 33:2b:105:PHE:O   | 33:2b:109:SER:OG   | 2.22                     | 0.54              |
| 33:1b:15:VAL:HG12 | 33:1b:16:HIS:CD2   | 2.43                     | 0.54              |
| 1:2A:1067:A:H4'   | 1:2A:1068:G:OP2    | 2.08                     | 0.54              |
| 26:24:48:ARG:HG3  | 26:24:52:THR:HG23  | 1.88                     | 0.54              |
| 32:2a:433:C:H2'   | 32:2a:434:U:H6     | 1.70                     | 0.54              |
| 32:2a:964:A:N3    | 32:2a:969:A:O2'    | 2.33                     | 0.54              |
| 32:2a:1258:G:H2'  | 32:2a:1259:C:C6    | 2.43                     | 0.54              |
| 1:1A:1468:C:OP1   | 60:1A:4181:HOH:O   | 2.18                     | 0.54              |
| 1:1A:1810:A:H2'   | 1:1A:1811:G:O4'    | 2.08                     | 0.54              |
| 1:1A:2492:U:H2'   | 1:1A:2493:U:C6     | 2.43                     | 0.54              |
| 32:1a:405:U:O4    | 35:1d:2:GLY:N      | 2.41                     | 0.54              |
| 1:2A:1047:G:H21   | 1:2A:1111:A:H62    | 1.54                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:2A:2331:G:O2'    | 22:20:43:THR:HG22  | 2.08                     | 0.54              |
| 1:2A:2567:G:H2'    | 1:2A:2568:C:C6     | 2.43                     | 0.54              |
| 5:2F:184:TYR:CE2   | 5:2F:188:ARG:HD2   | 2.43                     | 0.54              |
| 14:2S:25:ARG:NH1   | 14:2S:42:ASP:OD1   | 2.41                     | 0.54              |
| 32:2a:258:G:H2'    | 32:2a:259:G:H8     | 1.72                     | 0.54              |
| 32:2a:1031:G:H2'   | 32:2a:1032:G:C8    | 2.43                     | 0.54              |
| 33:2b:71:VAL:HA    | 33:2b:93:VAL:HG22  | 1.89                     | 0.54              |
| 40:2i:3:GLN:HE21   | 40:2i:20:ARG:HH21  | 1.56                     | 0.54              |
| 49:2r:51:LEU:HD22  | 49:2r:55:ARG:HE    | 1.72                     | 0.54              |
| 1:1A:2121:G:H1     | 1:1A:2177:C:H42    | 1.56                     | 0.54              |
| 3:1D:69:ARG:NH1    | 60:1D:409:HOH:O    | 2.41                     | 0.54              |
| 3:1D:108:PRO:HG3   | 3:1D:143:HIS:CE1   | 2.43                     | 0.54              |
| 23:11:64:ALA:HA    | 23:11:67:ILE:HG13  | 1.90                     | 0.54              |
| 32:1a:116:A:H61    | 32:1a:313:A:H1'    | 1.72                     | 0.54              |
| 32:1a:540:G:H2'    | 32:1a:541:G:O4'    | 2.08                     | 0.54              |
| 36:1e:50:GLU:HB2   | 36:1e:53:LEU:HD13  | 1.89                     | 0.54              |
| 1:2A:2644:G:O6     | 60:2A:3876:HOH:O   | 2.16                     | 0.54              |
| 1:2A:2655:G:O2'    | 1:2A:2664:G:O6     | 2.26                     | 0.54              |
| 13:2R:100:LEU:HD11 | 13:2R:113:LEU:HD23 | 1.90                     | 0.54              |
| 35:2d:191:ARG:NH2  | 35:2d:200:GLU:OE1  | 2.28                     | 0.54              |
| 1:1A:153:C:OP2     | 23:11:92:LYS:NZ    | 2.41                     | 0.53              |
| 1:1A:271(L):U:H4'  | 8:1I:50:ARG:HH12   | 1.73                     | 0.53              |
| 1:1A:1165:U:H2'    | 1:1A:1166:C:C6     | 2.43                     | 0.53              |
| 1:1A:1823:G:OP1    | 3:1D:54:ARG:NH1    | 2.41                     | 0.53              |
| 1:1A:2547:U:O2     | 10:1O:23:ARG:NH2   | 2.38                     | 0.53              |
| 32:1a:524:G:H2'    | 32:1a:525:C:C6     | 2.43                     | 0.53              |
| 41:1j:42:THR:HG23  | 41:1j:68:HIS:HA    | 1.89                     | 0.53              |
| 1:2A:252:G:OP1     | 60:2A:3903:HOH:O   | 2.19                     | 0.53              |
| 1:2A:602:G:O2'     | 1:2A:655:A:N6      | 2.41                     | 0.53              |
| 1:2A:2115:G:H3'    | 1:2A:2116:G:H5'    | 1.89                     | 0.53              |
| 22:20:32:ARG:H     | 22:20:35:ASN:ND2   | 2.06                     | 0.53              |
| 31:29:3:VAL:HA     | 31:29:35:ARG:O     | 2.08                     | 0.53              |
| 32:2a:458:C:H2'    | 32:2a:460:G:O4'    | 2.07                     | 0.53              |
| 40:2i:28:VAL:HG22  | 40:2i:63:ILE:HB    | 1.91                     | 0.53              |
| 49:2r:73:ALA:HB3   | 49:2r:79:LEU:HD12  | 1.89                     | 0.53              |
| 53:2y:40:ILE:HB    | 53:2y:51:ASP:HB2   | 1.90                     | 0.53              |
| 1:1A:2683:C:H5'    | 15:1T:58:ASN:HD22  | 1.73                     | 0.53              |
| 11:1P:138:LEU:HD23 | 11:1P:145:PRO:HB3  | 1.89                     | 0.53              |
| 35:1d:65:ARG:NH1   | 35:1d:70:ILE:O     | 2.41                     | 0.53              |
| 1:2A:1833:U:O2'    | 1:2A:1969:A:N1     | 2.35                     | 0.53              |
| 20:2Y:6:HIS:CD2    | 20:2Y:7:VAL:H      | 2.26                     | 0.53              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 32:2a:736:C:H2'   | 32:2a:737:A:C8     | 2.43                     | 0.53              |
| 32:2a:1117:G:H5'  | 32:2a:1118:C:OP2   | 2.08                     | 0.53              |
| 10:1O:116:SER:HA  | 56:1a:1883:MPD:HM2 | 1.90                     | 0.53              |
| 15:1T:51:ARG:HG3  | 15:1T:98:LYS:HD2   | 1.90                     | 0.53              |
| 32:1a:108:G:H1    | 51:1t:15:ARG:HG2   | 1.72                     | 0.53              |
| 33:1b:55:PHE:HD1  | 33:1b:58:ILE:HD12  | 1.74                     | 0.53              |
| 40:1i:9:ARG:HG2   | 40:1i:14:VAL:HG22  | 1.91                     | 0.53              |
| 1:2A:479:A:N3     | 1:2A:481:G:H5''    | 2.24                     | 0.53              |
| 1:2A:973:A:H8     | 1:2A:973:A:OP1     | 1.91                     | 0.53              |
| 32:2a:407:G:OP1   | 35:2d:115:ARG:NH2  | 2.42                     | 0.53              |
| 32:2a:411:A:OP1   | 35:2d:30:LYS:NZ    | 2.32                     | 0.53              |
| 36:2e:122:GLU:O   | 36:2e:126:ARG:NH1  | 2.41                     | 0.53              |
| 53:2y:3:MET:HE3   | 53:2y:5:ILE:HD11   | 1.90                     | 0.53              |
| 1:1A:236:C:H2'    | 1:1A:237:C:C6      | 2.44                     | 0.53              |
| 1:1A:548:A:N6     | 17:1V:19:LYS:H     | 2.05                     | 0.53              |
| 1:1A:2801(A):A:N3 | 1:1A:2895:U:H1'    | 2.23                     | 0.53              |
| 4:1E:3:GLY:HA3    | 4:1E:81:ILE:HD12   | 1.91                     | 0.53              |
| 21:1Z:44:PHE:CZ   | 21:1Z:86:VAL:HG11  | 2.44                     | 0.53              |
| 32:1a:407:G:OP1   | 35:1d:115:ARG:NH2  | 2.41                     | 0.53              |
| 33:1b:215:LEU:O   | 33:1b:219:VAL:HG23 | 2.09                     | 0.53              |
| 44:1m:11:ARG:C    | 44:1m:13:LYS:H     | 2.17                     | 0.53              |
| 1:2A:2612:C:OP2   | 27:25:2:ALA:N      | 2.42                     | 0.53              |
| 7:2H:117:PRO:HG3  | 7:2H:123:PHE:CD2   | 2.43                     | 0.53              |
| 27:25:57:VAL:HG12 | 27:25:58:LEU:HB2   | 1.90                     | 0.53              |
| 32:2a:1320:C:H1'  | 50:2s:73:GLU:HG2   | 1.90                     | 0.53              |
| 46:2o:87:ILE:HG22 | 46:2o:88:ARG:H     | 1.73                     | 0.53              |
| 1:1A:1416:G:O2'   | 1:1A:1417:C:OP2    | 2.25                     | 0.53              |
| 1:1A:1429:G:H2'   | 1:1A:1430:C:C6     | 2.42                     | 0.53              |
| 1:1A:1969:A:O2'   | 1:1A:1972:A:N3     | 2.41                     | 0.53              |
| 32:1a:945:G:OP1   | 60:1a:1933:HOH:O   | 2.19                     | 0.53              |
| 1:2A:107:C:H2'    | 1:2A:108:U:H6      | 1.74                     | 0.53              |
| 1:2A:218:A:OP2    | 60:2A:3899:HOH:O   | 2.18                     | 0.53              |
| 1:2A:530:G:O6     | 60:2A:3885:HOH:O   | 2.17                     | 0.53              |
| 1:2A:855:G:O6     | 60:2A:3892:HOH:O   | 2.17                     | 0.53              |
| 1:2A:1278:A:HO2'  | 13:2R:27:SER:HG    | 1.55                     | 0.53              |
| 5:2F:192:LEU:HD13 | 5:2F:194:MET:HE2   | 1.90                     | 0.53              |
| 13:2R:2:ARG:NH1   | 13:2R:5:LYS:O      | 2.42                     | 0.53              |
| 21:2Z:48:PHE:HE1  | 21:2Z:71:VAL:HG11  | 1.74                     | 0.53              |
| 21:2Z:52:SER:OG   | 21:2Z:53:ILE:N     | 2.28                     | 0.53              |
| 32:2a:1346:A:OP1  | 40:2i:120:ARG:NH1  | 2.40                     | 0.53              |
| 33:2b:216:SER:O   | 33:2b:220:ASP:N    | 2.40                     | 0.53              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:1A:2478:A:OP2    | 31:19:2:LYS:NZ     | 2.34                     | 0.53              |
| 7:1H:7:LEU:HD12    | 7:1H:8:PRO:HD2     | 1.90                     | 0.53              |
| 8:1I:27:ARG:HD2    | 23:11:71:TYR:CE2   | 2.43                     | 0.53              |
| 32:1a:7:G:H5'      | 32:1a:298:A:O4'    | 2.09                     | 0.53              |
| 32:1a:1025:U:C2    | 32:1a:1036:G:O6    | 2.61                     | 0.53              |
| 32:1a:1071:C:H2'   | 32:1a:1072:G:H8    | 1.73                     | 0.53              |
| 32:1a:1314:C:OP2   | 50:1s:4:SER:OG     | 2.15                     | 0.53              |
| 34:1c:135:LYS:HZ3  | 36:1e:53:LEU:HD11  | 1.74                     | 0.53              |
| 39:1h:81:HIS:N     | 39:1h:138:TRP:O    | 2.42                     | 0.53              |
| 42:1k:99:GLN:HG2   | 42:1k:105:VAL:HG21 | 1.91                     | 0.53              |
| 1:2A:363:G:H2'     | 1:2A:363(A):A:H8   | 1.73                     | 0.53              |
| 1:2A:1889:A:H2'    | 1:2A:1890:A:C8     | 2.43                     | 0.53              |
| 9:2N:67:LEU:O      | 9:2N:88:GLU:HG3    | 2.08                     | 0.53              |
| 15:2T:19:LEU:HD13  | 15:2T:86:ILE:HD12  | 1.91                     | 0.53              |
| 15:2T:24:PRO:HA    | 15:2T:49:VAL:HG23  | 1.89                     | 0.53              |
| 32:2a:451:A:N6     | 32:2a:480:U:H2'    | 2.24                     | 0.53              |
| 32:2a:1151:A:H5''  | 41:2j:41:PRO:HA    | 1.91                     | 0.53              |
| 39:2h:20:TYR:HA    | 39:2h:65:TYR:CZ    | 2.44                     | 0.53              |
| 39:2h:25:ASP:N     | 39:2h:25:ASP:OD1   | 2.39                     | 0.53              |
| 1:1A:2452:C:OP1    | 60:1A:4183:HOH:O   | 2.18                     | 0.53              |
| 4:1E:2:LYS:HB2     | 4:1E:95:ILE:HD12   | 1.91                     | 0.53              |
| 5:1F:188:ARG:NH2   | 60:1F:407:HOH:O    | 2.41                     | 0.53              |
| 6:1G:101:ILE:HD13  | 26:14:25:TYR:HB2   | 1.89                     | 0.53              |
| 7:1H:27:LYS:HG2    | 7:1H:32:GLU:HG2    | 1.91                     | 0.53              |
| 8:1I:38:LEU:HB3    | 8:1I:40:THR:HG23   | 1.91                     | 0.53              |
| 32:1a:165:C:H2'    | 32:1a:166:G:C8     | 2.44                     | 0.53              |
| 32:1a:741:G:H2'    | 32:1a:742:G:O4'    | 2.09                     | 0.53              |
| 36:1e:143:ARG:NH1  | 39:1h:77:GLU:OE2   | 2.42                     | 0.53              |
| 1:2A:581:C:H2'     | 1:2A:582:G:C8      | 2.44                     | 0.53              |
| 7:2H:12:PRO:O      | 7:2H:15:VAL:HG22   | 2.09                     | 0.53              |
| 8:2I:104:GLN:HE22  | 8:2I:105:HIS:CE1   | 2.27                     | 0.53              |
| 32:2a:1040:U:H2'   | 32:2a:1041:A:O4'   | 2.07                     | 0.53              |
| 32:2a:1292:U:OP2   | 38:2g:41:ARG:NH2   | 2.42                     | 0.53              |
| 38:2g:68:ASN:HD22  | 38:2g:128:ALA:HA   | 1.73                     | 0.53              |
| 6:1G:44:GLY:HA2    | 6:1G:88:ILE:HG22   | 1.91                     | 0.53              |
| 32:1a:190:U:H2'    | 32:1a:191:G:H8     | 1.72                     | 0.53              |
| 1:2A:1178:C:H2'    | 1:2A:1179:C:C6     | 2.44                     | 0.53              |
| 6:2G:145:THR:HG23  | 6:2G:147:ASP:H     | 1.73                     | 0.53              |
| 10:2O:115:VAL:HG13 | 10:2O:121:VAL:HG21 | 1.91                     | 0.53              |
| 32:2a:222:U:H2'    | 32:2a:223:U:C6     | 2.44                     | 0.53              |
| 53:2y:3:MET:HA     | 53:2y:37:PRO:HG2   | 1.91                     | 0.53              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 1:1A:2181:G:H2'     | 1:1A:2182:G:C8     | 2.44                     | 0.53              |
| 12:1Q:110:THR:HG23  | 12:1Q:113:GLN:OE1  | 2.09                     | 0.53              |
| 25:13:55:ARG:NH1    | 25:13:57:GLU:OE1   | 2.38                     | 0.53              |
| 33:1b:163:PHE:CD1   | 33:1b:185:ILE:HB   | 2.43                     | 0.53              |
| 1:2A:1523:U:H2'     | 1:2A:1524:G:C8     | 2.44                     | 0.53              |
| 1:2A:1688:U:O2      | 1:2A:1700:A:H5'    | 2.09                     | 0.53              |
| 2:2B:90:A:C5        | 2:2B:91:C:H1'      | 2.43                     | 0.53              |
| 9:2N:58:ASP:N       | 9:2N:58:ASP:OD1    | 2.38                     | 0.53              |
| 9:2N:97:ARG:HA      | 9:2N:100:GLU:HB2   | 1.91                     | 0.53              |
| 10:2O:120:GLU:HG2   | 10:2O:122:LEU:HG   | 1.91                     | 0.53              |
| 32:2a:1305:G:N2     | 32:2a:1331:G:H1'   | 2.24                     | 0.53              |
| 32:2a:1515:C:H2'    | 32:2a:1516:G:C8    | 2.44                     | 0.53              |
| 39:2h:4:ASP:OD2     | 39:2h:85:ARG:NH1   | 2.42                     | 0.53              |
| 48:2q:12:SER:HB3    | 48:2q:20:THR:HB    | 1.91                     | 0.53              |
| 4:1E:9:VAL:HB       | 15:1T:3:ARG:HG2    | 1.90                     | 0.53              |
| 6:1G:142:PRO:HB2    | 26:14:31:ILE:HG21  | 1.91                     | 0.53              |
| 32:1a:17:U:H2'      | 32:1a:18:C:C6      | 2.43                     | 0.53              |
| 37:1f:3:ARG:HD3     | 37:1f:64:GLN:NE2   | 2.24                     | 0.53              |
| 42:1k:81:ASP:N      | 42:1k:81:ASP:OD1   | 2.39                     | 0.53              |
| 51:1t:53:LEU:HB2    | 51:1t:100:ILE:HG13 | 1.90                     | 0.53              |
| 1:2A:945:A:OP2      | 60:2A:3897:HOH:O   | 2.18                     | 0.53              |
| 1:2A:1292:U:H2'     | 1:2A:1293:C:C6     | 2.44                     | 0.53              |
| 1:2A:2115:G:H22     | 1:2A:2119:A:H5'    | 1.73                     | 0.53              |
| 26:24:41:PRO:HG3    | 26:24:49:PHE:CE2   | 2.44                     | 0.53              |
| 32:2a:325:A:OP2     | 51:2t:70:SER:OG    | 2.24                     | 0.53              |
| 32:2a:881:G:P       | 43:2l:12:ARG:HH22  | 2.31                     | 0.53              |
| 32:2a:1030(C):G:H2' | 32:2a:1030(D):A:C8 | 2.44                     | 0.53              |
| 44:2m:80:ARG:O      | 44:2m:84:ILE:HG23  | 2.09                     | 0.53              |
| 1:1A:1486:A:H2'     | 1:1A:1487:G:H8     | 1.74                     | 0.52              |
| 1:1A:1578:U:H2'     | 1:1A:1579:A:H5'    | 1.90                     | 0.52              |
| 1:1A:2870:C:H2'     | 1:1A:2871:C:O4'    | 2.08                     | 0.52              |
| 33:1b:219:VAL:HA    | 33:1b:222:ILE:HD12 | 1.91                     | 0.52              |
| 1:2A:1076:C:H4'     | 1:2A:1077:A:OP1    | 2.08                     | 0.52              |
| 1:2A:1379:A:H4'     | 1:2A:1380:G:OP2    | 2.08                     | 0.52              |
| 8:2I:4:ILE:HD11     | 8:2I:44:LEU:HD13   | 1.91                     | 0.52              |
| 13:2R:97:VAL:HG22   | 13:2R:114:VAL:HG13 | 1.89                     | 0.52              |
| 32:2a:266:G:H3'     | 48:2q:67:LYS:HB2   | 1.91                     | 0.52              |
| 32:2a:1513:A:H2'    | 32:2a:1514:C:C6    | 2.44                     | 0.52              |
| 36:2e:78:HIS:HA     | 39:2h:105:ARG:HG3  | 1.91                     | 0.52              |
| 14:1S:52:SER:HB2    | 14:1S:55:ALA:H     | 1.73                     | 0.52              |
| 32:1a:1036:G:H5''   | 32:1a:1037:C:C5    | 2.44                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:2A:1960:A:OP2    | 60:2A:3904:HOH:O   | 2.19                     | 0.52              |
| 1:2A:2092:U:OP1    | 60:2A:3905:HOH:O   | 2.19                     | 0.52              |
| 9:2N:12:ARG:HH22   | 9:2N:138:LEU:HD11  | 1.74                     | 0.52              |
| 19:2X:57:LEU:HD21  | 19:2X:78:LYS:HE2   | 1.90                     | 0.52              |
| 34:2c:6:HIS:HD2    | 34:2c:8:ILE:H      | 1.57                     | 0.52              |
| 1:1A:1176:G:H1'    | 1:1A:1177:A:C5'    | 2.38                     | 0.52              |
| 1:1A:2747:G:O6     | 1:1A:2755:C:H5''   | 2.10                     | 0.52              |
| 4:1E:47:VAL:HG12   | 4:1E:49:LEU:HD13   | 1.91                     | 0.52              |
| 32:1a:78:G:H1      | 32:1a:91:C:N4      | 2.06                     | 0.52              |
| 33:1b:112:VAL:HG12 | 33:1b:149:LEU:HD13 | 1.90                     | 0.52              |
| 1:2A:414:C:H2'     | 1:2A:415:A:C8      | 2.44                     | 0.52              |
| 1:2A:674:G:H1'     | 5:2F:74:ARG:HD2    | 1.91                     | 0.52              |
| 1:2A:2870:C:H2'    | 1:2A:2871:C:O4'    | 2.09                     | 0.52              |
| 2:2B:17:C:H2'      | 2:2B:18:G:O4'      | 2.09                     | 0.52              |
| 5:2F:60:SER:OG     | 5:2F:61:GLY:N      | 2.42                     | 0.52              |
| 8:2I:85:GLU:HG3    | 8:2I:86:THR:H      | 1.75                     | 0.52              |
| 33:2b:88:ALA:HB1   | 33:2b:90:MET:HG3   | 1.90                     | 0.52              |
| 1:1A:1025:G:C4     | 1:1A:1135:C:H1'    | 2.45                     | 0.52              |
| 1:1A:2130:U:O2'    | 1:1A:2133:G:O2'    | 2.14                     | 0.52              |
| 1:1A:2291:U:OP1    | 1:1A:2380:C:O2'    | 2.22                     | 0.52              |
| 32:1a:509:A:N3     | 32:1a:543:C:O2'    | 2.35                     | 0.52              |
| 32:1a:974:A:H8     | 32:1a:974:A:OP1    | 1.92                     | 0.52              |
| 35:1d:187:ARG:NH2  | 35:1d:193:ASP:OD2  | 2.43                     | 0.52              |
| 44:1m:65:LYS:HE2   | 44:1m:69:GLU:HG2   | 1.90                     | 0.52              |
| 1:2A:2360:A:H2'    | 1:2A:2361:A:O4'    | 2.09                     | 0.52              |
| 4:2E:116:VAL:HG13  | 4:2E:122:PHE:HB2   | 1.90                     | 0.52              |
| 32:2a:406:G:H21    | 35:2d:119:GLN:NE2  | 2.08                     | 0.52              |
| 32:2a:429:U:OP1    | 35:2d:13:ARG:NH2   | 2.43                     | 0.52              |
| 33:2b:16:HIS:O     | 33:2b:18:GLY:N     | 2.42                     | 0.52              |
| 33:2b:179:LYS:HA   | 39:2h:72:PRO:HG3   | 1.91                     | 0.52              |
| 39:2h:11:THR:HG22  | 39:2h:15:ASN:HD21  | 1.73                     | 0.52              |
| 7:1H:11:VAL:HG21   | 7:1H:50:VAL:HG23   | 1.89                     | 0.52              |
| 32:1a:1348:U:H2'   | 32:1a:1349:A:C8    | 2.44                     | 0.52              |
| 35:1d:4:TYR:O      | 35:1d:6:GLY:N      | 2.42                     | 0.52              |
| 1:2A:2127:G:H2'    | 1:2A:2128:C:O4'    | 2.10                     | 0.52              |
| 13:2R:87:TYR:OH    | 13:2R:117:VAL:O    | 2.23                     | 0.52              |
| 14:2S:14:VAL:O     | 14:2S:18:ILE:HG12  | 2.10                     | 0.52              |
| 17:2V:29:PRO:HA    | 17:2V:61:VAL:HG23  | 1.91                     | 0.52              |
| 19:2X:1:MET:HE1    | 24:22:26:ARG:HH21  | 1.74                     | 0.52              |
| 21:2Z:28:MET:HE1   | 21:2Z:61:LEU:HD11  | 1.92                     | 0.52              |
| 26:24:59:PHE:HB3   | 26:24:61:ARG:HB3   | 1.90                     | 0.52              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 32:2a:1008:C:H2'  | 32:2a:1009:G:C8    | 2.44                     | 0.52              |
| 32:2a:1071:C:H2'  | 32:2a:1072:G:H8    | 1.73                     | 0.52              |
| 41:2j:6:ILE:HD13  | 41:2j:98:ILE:HG12  | 1.91                     | 0.52              |
| 50:2s:19:VAL:O    | 50:2s:23:ASN:ND2   | 2.42                     | 0.52              |
| 1:1A:1045:A:O2'   | 1:1A:1047:G:C4     | 2.62                     | 0.52              |
| 1:1A:1754:C:H5    | 15:1T:96:ARG:NH2   | 2.08                     | 0.52              |
| 1:1A:2022:U:O2'   | 1:1A:2617:C:H5'    | 2.09                     | 0.52              |
| 1:1A:2749:A:OP1   | 7:1H:3:ARG:NH1     | 2.43                     | 0.52              |
| 10:1O:64:ARG:HB2  | 10:1O:79:PHE:CD2   | 2.45                     | 0.52              |
| 32:1a:41:G:H2'    | 32:1a:42:G:C8      | 2.45                     | 0.52              |
| 32:1a:1240:U:OP1  | 38:1g:119:ARG:NH2  | 2.38                     | 0.52              |
| 35:1d:15:GLU:OE2  | 35:1d:66:ARG:NH1   | 2.42                     | 0.52              |
| 36:1e:8:GLU:OE2   | 36:1e:63:ARG:NH2   | 2.42                     | 0.52              |
| 1:2A:2611:U:C4    | 27:25:3:LYS:HG2    | 2.45                     | 0.52              |
| 1:2A:2803:C:H2'   | 1:2A:2804:C:H6     | 1.75                     | 0.52              |
| 32:2a:1356:G:H2'  | 32:2a:1357:A:C8    | 2.44                     | 0.52              |
| 1:1A:2314:C:H2'   | 1:1A:2315:G:C8     | 2.45                     | 0.52              |
| 1:1A:2690:C:OP1   | 13:1R:17:ARG:NH2   | 2.42                     | 0.52              |
| 5:1F:185:ASP:OD1  | 5:1F:188:ARG:NH1   | 2.42                     | 0.52              |
| 13:1R:98:LEU:HB2  | 13:1R:113:LEU:HD11 | 1.92                     | 0.52              |
| 32:1a:346:G:H3'   | 56:1a:1883:MPD:H51 | 1.90                     | 0.52              |
| 35:1d:180:GLY:O   | 35:1d:182:LYS:NZ   | 2.42                     | 0.52              |
| 1:2A:1309:G:H4'   | 29:27:7:PRO:HB2    | 1.90                     | 0.52              |
| 8:2I:57:ARG:O     | 8:2I:61:ARG:HG2    | 2.10                     | 0.52              |
| 9:2N:39:ARG:HD2   | 60:2N:303:HOH:O    | 2.10                     | 0.52              |
| 35:2d:103:ASN:OD1 | 35:2d:114:ARG:NE   | 2.35                     | 0.52              |
| 40:2i:53:VAL:HG11 | 40:2i:92:TYR:CE1   | 2.45                     | 0.52              |
| 1:1A:236:C:H2'    | 1:1A:237:C:H6      | 1.73                     | 0.52              |
| 1:1A:559:G:H22    | 16:1U:49:HIS:CE1   | 2.28                     | 0.52              |
| 1:1A:1937:A:H1'   | 1:1A:1939:5MU:H72  | 1.92                     | 0.52              |
| 1:1A:2751:G:C4    | 7:1H:2:SER:HA      | 2.45                     | 0.52              |
| 4:1E:54:GLN:OE1   | 4:1E:55:ASN:N      | 2.42                     | 0.52              |
| 16:1U:113:ALA:O   | 16:1U:117:GLN:NE2  | 2.42                     | 0.52              |
| 32:1a:763:G:H2'   | 32:1a:764:C:C6     | 2.45                     | 0.52              |
| 32:1a:1456:G:N1   | 51:1t:51:GLU:OE2   | 2.34                     | 0.52              |
| 1:2A:2647:U:H2'   | 1:2A:2648:C:C6     | 2.45                     | 0.52              |
| 1:2A:2685:G:P     | 15:2T:51:ARG:HH22  | 2.33                     | 0.52              |
| 9:2N:99:LEU:HD22  | 9:2N:103:VAL:HG23  | 1.91                     | 0.52              |
| 32:2a:632:A:H5'   | 32:2a:633:G:OP2    | 2.10                     | 0.52              |
| 32:2a:1286:A:H8   | 32:2a:1287:A:H4'   | 1.75                     | 0.52              |
| 48:2q:4:LYS:H     | 48:2q:61:GLU:HG2   | 1.75                     | 0.52              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:1A:1040:C:H2'   | 1:1A:1041:C:O4'    | 2.10                     | 0.52              |
| 1:2A:2022:U:O2'   | 1:2A:2617:C:H5'    | 2.10                     | 0.52              |
| 2:2B:95:C:H2'     | 2:2B:96:U:C6       | 2.45                     | 0.52              |
| 7:2H:24:VAL:HG21  | 7:2H:72:ILE:HG12   | 1.92                     | 0.52              |
| 17:2V:24:LYS:HA   | 17:2V:92:THR:OG1   | 2.10                     | 0.52              |
| 32:2a:17:U:H2'    | 32:2a:18:C:C6      | 2.45                     | 0.52              |
| 32:2a:1004:A:H2'  | 32:2a:1038:C:H1'   | 1.91                     | 0.52              |
| 32:2a:1372:U:OP1  | 40:2i:72:GLY:N     | 2.42                     | 0.52              |
| 32:2a:1505:G:H4'  | 32:2a:1506:U:H5''  | 1.92                     | 0.52              |
| 36:2e:139:LEU:HA  | 36:2e:142:LEU:HD12 | 1.91                     | 0.52              |
| 38:2g:48:LYS:O    | 38:2g:52:GLU:HG2   | 2.09                     | 0.52              |
| 51:2t:16:HIS:O    | 51:2t:19:SER:OG    | 2.23                     | 0.52              |
| 1:1A:1508:A:H4'   | 1:1A:1509(A):A:C4  | 2.45                     | 0.52              |
| 1:1A:2165:G:H2'   | 1:1A:2166:G:C8     | 2.45                     | 0.52              |
| 1:1A:2445:G:OP1   | 5:1F:74:ARG:NH2    | 2.43                     | 0.52              |
| 17:1V:40:LEU:HB2  | 17:1V:46:VAL:HG13  | 1.91                     | 0.52              |
| 22:10:70:GLN:HG2  | 22:10:72:ARG:HG3   | 1.91                     | 0.52              |
| 47:1p:1:MET:N     | 47:1p:1:MET:HE2    | 2.25                     | 0.52              |
| 1:2A:116:C:H2'    | 1:2A:117:G:O4'     | 2.09                     | 0.52              |
| 1:2A:639:U:H2'    | 1:2A:640:C:C6      | 2.45                     | 0.52              |
| 1:2A:889:C:HO2'   | 1:2A:890:A:H8      | 1.58                     | 0.52              |
| 18:2W:86:LEU:HD22 | 18:2W:96:ILE:HD11  | 1.92                     | 0.52              |
| 33:2b:127:ILE:C   | 33:2b:129:GLU:H    | 2.18                     | 0.52              |
| 42:2k:27:ASN:OD1  | 42:2k:28:THR:N     | 2.41                     | 0.52              |
| 1:1A:1358:G:N1    | 1:1A:1372:U:OP2    | 2.29                     | 0.51              |
| 42:1k:86:GLY:N    | 42:1k:112:THR:OG1  | 2.42                     | 0.51              |
| 50:1s:43:GLU:OE1  | 50:1s:43:GLU:N     | 2.43                     | 0.51              |
| 1:2A:898:C:H2'    | 1:2A:899:A:O4'     | 2.10                     | 0.51              |
| 1:2A:1027:A:C2    | 1:2A:2488:A:H5'    | 2.45                     | 0.51              |
| 5:2F:167:ALA:HB1  | 5:2F:173:VAL:HG11  | 1.92                     | 0.51              |
| 32:2a:224:C:H2'   | 32:2a:225:C:H6     | 1.75                     | 0.51              |
| 35:2d:12:CYS:HB3  | 59:2d:501:SF4:S2   | 2.49                     | 0.51              |
| 1:1A:971:C:OP2    | 60:1A:4185:HOH:O   | 2.19                     | 0.51              |
| 1:1A:2646:C:OP2   | 1:1A:2732:G:O2'    | 2.23                     | 0.51              |
| 32:1a:1162:C:H42  | 32:1a:1174:G:H1    | 1.59                     | 0.51              |
| 38:1g:90:GLU:N    | 38:1g:90:GLU:OE1   | 2.41                     | 0.51              |
| 47:1p:29:ASP:OD1  | 47:1p:29:ASP:N     | 2.43                     | 0.51              |
| 1:2A:330:A:HO2'   | 1:2A:331:A:H8      | 1.52                     | 0.51              |
| 1:2A:1169:G:H1    | 1:2A:1180:C:H42    | 1.58                     | 0.51              |
| 1:2A:2128:C:H3'   | 1:2A:2129:C:H5''   | 1.92                     | 0.51              |
| 1:2A:2657:A:O3'   | 7:2H:160:LYS:NZ    | 2.43                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:2A:2849:U:H4'    | 1:2A:2868:A:C2     | 2.46                     | 0.51              |
| 32:2a:149:A:H2'    | 32:2a:150:C:C6     | 2.45                     | 0.51              |
| 32:2a:176:C:H2'    | 32:2a:177:C:H6     | 1.75                     | 0.51              |
| 32:2a:1004:A:N7    | 32:2a:1037:C:H2'   | 2.25                     | 0.51              |
| 1:1A:492:A:H2'     | 1:1A:493:G:O4'     | 2.10                     | 0.51              |
| 1:1A:1594:G:O6     | 60:1A:4170:HOH:O   | 2.17                     | 0.51              |
| 16:1U:17:ILE:HG23  | 16:1U:39:LEU:HD12  | 1.91                     | 0.51              |
| 44:1m:37:THR:O     | 44:1m:55:ARG:NH1   | 2.24                     | 0.51              |
| 1:2A:240:G:O6      | 60:2A:3906:HOH:O   | 2.19                     | 0.51              |
| 1:2A:581:C:H2'     | 1:2A:582:G:H8      | 1.75                     | 0.51              |
| 1:2A:1651:G:OP1    | 13:2R:40:LYS:NZ    | 2.35                     | 0.51              |
| 1:2A:1657:C:H2'    | 1:2A:1658:C:C6     | 2.45                     | 0.51              |
| 1:2A:1669:A:H5''   | 1:2A:2550:G:OP1    | 2.10                     | 0.51              |
| 6:2G:64:THR:HB     | 6:2G:94:LEU:HD21   | 1.91                     | 0.51              |
| 20:2Y:38:ILE:HD11  | 20:2Y:66:PRO:HG3   | 1.93                     | 0.51              |
| 32:2a:826:C:H4'    | 39:2h:12:ARG:HG2   | 1.93                     | 0.51              |
| 32:2a:974:A:H8     | 32:2a:974:A:OP1    | 1.93                     | 0.51              |
| 32:2a:1009:G:H1    | 32:2a:1020:U:H3    | 1.57                     | 0.51              |
| 40:2i:53:VAL:C     | 40:2i:55:ALA:H     | 2.19                     | 0.51              |
| 40:2i:85:LEU:HB3   | 40:2i:92:TYR:CD2   | 2.45                     | 0.51              |
| 1:1A:2115:G:H2'    | 1:1A:2117:A:H62    | 1.74                     | 0.51              |
| 13:1R:67:LEU:HD13  | 13:1R:76:VAL:HG21  | 1.90                     | 0.51              |
| 22:10:38:VAL:HB    | 22:10:59:LEU:HB2   | 1.92                     | 0.51              |
| 32:1a:79:G:N1      | 32:1a:90:U:N3      | 2.59                     | 0.51              |
| 32:1a:1272:G:H2'   | 32:1a:1273:G:O4'   | 2.11                     | 0.51              |
| 33:1b:138:LEU:O    | 33:1b:142:LEU:N    | 2.43                     | 0.51              |
| 34:1c:36:ASP:N     | 34:1c:36:ASP:OD1   | 2.43                     | 0.51              |
| 45:1n:4:LYS:HA     | 45:1n:7:ILE:HG23   | 1.91                     | 0.51              |
| 1:2A:1324:G:O2'    | 1:2A:1326:U:OP2    | 2.25                     | 0.51              |
| 4:2E:52:LEU:HB3    | 4:2E:53:PRO:HD2    | 1.91                     | 0.51              |
| 32:2a:719:C:O2'    | 49:2r:50:ILE:O     | 2.28                     | 0.51              |
| 32:2a:1362:C:H2'   | 32:2a:1363:C:H5''  | 1.91                     | 0.51              |
| 34:2c:87:LEU:O     | 34:2c:91:LEU:N     | 2.43                     | 0.51              |
| 35:2d:121:VAL:HG22 | 35:2d:126:ILE:HG13 | 1.91                     | 0.51              |
| 48:2q:62:SER:OG    | 48:2q:72:ARG:HG3   | 2.10                     | 0.51              |
| 1:1A:1939:5MU:OP1  | 1:1A:2604:U:O2'    | 2.27                     | 0.51              |
| 5:1F:95:ARG:HD3    | 5:1F:97:TYR:CZ     | 2.46                     | 0.51              |
| 30:18:45:GLY:HA3   | 60:18:222:HOH:O    | 2.10                     | 0.51              |
| 32:1a:269:C:H2'    | 32:1a:270:A:H8     | 1.73                     | 0.51              |
| 32:1a:1292:U:OP2   | 38:1g:41:ARG:NH2   | 2.44                     | 0.51              |
| 37:1f:19:LEU:HD11  | 37:1f:59:TYR:CZ    | 2.46                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 41:1j:39:PRO:HA   | 41:1j:70:ARG:HD3  | 1.91                     | 0.51              |
| 1:2A:644:A:H4'    | 1:2A:645:C:H5     | 1.76                     | 0.51              |
| 1:2A:1778:U:OP2   | 60:2A:3907:HOH:O  | 2.19                     | 0.51              |
| 1:2A:2781:A:H5''  | 1:2A:2782:G:H5'   | 1.93                     | 0.51              |
| 5:2F:178:PRO:HB2  | 5:2F:201:VAL:HG21 | 1.91                     | 0.51              |
| 32:2a:620:C:C2    | 35:2d:135:LEU:HG  | 2.46                     | 0.51              |
| 1:1A:2162:G:H4'   | 1:1A:2172:U:O2'   | 2.09                     | 0.51              |
| 4:1E:14:ILE:HG12  | 4:1E:21:VAL:HG23  | 1.92                     | 0.51              |
| 32:1a:486:U:H2'   | 32:1a:487:A:C8    | 2.43                     | 0.51              |
| 32:1a:596:C:OP2   | 60:1a:1919:HOH:O  | 2.18                     | 0.51              |
| 32:1a:1273:G:H3'  | 32:1a:1274:G:H8   | 1.74                     | 0.51              |
| 33:1b:84:GLU:HG3  | 33:1b:215:LEU:HB3 | 1.93                     | 0.51              |
| 34:1c:18:TRP:H    | 34:1c:18:TRP:HE3  | 1.59                     | 0.51              |
| 47:1p:20:VAL:HG23 | 47:1p:35:LYS:HA   | 1.92                     | 0.51              |
| 53:1y:74:ILE:O    | 53:1y:78:ILE:HG12 | 2.11                     | 0.51              |
| 1:2A:1650:G:O6    | 60:2A:3886:HOH:O  | 2.17                     | 0.51              |
| 11:2P:63:PRO:HG2  | 30:28:25:MET:HB2  | 1.93                     | 0.51              |
| 32:2a:1320:C:H2'  | 32:2a:1321:C:O4'  | 2.11                     | 0.51              |
| 32:1a:1510:U:H2'  | 32:1a:1511:G:C8   | 2.45                     | 0.51              |
| 1:2A:526:A:OP1    | 60:2A:3913:HOH:O  | 2.19                     | 0.51              |
| 1:2A:760:G:H2'    | 1:2A:761:A:O4'    | 2.11                     | 0.51              |
| 1:2A:1588:C:H2'   | 1:2A:1589:C:C6    | 2.46                     | 0.51              |
| 1:2A:1593:G:H2'   | 1:2A:1594:G:C8    | 2.45                     | 0.51              |
| 2:2B:31:C:H4'     | 6:2G:29:TRP:CZ2   | 2.46                     | 0.51              |
| 3:2D:142:VAL:HG23 | 3:2D:193:VAL:HA   | 1.93                     | 0.51              |
| 32:2a:328:C:H4'   | 32:2a:329:A:H5'   | 1.93                     | 0.51              |
| 32:2a:392:G:H2'   | 32:2a:393:A:H8    | 1.74                     | 0.51              |
| 32:2a:627:G:H2'   | 32:2a:628:G:C8    | 2.46                     | 0.51              |
| 32:2a:673:G:O3'   | 37:2f:87:ARG:NH2  | 2.44                     | 0.51              |
| 52:2u:6:ARG:O     | 52:2u:8:THR:N     | 2.42                     | 0.51              |
| 1:1A:185:U:H2'    | 1:1A:186:G:C8     | 2.46                     | 0.51              |
| 12:1Q:137:TYR:O   | 12:1Q:141:GLN:HG2 | 2.11                     | 0.51              |
| 15:1T:100:TYR:O   | 15:1T:103:ARG:HG3 | 2.11                     | 0.51              |
| 32:1a:370:C:H2'   | 32:1a:371:G:C8    | 2.46                     | 0.51              |
| 33:1b:15:VAL:HG12 | 33:1b:16:HIS:HD2  | 1.76                     | 0.51              |
| 50:1s:41:VAL:HG13 | 50:1s:43:GLU:H    | 1.75                     | 0.51              |
| 1:2A:876:C:H2'    | 1:2A:877:U:O4'    | 2.11                     | 0.51              |
| 1:2A:1200:C:H5'   | 60:2A:3860:HOH:O  | 2.10                     | 0.51              |
| 1:2A:1796:U:H2'   | 1:2A:1797:C:C6    | 2.46                     | 0.51              |
| 8:2I:72:LEU:HA    | 8:2I:75:LEU:HB3   | 1.91                     | 0.51              |
| 17:2V:5:VAL:HG12  | 17:2V:37:VAL:HG22 | 1.93                     | 0.51              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 32:2a:1132:C:H2'   | 32:2a:1133:G:H8   | 1.76                     | 0.51              |
| 32:2a:1141:C:H2'   | 32:2a:1142:G:H8   | 1.75                     | 0.51              |
| 32:2a:1200:C:OP1   | 60:2a:3226:HOH:O  | 2.19                     | 0.51              |
| 1:1A:489:G:N7      | 18:1W:49:LYS:NZ   | 2.59                     | 0.51              |
| 1:1A:628:G:H2'     | 1:1A:629:G:C8     | 2.46                     | 0.51              |
| 1:1A:1050:A:H2'    | 1:1A:1051:G:O4'   | 2.11                     | 0.51              |
| 1:1A:1056:G:N1     | 1:1A:1102:C:OP2   | 2.38                     | 0.51              |
| 1:1A:2048:G:O6     | 60:1A:4179:HOH:O  | 2.18                     | 0.51              |
| 6:1G:31:VAL:O      | 60:1G:301:HOH:O   | 2.19                     | 0.51              |
| 35:1d:128:VAL:HG12 | 35:1d:129:ASN:ND2 | 2.25                     | 0.51              |
| 1:2A:817:C:H2'     | 1:2A:818:G:O4'    | 2.11                     | 0.51              |
| 1:2A:1275:A:H4'    | 60:2A:3872:HOH:O  | 2.10                     | 0.51              |
| 1:2A:1754:C:OP1    | 15:2T:96:ARG:NH1  | 2.44                     | 0.51              |
| 1:2A:2114:A:H2'    | 1:2A:2115:G:O4'   | 2.11                     | 0.51              |
| 6:2G:110:ALA:HB1   | 6:2G:140:ILE:HG22 | 1.93                     | 0.51              |
| 12:2Q:57:HIS:NE2   | 12:2Q:116:GLU:HB3 | 2.26                     | 0.51              |
| 32:2a:49:U:OP2     | 60:2a:3224:HOH:O  | 2.17                     | 0.51              |
| 32:2a:273:A:H1'    | 48:2q:16:GLN:HE21 | 1.75                     | 0.51              |
| 32:2a:448:A:P      | 32:2a:485:G:H22   | 2.34                     | 0.51              |
| 33:2b:74:LYS:HB3   | 33:2b:169:LYS:HE3 | 1.92                     | 0.51              |
| 48:2q:41:LYS:HZ1   | 48:2q:92:ARG:HH21 | 1.57                     | 0.51              |
| 4:1E:48:GLN:HE21   | 4:1E:78:LEU:HG    | 1.76                     | 0.51              |
| 32:1a:222:U:H2'    | 32:1a:223:U:C6    | 2.46                     | 0.51              |
| 32:1a:1347:G:N2    | 32:1a:1373:G:H2'  | 2.26                     | 0.51              |
| 32:1a:1513:A:H2'   | 32:1a:1514:C:C6   | 2.46                     | 0.51              |
| 1:2A:1141:U:OP2    | 9:2N:63:THR:OG1   | 2.22                     | 0.51              |
| 1:2A:1653:G:H3'    | 13:2R:2:ARG:HB2   | 1.93                     | 0.51              |
| 1:2A:1815:A:OP2    | 60:2A:3908:HOH:O  | 2.19                     | 0.51              |
| 12:2Q:97:VAL:HG11  | 12:2Q:103:MET:HE3 | 1.93                     | 0.51              |
| 19:2X:11:PRO:HG2   | 19:2X:13:LEU:HD21 | 1.93                     | 0.51              |
| 32:2a:70:G:H1      | 32:2a:99:U:H3     | 1.57                     | 0.51              |
| 32:2a:1030:C:H42   | 32:2a:1031:G:H1   | 1.59                     | 0.51              |
| 1:1A:774:A:N3      | 1:1A:774:A:H2'    | 2.26                     | 0.50              |
| 6:1G:67:LYS:H      | 26:14:6:HIS:CE1   | 2.28                     | 0.50              |
| 9:1N:48:MET:HE3    | 9:1N:48:MET:C     | 2.36                     | 0.50              |
| 23:11:3:LYS:HG3    | 23:11:4:VAL:H     | 1.76                     | 0.50              |
| 26:14:34:GLU:HG2   | 26:14:35:VAL:HG12 | 1.93                     | 0.50              |
| 35:1d:178:VAL:O    | 35:1d:180:GLY:N   | 2.39                     | 0.50              |
| 1:2A:1010:A:OP2    | 60:2A:3916:HOH:O  | 2.20                     | 0.50              |
| 1:2A:1091:G:C2     | 1:2A:1092:C:H5    | 2.28                     | 0.50              |
| 1:2A:1272:A:OP1    | 60:2A:3912:HOH:O  | 2.19                     | 0.50              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 1:2A:1568:G:N7      | 60:2A:4078:HOH:O   | 2.35                     | 0.50              |
| 1:2A:2551:C:OP2     | 60:2A:3909:HOH:O   | 2.19                     | 0.50              |
| 4:2E:143:ASN:HD22   | 4:2E:147:PRO:HD3   | 1.75                     | 0.50              |
| 7:2H:137:ASP:HB3    | 7:2H:140:LYS:HB3   | 1.93                     | 0.50              |
| 11:2P:18:ARG:NH1    | 60:2P:308:HOH:O    | 2.44                     | 0.50              |
| 32:2a:667:G:OP1     | 32:2a:732:C:O2'    | 2.19                     | 0.50              |
| 32:2a:1073:U:H2'    | 32:2a:1074:G:H8    | 1.76                     | 0.50              |
| 32:2a:1203:C:H2'    | 32:2a:1204:A:C8    | 2.46                     | 0.50              |
| 32:2a:1323:G:H2'    | 32:2a:1324:A:C8    | 2.47                     | 0.50              |
| 36:2e:53:LEU:HA     | 36:2e:56:GLN:HB2   | 1.92                     | 0.50              |
| 1:1A:1011:G:OP1     | 16:1U:77:SER:OG    | 2.28                     | 0.50              |
| 9:1N:42:TRP:CH2     | 9:1N:44:PRO:HB3    | 2.47                     | 0.50              |
| 32:1a:376:G:H5''    | 47:1p:5:ARG:HB2    | 1.93                     | 0.50              |
| 32:1a:620:C:C2      | 35:1d:135:LEU:HG   | 2.45                     | 0.50              |
| 47:1p:1:MET:HE3     | 47:1p:3:LYS:HD2    | 1.92                     | 0.50              |
| 1:2A:753:C:H2'      | 1:2A:754:C:H6      | 1.75                     | 0.50              |
| 1:2A:807:U:OP2      | 11:2P:41:ARG:NH2   | 2.44                     | 0.50              |
| 1:2A:1404:C:O2'     | 1:2A:1405:U:H5'    | 2.11                     | 0.50              |
| 1:2A:2115:G:H3'     | 1:2A:2116:G:C5'    | 2.41                     | 0.50              |
| 1:2A:2687:U:H2'     | 1:2A:2688:U:O4'    | 2.11                     | 0.50              |
| 5:2F:21:ALA:CB      | 5:2F:22:ALA:HA     | 2.39                     | 0.50              |
| 8:2I:93:THR:O       | 8:2I:96:ASP:N      | 2.44                     | 0.50              |
| 17:2V:5:VAL:HG11    | 17:2V:57:VAL:HG21  | 1.92                     | 0.50              |
| 19:2X:44:GLU:HG3    | 19:2X:51:VAL:HG23  | 1.93                     | 0.50              |
| 32:2a:41:G:H2'      | 32:2a:42:G:H8      | 1.76                     | 0.50              |
| 35:2d:162:LEU:HD22  | 35:2d:178:VAL:HG13 | 1.93                     | 0.50              |
| 36:2e:10:MET:HB2    | 36:2e:13:ILE:HD11  | 1.93                     | 0.50              |
| 41:2j:40:LEU:HD11   | 41:2j:71:LEU:HD12  | 1.93                     | 0.50              |
| 32:1a:495:A:H4'     | 32:1a:496:A:OP1    | 2.11                     | 0.50              |
| 32:1a:1172:C:H2'    | 32:1a:1173:G:H8    | 1.77                     | 0.50              |
| 42:1k:91:ARG:HG3    | 42:1k:92:GLU:N     | 2.25                     | 0.50              |
| 42:1k:124:LYS:HE3   | 42:1k:125:PHE:CE2  | 2.47                     | 0.50              |
| 1:2A:572:A:OP2      | 17:2V:78:LYS:NZ    | 2.44                     | 0.50              |
| 1:2A:2438:U:O2'     | 1:2A:2440:C:OP1    | 2.26                     | 0.50              |
| 32:2a:489:C:H2'     | 32:2a:490:G:H8     | 1.77                     | 0.50              |
| 32:2a:1030(B):C:H41 | 32:2a:1030(C):G:N2 | 2.06                     | 0.50              |
| 32:2a:1187:G:N2     | 45:2n:60:SER:OG    | 2.31                     | 0.50              |
| 32:2a:1493:A:H5'    | 32:2a:1494:G:OP2   | 2.12                     | 0.50              |
| 34:2c:91:LEU:HD22   | 34:2c:101:LEU:HD22 | 1.92                     | 0.50              |
| 39:2h:121:ASP:N     | 39:2h:121:ASP:OD1  | 2.43                     | 0.50              |
| 47:2p:1:MET:HE2     | 47:2p:1:MET:N      | 2.26                     | 0.50              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:1A:1140:C:OP2   | 9:1N:66:LYS:NZ     | 2.40                     | 0.50              |
| 1:1A:2405:G:O2'   | 1:1A:2411:A:N6     | 2.44                     | 0.50              |
| 11:1P:140:ALA:O   | 25:23:38:GLU:HG2   | 2.12                     | 0.50              |
| 12:1Q:38:GLU:HA   | 12:1Q:99:PRO:HG3   | 1.93                     | 0.50              |
| 24:12:51:ARG:HD3  | 24:12:55:ARG:NH1   | 2.25                     | 0.50              |
| 32:1a:1144:G:N2   | 32:1a:1146:A:H62   | 2.10                     | 0.50              |
| 32:1a:1187:G:H5'  | 40:1i:113:LYS:NZ   | 2.25                     | 0.50              |
| 35:1d:88:VAL:O    | 35:1d:92:VAL:HG23  | 2.12                     | 0.50              |
| 39:1h:41:ARG:HB3  | 39:1h:41:ARG:CZ    | 2.42                     | 0.50              |
| 1:2A:2050:C:H1'   | 4:2E:156:MET:HE2   | 1.93                     | 0.50              |
| 1:2A:2053:G:OP1   | 60:2A:3914:HOH:O   | 2.19                     | 0.50              |
| 3:2D:73:VAL:HG13  | 3:2D:120:GLY:HA3   | 1.92                     | 0.50              |
| 10:2O:35:VAL:HG13 | 10:2O:65:THR:HG23  | 1.94                     | 0.50              |
| 15:2T:120:ARG:HA  | 15:2T:123:GLN:HB2  | 1.92                     | 0.50              |
| 30:28:56:GLU:HA   | 30:28:59:LYS:HB2   | 1.93                     | 0.50              |
| 32:2a:1316:G:H5'' | 45:2n:17:LYS:NZ    | 2.26                     | 0.50              |
| 36:2e:83:GLU:HG2  | 36:2e:88:LYS:HG3   | 1.92                     | 0.50              |
| 44:2m:4:ILE:HG13  | 44:2m:57:ARG:HB2   | 1.94                     | 0.50              |
| 1:1A:1174:A:H1'   | 1:1A:1175:U:O4'    | 2.11                     | 0.50              |
| 12:1Q:57:HIS:CD2  | 12:1Q:117:ALA:HB2  | 2.46                     | 0.50              |
| 16:1U:49:HIS:HA   | 16:1U:52:ARG:HG2   | 1.93                     | 0.50              |
| 21:1Z:53:ILE:HG22 | 21:1Z:71:VAL:HG12  | 1.93                     | 0.50              |
| 21:1Z:63:ASP:O    | 21:1Z:65:GLN:N     | 2.43                     | 0.50              |
| 30:18:15:LYS:HB3  | 56:18:104:MPD:H52  | 1.94                     | 0.50              |
| 1:2A:184:C:H2'    | 1:2A:185:U:C6      | 2.47                     | 0.50              |
| 1:2A:300:A:H1'    | 1:2A:319:C:H1'     | 1.93                     | 0.50              |
| 1:2A:1341:U:OP2   | 1:2A:1394:U:O2'    | 2.23                     | 0.50              |
| 7:2H:98:LEU:HD22  | 7:2H:125:VAL:HG23  | 1.93                     | 0.50              |
| 9:2N:42:TRP:CH2   | 9:2N:44:PRO:HB3    | 2.46                     | 0.50              |
| 13:2R:55:ALA:HB2  | 13:2R:79:LEU:HD13  | 1.93                     | 0.50              |
| 20:2Y:35:TYR:CE2  | 20:2Y:69:ALA:HB3   | 2.46                     | 0.50              |
| 34:2c:6:HIS:CD2   | 34:2c:8:ILE:H      | 2.30                     | 0.50              |
| 1:1A:2137:C:N4    | 1:1A:2154:G:H1     | 2.10                     | 0.50              |
| 3:1D:102:LYS:C    | 3:1D:103:ARG:HG2   | 2.36                     | 0.50              |
| 6:1G:146:TYR:O    | 6:1G:149:VAL:HG12  | 2.11                     | 0.50              |
| 27:15:16:ARG:HG3  | 27:15:17:ASP:N     | 2.27                     | 0.50              |
| 40:1i:9:ARG:HB3   | 40:1i:104:ARG:HH21 | 1.77                     | 0.50              |
| 41:1j:37:PRO:HB3  | 41:1j:72:VAL:HG12  | 1.92                     | 0.50              |
| 1:2A:1084:A:N6    | 1:2A:1086:A:N7     | 2.60                     | 0.50              |
| 1:2A:1269:A:OP1   | 60:2A:3915:HOH:O   | 2.20                     | 0.50              |
| 6:2G:145:THR:HG22 | 6:2G:148:MET:HG2   | 1.94                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 30:28:63:PRO:HG2  | 30:28:64:TYR:CE2  | 2.47                     | 0.50              |
| 32:2a:1014:A:H2   | 32:2a:1219:U:H1'  | 1.75                     | 0.50              |
| 32:2a:1277:C:H4'  | 32:2a:1281:U:H5   | 1.76                     | 0.50              |
| 1:1A:1178:C:H2'   | 1:1A:1179:C:C6    | 2.47                     | 0.50              |
| 5:1F:161:GLU:O    | 5:1F:165:ARG:HG3  | 2.11                     | 0.50              |
| 9:1N:12:ARG:NH1   | 9:1N:50:ASP:OD2   | 2.45                     | 0.50              |
| 12:1Q:135:ASP:N   | 12:1Q:138:ASP:OD2 | 2.42                     | 0.50              |
| 51:1t:83:ARG:HA   | 51:1t:86:ARG:HH11 | 1.76                     | 0.50              |
| 1:2A:511:U:OP2    | 60:2A:3917:HOH:O  | 2.20                     | 0.50              |
| 1:2A:1065:U:H3    | 1:2A:1073:A:N6    | 2.00                     | 0.50              |
| 6:2G:77:ILE:HG22  | 6:2G:80:PHE:H     | 1.77                     | 0.50              |
| 10:2O:98:VAL:HG22 | 10:2O:118:ALA:HA  | 1.94                     | 0.50              |
| 32:2a:176:C:H2'   | 32:2a:177:C:C6    | 2.47                     | 0.50              |
| 37:2f:99:ALA:HB2  | 49:2r:31:LEU:HD11 | 1.92                     | 0.50              |
| 41:2j:32:ALA:HB1  | 41:2j:33:GLN:HA   | 1.93                     | 0.50              |
| 1:1A:548:A:O2'    | 1:1A:549:G:OP1    | 2.27                     | 0.50              |
| 1:1A:1688:U:O2    | 1:1A:1700:A:H5'   | 2.12                     | 0.50              |
| 1:1A:2811:G:N2    | 1:1A:2891:G:H1'   | 2.27                     | 0.50              |
| 4:1E:31:CYS:HB3   | 4:1E:49:LEU:HG    | 1.93                     | 0.50              |
| 5:1F:38:ARG:NH2   | 60:1F:408:HOH:O   | 2.44                     | 0.50              |
| 21:1Z:103:ARG:HD3 | 21:1Z:136:PHE:CG  | 2.47                     | 0.50              |
| 25:13:3:ARG:NH1   | 25:13:60:GLU:OE2  | 2.41                     | 0.50              |
| 32:1a:584:G:H5'   | 48:1q:91:ARG:HH21 | 1.76                     | 0.50              |
| 32:1a:763:G:H2'   | 32:1a:764:C:H6    | 1.75                     | 0.50              |
| 32:1a:1166:G:N2   | 32:1a:1170:A:OP2  | 2.37                     | 0.50              |
| 34:1c:6:HIS:HD2   | 34:1c:8:ILE:H     | 1.59                     | 0.50              |
| 44:1m:32:GLU:HG2  | 44:1m:64:TRP:HZ2  | 1.76                     | 0.50              |
| 1:2A:1096:A:H2'   | 1:2A:1097:U:H6    | 1.76                     | 0.50              |
| 1:2A:2114:A:H3'   | 1:2A:2115:G:H8    | 1.77                     | 0.50              |
| 6:2G:17:PRO:HA    | 6:2G:20:ILE:HD12  | 1.94                     | 0.50              |
| 32:2a:1256:A:N6   | 32:2a:1278:U:H1'  | 2.27                     | 0.50              |
| 39:2h:10:LEU:HD22 | 39:2h:83:ILE:HD11 | 1.92                     | 0.50              |
| 39:2h:81:HIS:N    | 39:2h:138:TRP:O   | 2.42                     | 0.50              |
| 1:1A:330:A:HO2'   | 1:1A:331:A:H8     | 1.54                     | 0.50              |
| 1:1A:878:A:H2'    | 1:1A:879:G:H5'    | 1.94                     | 0.50              |
| 1:1A:1250:G:H5''  | 60:1U:319:HOH:O   | 2.11                     | 0.50              |
| 1:1A:2285:C:OP2   | 28:16:6:ARG:NH1   | 2.45                     | 0.50              |
| 1:1A:2811:G:N7    | 60:1A:4381:HOH:O  | 2.34                     | 0.50              |
| 60:1A:5280:HOH:O  | 4:1E:144:ARG:HD3  | 2.12                     | 0.50              |
| 32:1a:192:U:O2'   | 51:1t:60:GLU:OE1  | 2.23                     | 0.50              |
| 32:1a:743:U:H2'   | 32:1a:744:C:C6    | 2.46                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 32:1a:971:G:H22    | 32:1a:1363(A):A:P  | 2.35                     | 0.50              |
| 32:1a:1409:C:H2'   | 32:1a:1410:G:H8    | 1.76                     | 0.50              |
| 40:1i:17:VAL:HG21  | 40:1i:81:ILE:HG22  | 1.94                     | 0.50              |
| 48:1q:59:ILE:HG22  | 48:1q:73:VAL:HA    | 1.93                     | 0.50              |
| 53:1y:44:GLU:HG3   | 53:1y:46:GLN:H     | 1.77                     | 0.50              |
| 1:2A:842:G:N7      | 60:2A:4081:HOH:O   | 2.35                     | 0.50              |
| 6:2G:101:ILE:HG21  | 26:24:25:TYR:HB2   | 1.93                     | 0.50              |
| 21:2Z:27:VAL:HG23  | 21:2Z:36:LYS:HA    | 1.94                     | 0.50              |
| 32:2a:110:C:H2'    | 32:2a:111:G:O4'    | 2.12                     | 0.50              |
| 32:2a:164:U:H2'    | 32:2a:165:C:C6     | 2.46                     | 0.50              |
| 32:2a:255:G:H2'    | 32:2a:256:U:C6     | 2.47                     | 0.50              |
| 32:2a:474:G:H2'    | 32:2a:475:G:H8     | 1.76                     | 0.50              |
| 48:2q:27:PHE:CZ    | 48:2q:36:ILE:HD11  | 2.47                     | 0.50              |
| 1:1A:307:G:H21     | 1:1A:330:A:N6      | 2.10                     | 0.49              |
| 1:1A:375:C:H2'     | 1:1A:376:C:C6      | 2.47                     | 0.49              |
| 7:1H:97:ARG:NE     | 7:1H:104:GLU:OE2   | 2.42                     | 0.49              |
| 21:1Z:146:ILE:HG12 | 21:1Z:174:VAL:HG12 | 1.93                     | 0.49              |
| 32:1a:1346:A:H5''  | 40:1i:120:ARG:HH12 | 1.76                     | 0.49              |
| 33:1b:15:VAL:HG22  | 33:1b:209:ARG:HD2  | 1.93                     | 0.49              |
| 33:1b:157:ARG:HG2  | 33:1b:158:LEU:H    | 1.77                     | 0.49              |
| 34:1c:6:HIS:HB3    | 45:1n:49:HIS:ND1   | 2.27                     | 0.49              |
| 44:1m:2:ALA:HA     | 44:1m:8:GLU:HB2    | 1.93                     | 0.49              |
| 47:1p:40:ASP:HB3   | 47:1p:48:TRP:HB2   | 1.92                     | 0.49              |
| 1:2A:796:C:H2'     | 1:2A:797:C:C6      | 2.47                     | 0.49              |
| 1:2A:815:C:H2'     | 1:2A:816:C:H6      | 1.77                     | 0.49              |
| 1:2A:2647:U:H2'    | 1:2A:2648:C:H6     | 1.76                     | 0.49              |
| 3:2D:177:LEU:HD12  | 3:2D:181:GLU:HB3   | 1.93                     | 0.49              |
| 7:2H:3:ARG:HH22    | 7:2H:65:HIS:HB3    | 1.76                     | 0.49              |
| 24:22:4:SER:HA     | 24:22:7:ARG:NH1    | 2.27                     | 0.49              |
| 32:2a:1218:C:H2'   | 32:2a:1219:U:C6    | 2.47                     | 0.49              |
| 33:2b:15:VAL:HG23  | 33:2b:16:HIS:HD2   | 1.76                     | 0.49              |
| 33:2b:140:HIS:O    | 33:2b:144:ARG:N    | 2.38                     | 0.49              |
| 34:2c:181:ASN:N    | 34:2c:205:GLY:O    | 2.42                     | 0.49              |
| 47:2p:43:LYS:HG2   | 47:2p:48:TRP:CD2   | 2.47                     | 0.49              |
| 1:1A:71:A:N7       | 19:1X:31:HIS:HE1   | 2.10                     | 0.49              |
| 1:1A:2023:G:H5'    | 1:1A:2617:C:H4'    | 1.94                     | 0.49              |
| 1:1A:2788:C:O2'    | 1:1A:2809:A:N3     | 2.40                     | 0.49              |
| 4:1E:77:ILE:HG21   | 4:1E:195:LEU:HD11  | 1.94                     | 0.49              |
| 11:1P:65:ARG:HD2   | 30:18:25:MET:SD    | 2.52                     | 0.49              |
| 11:1P:106:LEU:HD22 | 11:1P:112:LEU:HG   | 1.94                     | 0.49              |
| 32:1a:92:C:H2'     | 32:1a:93:G:C8      | 2.47                     | 0.49              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:2A:61:G:H5'     | 24:22:50:ILE:HG21  | 1.95                     | 0.49              |
| 1:2A:660:G:O3'    | 5:2F:38:ARG:NH2    | 2.45                     | 0.49              |
| 1:2A:888:C:P      | 44:2m:93:ARG:HD2   | 2.52                     | 0.49              |
| 1:2A:1814:G:OP1   | 60:2A:3895:HOH:O   | 2.18                     | 0.49              |
| 1:2A:2128:C:H5'   | 1:2A:2129:C:OP2    | 2.11                     | 0.49              |
| 4:2E:181:LEU:HD11 | 15:2T:6:LEU:HD23   | 1.94                     | 0.49              |
| 19:2X:88:LYS:HD2  | 19:2X:93:GLU:HG3   | 1.94                     | 0.49              |
| 32:2a:137:C:H2'   | 32:2a:138:G:C8     | 2.47                     | 0.49              |
| 32:2a:811:C:O2'   | 32:2a:901:A:N1     | 2.42                     | 0.49              |
| 32:2a:1062:U:H2'  | 32:2a:1063:C:C6    | 2.47                     | 0.49              |
| 40:2i:26:VAL:HG11 | 40:2i:33:PHE:HD1   | 1.76                     | 0.49              |
| 47:2p:43:LYS:HG2  | 47:2p:48:TRP:CG    | 2.48                     | 0.49              |
| 1:1A:271(H):G:O2' | 1:1A:271(I):G:OP2  | 2.26                     | 0.49              |
| 1:1A:1041:C:H5'   | 1:1A:1042:G:OP2    | 2.12                     | 0.49              |
| 1:1A:2111:C:H42   | 1:1A:2147:G:N2     | 2.11                     | 0.49              |
| 1:1A:2134:A:H62   | 1:1A:2157:G:C4'    | 2.25                     | 0.49              |
| 1:1A:2273:A:H2'   | 1:1A:2274:A:C8     | 2.47                     | 0.49              |
| 1:1A:2365:G:O6    | 30:18:39:LYS:HE3   | 2.11                     | 0.49              |
| 14:1S:78:LEU:HD11 | 14:1S:109:GLY:HA3  | 1.94                     | 0.49              |
| 32:1a:619:U:N3    | 35:1d:134:ASP:OD1  | 2.43                     | 0.49              |
| 42:1k:87:THR:O    | 42:1k:87:THR:OG1   | 2.23                     | 0.49              |
| 1:2A:2557:G:H2'   | 1:2A:2558:C:C6     | 2.47                     | 0.49              |
| 10:2O:65:THR:OG1  | 10:2O:67:LYS:O     | 2.30                     | 0.49              |
| 15:2T:26:ASP:O    | 15:2T:49:VAL:HG22  | 2.13                     | 0.49              |
| 16:2U:75:ASN:OD1  | 16:2U:78:THR:N     | 2.42                     | 0.49              |
| 32:2a:401:C:O2'   | 32:2a:621:A:N3     | 2.41                     | 0.49              |
| 1:1A:2893:G:H4'   | 1:1A:2894:G:O5'    | 2.12                     | 0.49              |
| 18:1W:18:ARG:NH1  | 18:1W:76:VAL:O     | 2.46                     | 0.49              |
| 22:10:25:ARG:HD3  | 22:10:29:GLN:HE21  | 1.78                     | 0.49              |
| 24:12:29:LYS:HG2  | 24:12:57:ILE:HD13  | 1.95                     | 0.49              |
| 32:1a:1030:C:N4   | 32:1a:1032:G:O6    | 2.45                     | 0.49              |
| 34:1c:87:LEU:O    | 34:1c:91:LEU:N     | 2.41                     | 0.49              |
| 1:2A:910:A:C5     | 12:2Q:13:GLN:HG3   | 2.47                     | 0.49              |
| 1:2A:1187:G:N2    | 1:2A:1188:U:O4     | 2.46                     | 0.49              |
| 1:2A:2564:A:C2    | 1:2A:2647:U:H4'    | 2.48                     | 0.49              |
| 1:2A:2823:A:OP1   | 4:2E:113:PHE:HB2   | 2.12                     | 0.49              |
| 2:2B:13:A:N1      | 2:2B:69:G:O2'      | 2.42                     | 0.49              |
| 11:2P:35:HIS:O    | 60:2P:304:HOH:O    | 2.20                     | 0.49              |
| 12:2Q:38:GLU:HG3  | 12:2Q:127:ILE:HG22 | 1.94                     | 0.49              |
| 19:2X:35:THR:HG22 | 19:2X:37:THR:N     | 2.26                     | 0.49              |
| 32:2a:1151:A:HO2' | 32:2a:1152:A:H8    | 1.58                     | 0.49              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 38:2g:132:GLY:O   | 38:2g:136:LYS:HG2  | 2.12                     | 0.49              |
| 1:1A:264:C:O2'    | 1:1A:265:A:H2'     | 2.11                     | 0.49              |
| 1:1A:2277:G:OP2   | 22:10:10:THR:HG21  | 2.13                     | 0.49              |
| 11:1P:91:PHE:HE1  | 11:1P:99:LEU:HD22  | 1.77                     | 0.49              |
| 18:1W:18:ARG:HG3  | 18:1W:76:VAL:HB    | 1.94                     | 0.49              |
| 22:10:40:GLN:OE1  | 22:10:44:ARG:N     | 2.46                     | 0.49              |
| 32:1a:155:C:H2'   | 32:1a:156:G:O4'    | 2.12                     | 0.49              |
| 32:1a:174:C:H2'   | 32:1a:175:C:C6     | 2.48                     | 0.49              |
| 32:1a:347:G:OP2   | 56:1a:1883:MPD:H53 | 2.12                     | 0.49              |
| 32:1a:567:G:N3    | 60:1a:1982:HOH:O   | 2.35                     | 0.49              |
| 32:1a:762:C:H2'   | 32:1a:763:G:H8     | 1.76                     | 0.49              |
| 32:1a:1252:A:H2'  | 32:1a:1253:G:O4'   | 2.12                     | 0.49              |
| 38:1g:76:ARG:HE   | 38:1g:89:MET:HG3   | 1.77                     | 0.49              |
| 1:2A:443:A:H1'    | 1:2A:1201:C:O4'    | 2.12                     | 0.49              |
| 1:2A:614(C):A:C4  | 5:2F:180:GLY:HA2   | 2.48                     | 0.49              |
| 6:2G:107:LEU:HA   | 6:2G:111:LEU:HG    | 1.94                     | 0.49              |
| 6:2G:112:PRO:HG3  | 26:24:43:TYR:HE2   | 1.76                     | 0.49              |
| 7:2H:46:GLU:HB2   | 7:2H:49:VAL:HG12   | 1.95                     | 0.49              |
| 8:2I:96:ASP:N     | 8:2I:96:ASP:OD1    | 2.43                     | 0.49              |
| 12:2Q:29:PHE:O    | 21:2Z:122:ARG:NH2  | 2.45                     | 0.49              |
| 32:2a:769:G:H4'   | 32:2a:1513:A:H4'   | 1.95                     | 0.49              |
| 36:2e:15:ARG:HD2  | 36:2e:26:PHE:CG    | 2.48                     | 0.49              |
| 39:2h:73:ASP:OD1  | 39:2h:75:ARG:HG3   | 2.13                     | 0.49              |
| 44:2m:3:ARG:HB3   | 44:2m:4:ILE:HG22   | 1.94                     | 0.49              |
| 1:1A:279:C:H42    | 1:1A:361:G:H1      | 1.60                     | 0.49              |
| 1:1A:531:C:H4'    | 1:1A:532:A:H5''    | 1.94                     | 0.49              |
| 1:1A:1083:U:H1'   | 1:1A:1086:A:N6     | 2.28                     | 0.49              |
| 1:1A:1086:A:H3'   | 1:1A:1086:A:N3     | 2.27                     | 0.49              |
| 1:1A:1094:U:O2'   | 1:1A:1096:A:N7     | 2.32                     | 0.49              |
| 1:1A:1175:U:O2'   | 1:1A:1176:G:O5'    | 2.22                     | 0.49              |
| 1:1A:2539:C:OP2   | 60:1A:4187:HOH:O   | 2.19                     | 0.49              |
| 3:1D:72:LYS:HB3   | 3:1D:75:ILE:HD12   | 1.94                     | 0.49              |
| 21:1Z:145:GLU:O   | 21:1Z:148:ASP:N    | 2.38                     | 0.49              |
| 30:18:47:LYS:NZ   | 56:18:104:MPD:H51  | 2.27                     | 0.49              |
| 39:1h:29:SER:HB3  | 39:1h:32:LYS:HG3   | 1.93                     | 0.49              |
| 1:2A:1518:U:H2'   | 1:2A:1519:G:O4'    | 2.12                     | 0.49              |
| 1:2A:2543:G:H2'   | 1:2A:2544:G:C8     | 2.47                     | 0.49              |
| 17:2V:57:VAL:HG12 | 17:2V:99:ILE:HG23  | 1.94                     | 0.49              |
| 25:23:3:ARG:HD2   | 25:23:36:VAL:HG12  | 1.93                     | 0.49              |
| 30:28:34:TRP:CG   | 30:28:35:GLN:N     | 2.81                     | 0.49              |
| 37:2f:91:VAL:HG11 | 49:2r:72:ARG:NH1   | 2.27                     | 0.49              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:1A:247:G:H4'    | 1:1A:386:G:C5      | 2.47                     | 0.49              |
| 1:1A:1193:G:OP1   | 11:1P:14:LYS:NZ    | 2.39                     | 0.49              |
| 10:1O:102:VAL:HB  | 10:1O:106:LEU:HD12 | 1.95                     | 0.49              |
| 21:1Z:70:LEU:HG   | 21:1Z:91:LEU:HD21  | 1.94                     | 0.49              |
| 32:1a:141:A:H2'   | 32:1a:142:G:H8     | 1.77                     | 0.49              |
| 32:1a:162:A:H3'   | 32:1a:163:C:O4'    | 2.13                     | 0.49              |
| 32:1a:431:A:H2'   | 32:1a:432:A:O4'    | 2.12                     | 0.49              |
| 32:1a:507:C:OP2   | 32:1a:508:C:O2'    | 2.28                     | 0.49              |
| 32:1a:1080:A:H5'  | 36:1e:14:ARG:HH21  | 1.76                     | 0.49              |
| 38:1g:113:GLU:HG2 | 38:1g:119:ARG:HG2  | 1.94                     | 0.49              |
| 1:2A:1802:A:N1    | 1:2A:1822:G:H1'    | 2.27                     | 0.49              |
| 3:2D:171:ASP:OD1  | 3:2D:171:ASP:N     | 2.46                     | 0.49              |
| 6:2G:15:VAL:HG22  | 6:2G:175:LEU:HB3   | 1.94                     | 0.49              |
| 32:2a:134:A:H61   | 47:2p:25:ARG:NH2   | 2.02                     | 0.49              |
| 32:2a:481:G:O2'   | 32:2a:483:C:N4     | 2.39                     | 0.49              |
| 32:2a:1239:A:H4'  | 32:2a:1240:U:H5''  | 1.94                     | 0.49              |
| 33:2b:17:PHE:HD1  | 33:2b:18:GLY:H     | 1.59                     | 0.49              |
| 33:2b:121:LEU:HG  | 33:2b:127:ILE:HG23 | 1.94                     | 0.49              |
| 40:2i:116:LYS:HD2 | 40:2i:122:ALA:HA   | 1.95                     | 0.49              |
| 41:2j:33:GLN:HB2  | 41:2j:75:ILE:H     | 1.76                     | 0.49              |
| 45:2n:29:ARG:HB3  | 45:2n:40:CYS:HB3   | 1.95                     | 0.49              |
| 1:1A:1002:G:H2'   | 1:1A:1003:G:O4'    | 2.12                     | 0.49              |
| 6:1G:33:ARG:NH1   | 60:1G:301:HOH:O    | 2.45                     | 0.49              |
| 32:1a:919:A:O2'   | 32:1a:1080:A:N1    | 2.43                     | 0.49              |
| 32:1a:1348:U:H2'  | 32:1a:1349:A:H8    | 1.78                     | 0.49              |
| 36:1e:90:VAL:O    | 36:1e:120:THR:HA   | 2.13                     | 0.49              |
| 1:2A:296:C:H2'    | 1:2A:297:C:H6      | 1.78                     | 0.49              |
| 1:2A:2168:G:H1'   | 1:2A:2170:A:N7     | 2.28                     | 0.49              |
| 10:2O:68:GLU:OE1  | 10:2O:78:ARG:NH1   | 2.45                     | 0.49              |
| 23:21:49:VAL:HG11 | 23:21:70:VAL:HG11  | 1.95                     | 0.49              |
| 28:26:6:ARG:NE    | 28:26:24:GLU:OE2   | 2.37                     | 0.49              |
| 37:2f:70:ASP:OD1  | 37:2f:70:ASP:N     | 2.41                     | 0.49              |
| 1:1A:2127:G:N2    | 1:1A:2173:A:H1'    | 2.16                     | 0.49              |
| 5:1F:32:LEU:HD11  | 5:1F:105:VAL:HG13  | 1.94                     | 0.49              |
| 32:1a:769:G:H4'   | 32:1a:1513:A:H4'   | 1.93                     | 0.49              |
| 33:1b:97:TRP:HZ2  | 33:1b:102:LEU:HD13 | 1.77                     | 0.49              |
| 36:1e:7:GLU:OE1   | 36:1e:37:ARG:NH2   | 2.35                     | 0.49              |
| 42:1k:124:LYS:HE3 | 42:1k:125:PHE:CZ   | 2.48                     | 0.49              |
| 43:1l:103:GLY:O   | 60:1l:301:HOH:O    | 2.20                     | 0.49              |
| 1:2A:324:A:N6     | 1:2A:338:G:O2'     | 2.44                     | 0.49              |
| 1:2A:2805:G:H2'   | 1:2A:2807:G:H8     | 1.75                     | 0.49              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 32:2a:399:G:H2'    | 32:2a:400:C:C6    | 2.47                     | 0.49              |
| 33:2b:116:GLU:HA   | 33:2b:119:GLU:HB2 | 1.95                     | 0.49              |
| 33:2b:187:LEU:HA   | 33:2b:201:ILE:HB  | 1.95                     | 0.49              |
| 43:2l:117:ARG:NH2  | 43:2l:124:LYS:HD2 | 2.28                     | 0.49              |
| 44:2m:15:VAL:HG13  | 44:2m:43:THR:O    | 2.13                     | 0.49              |
| 1:1A:1877:A:H5'    | 1:1A:1878:G:OP2   | 2.13                     | 0.49              |
| 1:1A:2224:G:H4'    | 1:1A:2226:C:C2    | 2.47                     | 0.49              |
| 1:1A:2356:C:O3'    | 22:10:20:ARG:HD3  | 2.13                     | 0.49              |
| 4:1E:144:ARG:HB3   | 4:1E:145:LYS:H    | 1.44                     | 0.49              |
| 21:1Z:63:ASP:C     | 21:1Z:65:GLN:H    | 2.19                     | 0.49              |
| 32:1a:836:G:OP1    | 49:1r:61:LYS:NZ   | 2.34                     | 0.49              |
| 32:1a:1318:A:H1'   | 50:1s:37:ARG:HH21 | 1.76                     | 0.49              |
| 50:1s:12:ASP:C     | 50:1s:14:HIS:H    | 2.21                     | 0.49              |
| 1:2A:1048:A:N6     | 1:2A:1111:A:H1'   | 2.28                     | 0.49              |
| 1:2A:2573:C:OP1    | 1:2A:2574:G:H5''  | 2.13                     | 0.49              |
| 2:2B:77:U:OP1      | 21:2Z:19:ARG:NH2  | 2.46                     | 0.49              |
| 11:2P:89:ALA:O     | 11:2P:121:LYS:NZ  | 2.32                     | 0.49              |
| 20:2Y:13:VAL:HG12  | 20:2Y:74:PRO:HA   | 1.95                     | 0.49              |
| 22:20:36:ILE:N     | 60:20:202:HOH:O   | 2.45                     | 0.49              |
| 32:2a:600:C:H2'    | 32:2a:601:C:C6    | 2.47                     | 0.49              |
| 33:2b:178:ARG:NH2  | 39:2h:74:PRO:HB3  | 2.27                     | 0.49              |
| 40:2i:9:ARG:O      | 40:2i:104:ARG:NE  | 2.40                     | 0.49              |
| 40:2i:108:VAL:HG12 | 40:2i:109:VAL:H   | 1.77                     | 0.49              |
| 40:2i:111:ARG:HG3  | 45:2n:61:TRP:HE1  | 1.78                     | 0.49              |
| 47:2p:58:TYR:O     | 47:2p:61:SER:OG   | 2.27                     | 0.49              |
| 1:1A:251:A:C5      | 1:1A:252:G:H1'    | 2.48                     | 0.48              |
| 1:1A:455:C:N3      | 1:1A:472:A:H2'    | 2.27                     | 0.48              |
| 1:1A:1579:A:H2'    | 1:1A:1580:A:C8    | 2.48                     | 0.48              |
| 1:1A:1790:C:H5''   | 1:1A:1791:A:OP1   | 2.13                     | 0.48              |
| 32:1a:559:A:OP1    | 36:1e:126:ARG:NH2 | 2.46                     | 0.48              |
| 32:1a:881:G:P      | 43:1l:12:ARG:HH22 | 2.36                     | 0.48              |
| 32:1a:1356:G:H2'   | 32:1a:1357:A:H8   | 1.77                     | 0.48              |
| 32:1a:1443:G:N2    | 32:1a:1460:A:H1'  | 2.28                     | 0.48              |
| 45:1n:23:ARG:NH1   | 45:1n:30:ALA:HB2  | 2.28                     | 0.48              |
| 1:2A:827:U:O2'     | 1:2A:2068:U:C2    | 2.63                     | 0.48              |
| 1:2A:1637:A:H4'    | 1:2A:2711:A:O2'   | 2.13                     | 0.48              |
| 1:2A:1657:C:H2'    | 1:2A:1658:C:H6    | 1.78                     | 0.48              |
| 6:2G:125:PHE:HB3   | 6:2G:166:ASP:OD1  | 2.12                     | 0.48              |
| 16:2U:102:GLU:HG3  | 17:2V:2:PHE:CZ    | 2.47                     | 0.48              |
| 30:28:34:TRP:O     | 60:28:202:HOH:O   | 2.19                     | 0.48              |
| 32:2a:1101:A:H4'   | 32:2a:1102:A:O5'  | 2.13                     | 0.48              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:1A:185:U:H4'    | 1:1A:218:A:H4'     | 1.96                     | 0.48              |
| 1:1A:1047:G:H2'   | 1:1A:1110:G:N2     | 2.28                     | 0.48              |
| 1:1A:1706:U:OP1   | 60:1A:4188:HOH:O   | 2.19                     | 0.48              |
| 3:1D:3:VAL:HG13   | 3:1D:17:THR:HB     | 1.94                     | 0.48              |
| 3:1D:134:ARG:NH1  | 3:1D:188:GLU:OE2   | 2.46                     | 0.48              |
| 4:1E:9:VAL:HG13   | 4:1E:25:VAL:O      | 2.14                     | 0.48              |
| 7:1H:124:GLU:HG3  | 7:1H:132:ARG:HB3   | 1.95                     | 0.48              |
| 8:1I:72:LEU:HD12  | 8:1I:138:ILE:HG21  | 1.96                     | 0.48              |
| 19:1X:32:PRO:HA   | 19:1X:77:LYS:HB2   | 1.95                     | 0.48              |
| 27:15:16:ARG:O    | 27:15:20:ARG:HG3   | 2.13                     | 0.48              |
| 32:1a:1121:U:H2'  | 32:1a:1122:U:H6    | 1.78                     | 0.48              |
| 32:1a:1505:G:OP1  | 60:1a:1905:HOH:O   | 2.20                     | 0.48              |
| 33:1b:86:GLU:C    | 33:1b:89:GLY:H     | 2.21                     | 0.48              |
| 39:1h:20:TYR:HE2  | 39:1h:75:ARG:HD2   | 1.77                     | 0.48              |
| 1:2A:465:G:O6     | 60:2A:3863:HOH:O   | 2.14                     | 0.48              |
| 1:2A:715:G:C2     | 46:2o:56:LEU:HD21  | 2.48                     | 0.48              |
| 1:2A:1081:U:H2'   | 1:2A:1082:U:H5''   | 1.94                     | 0.48              |
| 1:2A:2570:G:O6    | 60:2A:3889:HOH:O   | 2.17                     | 0.48              |
| 2:2B:56:G:H5'     | 6:2G:27:ASN:HD21   | 1.79                     | 0.48              |
| 6:2G:173:LEU:C    | 6:2G:178:PHE:HB2   | 2.37                     | 0.48              |
| 20:2Y:83:THR:OG1  | 20:2Y:84:ARG:N     | 2.46                     | 0.48              |
| 24:22:38:GLN:HB3  | 24:22:44:LEU:HB2   | 1.95                     | 0.48              |
| 46:2o:5:LYS:O     | 46:2o:9:GLN:HG2    | 2.13                     | 0.48              |
| 53:2y:47:GLY:HA2  | 53:2y:68:GLU:HA    | 1.93                     | 0.48              |
| 1:1A:1094:U:H1'   | 1:1A:1097:U:H5     | 1.78                     | 0.48              |
| 1:1A:2681:C:OP2   | 4:1E:109:LYS:NZ    | 2.35                     | 0.48              |
| 3:1D:70:TRP:HB3   | 3:1D:190:TYR:CE2   | 2.48                     | 0.48              |
| 22:10:18:ALA:O    | 22:10:20:ARG:NH1   | 2.46                     | 0.48              |
| 28:16:15:GLU:HG3  | 28:16:47:THR:HG23  | 1.95                     | 0.48              |
| 32:1a:54:C:N4     | 32:1a:353:A:OP2    | 2.43                     | 0.48              |
| 33:1b:75:LYS:HA   | 33:1b:78:GLN:HB2   | 1.95                     | 0.48              |
| 33:1b:84:GLU:HB3  | 33:1b:219:VAL:HG21 | 1.93                     | 0.48              |
| 1:2A:154(A):C:N4  | 1:2A:171:G:H1      | 2.10                     | 0.48              |
| 1:2A:1557:C:H5''  | 1:2A:1558:A:OP2    | 2.12                     | 0.48              |
| 1:2A:2023:G:H5'   | 1:2A:2617:C:H4'    | 1.95                     | 0.48              |
| 1:2A:2695:C:H2'   | 1:2A:2696:U:C6     | 2.49                     | 0.48              |
| 3:2D:132:PRO:HG3  | 3:2D:190:TYR:CE2   | 2.47                     | 0.48              |
| 6:2G:5:VAL:HG12   | 26:24:25:TYR:CE2   | 2.49                     | 0.48              |
| 15:2T:24:PRO:HD3  | 15:2T:52:ILE:HD12  | 1.95                     | 0.48              |
| 32:2a:741:G:H5''  | 46:2o:59:MET:HE1   | 1.96                     | 0.48              |
| 33:2b:87:ARG:HH21 | 33:2b:219:VAL:HB   | 1.79                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 39:2h:121:ASP:HB2  | 39:2h:125:ARG:NH2  | 2.28                     | 0.48              |
| 1:1A:2881:C:H2'    | 1:1A:2882:A:O4'    | 2.13                     | 0.48              |
| 4:1E:51:PHE:CD2    | 4:1E:52:LEU:HG     | 2.47                     | 0.48              |
| 10:1O:116:SER:O    | 56:1a:1883:MPD:H11 | 2.14                     | 0.48              |
| 32:1a:738:C:H2'    | 32:1a:739:C:C6     | 2.48                     | 0.48              |
| 32:1a:1014:A:C2    | 32:1a:1219:U:H1'   | 2.48                     | 0.48              |
| 32:1a:1036:G:H5''  | 32:1a:1037:C:H5    | 1.78                     | 0.48              |
| 39:1h:34:GLU:OE1   | 39:1h:37:ARG:NH2   | 2.36                     | 0.48              |
| 1:2A:387:U:OP1     | 60:2A:3911:HOH:O   | 2.19                     | 0.48              |
| 1:2A:1485:G:H2'    | 1:2A:1486:A:H8     | 1.79                     | 0.48              |
| 1:2A:1628:G:N7     | 60:2A:4086:HOH:O   | 2.35                     | 0.48              |
| 14:2S:61:ASN:O     | 14:2S:63:THR:N     | 2.47                     | 0.48              |
| 32:2a:1084:G:H5'   | 32:2a:1102:A:OP2   | 2.13                     | 0.48              |
| 32:2a:1187:G:H4'   | 40:2i:111:ARG:HH11 | 1.77                     | 0.48              |
| 32:2a:1258:G:H2'   | 32:2a:1259:C:H6    | 1.78                     | 0.48              |
| 32:2a:1264:C:H2'   | 32:2a:1265:G:C8    | 2.49                     | 0.48              |
| 41:2j:62:HIS:HB3   | 45:2n:59:ALA:HB3   | 1.94                     | 0.48              |
| 53:2y:64:SER:HA    | 53:2y:77:LEU:HD13  | 1.96                     | 0.48              |
| 53:2y:74:ILE:O     | 53:2y:78:ILE:HG12  | 2.13                     | 0.48              |
| 1:1A:1138:G:C2     | 9:1N:106:MET:HE2   | 2.48                     | 0.48              |
| 1:1A:1266:G:O5'    | 18:1W:15:ARG:NH2   | 2.47                     | 0.48              |
| 1:1A:2114:A:H3'    | 1:1A:2115:G:H8     | 1.78                     | 0.48              |
| 1:1A:2512:C:H2'    | 1:1A:2513:G:O4'    | 2.14                     | 0.48              |
| 8:1I:10:GLU:OE1    | 8:1I:10:GLU:N      | 2.45                     | 0.48              |
| 32:1a:826:C:H2'    | 32:1a:827:U:H6     | 1.78                     | 0.48              |
| 32:1a:1002:G:H1    | 32:1a:1038:C:N4    | 2.12                     | 0.48              |
| 32:1a:1190:G:H4'   | 34:1c:176:HIS:CE1  | 2.48                     | 0.48              |
| 32:1a:1287:A:H2    | 32:1a:1353:G:N3    | 2.10                     | 0.48              |
| 37:1f:19:LEU:O     | 37:1f:23:LYS:HG3   | 2.13                     | 0.48              |
| 1:2A:1462:C:H4'    | 1:2A:2703:C:H5'    | 1.94                     | 0.48              |
| 21:2Z:102:LEU:HD21 | 21:2Z:155:LEU:HD21 | 1.95                     | 0.48              |
| 21:2Z:182:LYS:HD2  | 60:2Z:302:HOH:O    | 2.13                     | 0.48              |
| 22:20:63:VAL:HG21  | 22:20:83:PRO:HG3   | 1.95                     | 0.48              |
| 50:2s:66:MET:HB2   | 50:2s:74:PHE:CZ    | 2.48                     | 0.48              |
| 1:1A:2147:G:H2'    | 1:1A:2148:G:O4'    | 2.13                     | 0.48              |
| 5:1F:160:ASN:ND2   | 5:1F:163:VAL:HG23  | 2.27                     | 0.48              |
| 18:1W:15:ARG:NH1   | 60:1W:310:HOH:O    | 2.47                     | 0.48              |
| 26:14:56:VAL:O     | 26:14:60:GLN:HB2   | 2.14                     | 0.48              |
| 32:1a:509:A:H5''   | 35:1d:55:ALA:HB2   | 1.95                     | 0.48              |
| 32:1a:685:G:O2'    | 32:1a:686:U:H5'    | 2.14                     | 0.48              |
| 32:1a:738:C:H2'    | 32:1a:739:C:H6     | 1.79                     | 0.48              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 32:1a:1292:U:H2'  | 32:1a:1293:G:C8    | 2.48                     | 0.48              |
| 33:1b:211:ILE:O   | 33:1b:215:LEU:HB2  | 2.14                     | 0.48              |
| 42:1k:92:GLU:O    | 42:1k:96:ARG:HG3   | 2.13                     | 0.48              |
| 51:1t:15:ARG:HA   | 51:1t:18:GLN:HG3   | 1.96                     | 0.48              |
| 51:1t:36:LEU:HD13 | 51:1t:58:LYS:HG3   | 1.95                     | 0.48              |
| 1:2A:2321:G:O2'   | 1:2A:2322:A:OP1    | 2.27                     | 0.48              |
| 7:2H:17:VAL:HG22  | 7:2H:26:VAL:HG22   | 1.96                     | 0.48              |
| 10:2O:2:ILE:HD12  | 10:2O:6:THR:HG21   | 1.96                     | 0.48              |
| 32:2a:999:C:N3    | 32:2a:1042:G:N2    | 2.57                     | 0.48              |
| 32:2a:1288:A:N1   | 32:2a:1371:G:H1'   | 2.28                     | 0.48              |
| 33:2b:82:ARG:HG3  | 33:2b:92:TYR:CZ    | 2.49                     | 0.48              |
| 36:2e:72:GLN:O    | 36:2e:75:THR:HG22  | 2.14                     | 0.48              |
| 46:2o:39:LEU:HD13 | 46:2o:56:LEU:HB2   | 1.95                     | 0.48              |
| 49:2r:31:LEU:HD13 | 49:2r:62:GLU:HB2   | 1.95                     | 0.48              |
| 1:1A:2065:C:H2'   | 1:1A:2066:C:H6     | 1.79                     | 0.48              |
| 6:1G:11:TYR:HA    | 6:1G:15:VAL:HB     | 1.95                     | 0.48              |
| 17:1V:21:ARG:HD3  | 17:1V:91:TYR:CE1   | 2.48                     | 0.48              |
| 19:1X:25:LYS:HA   | 19:1X:81:VAL:O     | 2.14                     | 0.48              |
| 32:1a:148:G:H2'   | 32:1a:149:A:C8     | 2.49                     | 0.48              |
| 32:1a:1090:U:H2'  | 32:1a:1091:U:C6    | 2.49                     | 0.48              |
| 33:1b:218:ALA:O   | 33:1b:222:ILE:HG13 | 2.12                     | 0.48              |
| 1:2A:815:C:H2'    | 1:2A:816:C:C6      | 2.49                     | 0.48              |
| 1:2A:2183:C:H2'   | 1:2A:2184:G:C8     | 2.48                     | 0.48              |
| 1:2A:2818:G:OP2   | 13:2R:42:LYS:NZ    | 2.47                     | 0.48              |
| 3:2D:275:LYS:HE3  | 3:2D:276:LYS:HA    | 1.96                     | 0.48              |
| 32:2a:1259:C:C4   | 32:2a:1260:C:H1'   | 2.49                     | 0.48              |
| 1:1A:858:U:O2     | 1:1A:2268:A:H2'    | 2.14                     | 0.48              |
| 1:1A:1231:G:H2'   | 1:1A:1232:G:C8     | 2.48                     | 0.48              |
| 1:1A:1486:A:H2'   | 1:1A:1487:G:C8     | 2.47                     | 0.48              |
| 1:1A:2721:A:H5''  | 60:1A:4331:HOH:O   | 2.13                     | 0.48              |
| 8:1I:72:LEU:O     | 8:1I:74:ASN:N      | 2.47                     | 0.48              |
| 19:1X:60:ARG:NH1  | 29:17:47:ARG:HH22  | 2.12                     | 0.48              |
| 32:1a:352:C:O2'   | 32:1a:354:G:OP1    | 2.30                     | 0.48              |
| 32:1a:674:G:H2'   | 32:1a:675:A:C8     | 2.48                     | 0.48              |
| 36:1e:103:GLY:O   | 36:1e:107:ARG:HB3  | 2.14                     | 0.48              |
| 1:2A:69:C:O2      | 1:2A:73:A:O2'      | 2.29                     | 0.48              |
| 1:2A:1278:A:OP1   | 13:2R:36:THR:HG23  | 2.13                     | 0.48              |
| 1:2A:1839:G:C8    | 1:2A:1927:A:H1'    | 2.49                     | 0.48              |
| 1:2A:2748:A:N3    | 7:2H:63:SER:OG     | 2.46                     | 0.48              |
| 9:2N:91:LEU:HD23  | 9:2N:91:LEU:HA     | 1.73                     | 0.48              |
| 14:2S:36:TYR:N    | 14:2S:36:TYR:CD1   | 2.82                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 18:2W:88:ARG:O    | 60:2W:303:HOH:O   | 2.20                     | 0.48              |
| 32:2a:1246:C:H2'  | 32:2a:1247:U:H6   | 1.78                     | 0.48              |
| 33:2b:204:ASN:O   | 33:2b:210:SER:OG  | 2.20                     | 0.48              |
| 37:2f:10:LEU:HD13 | 37:2f:61:LEU:HD13 | 1.96                     | 0.48              |
| 1:1A:1778:U:OP2   | 60:1A:4194:HOH:O  | 2.20                     | 0.48              |
| 8:1I:132:PRO:HD2  | 8:1I:136:VAL:O    | 2.13                     | 0.48              |
| 32:1a:920:U:H2'   | 32:1a:921:U:C6    | 2.49                     | 0.48              |
| 32:1a:950:U:OP2   | 44:1m:102:ARG:HD2 | 2.14                     | 0.48              |
| 35:1d:53:ASP:HB3  | 35:1d:57:ARG:NH1  | 2.27                     | 0.48              |
| 35:1d:98:GLU:OE1  | 35:1d:103:ASN:ND2 | 2.36                     | 0.48              |
| 35:1d:104:VAL:HA  | 35:1d:107:ARG:HB2 | 1.96                     | 0.48              |
| 53:1y:55:ASN:OD1  | 53:1y:60:VAL:HG12 | 2.14                     | 0.48              |
| 1:2A:1810:A:H2'   | 1:2A:1811:G:O4'   | 2.14                     | 0.48              |
| 1:2A:2130:U:H2'   | 1:2A:2158:A:N6    | 2.18                     | 0.48              |
| 32:2a:255:G:H2'   | 32:2a:256:U:H6    | 1.79                     | 0.48              |
| 32:2a:514:C:H2'   | 32:2a:515:G:H8    | 1.78                     | 0.48              |
| 32:2a:542:G:P     | 35:2d:10:ARG:HH22 | 2.37                     | 0.48              |
| 32:2a:863:U:O2'   | 32:2a:865:A:N7    | 2.31                     | 0.48              |
| 34:2c:117:ALA:HB2 | 34:2c:200:ALA:HB2 | 1.95                     | 0.48              |
| 35:2d:72:GLU:OE2  | 35:2d:207:TYR:OH  | 2.29                     | 0.48              |
| 44:2m:17:VAL:O    | 44:2m:20:THR:OG1  | 2.31                     | 0.48              |
| 1:1A:642:G:N2     | 1:1A:645:C:OP2    | 2.43                     | 0.48              |
| 1:1A:868:U:C4     | 1:1A:869:G:N7     | 2.81                     | 0.48              |
| 1:1A:1296:G:OP1   | 1:1A:2709:G:O2'   | 2.26                     | 0.48              |
| 1:1A:2693:A:H2'   | 1:1A:2694:G:C8    | 2.48                     | 0.48              |
| 4:1E:12:THR:HG21  | 15:1T:11:GLU:OE2  | 2.14                     | 0.48              |
| 7:1H:41:MET:HE2   | 7:1H:65:HIS:HA    | 1.95                     | 0.48              |
| 12:1Q:103:MET:HE2 | 12:1Q:104:PHE:HE2 | 1.79                     | 0.48              |
| 20:1Y:35:TYR:CE2  | 20:1Y:69:ALA:HB3  | 2.49                     | 0.48              |
| 28:16:14:THR:HG21 | 28:16:48:VAL:HG13 | 1.96                     | 0.48              |
| 32:1a:458:C:H2'   | 32:1a:460:G:O4'   | 2.14                     | 0.48              |
| 32:1a:911:U:H2'   | 32:1a:912:C:C6    | 2.49                     | 0.48              |
| 32:1a:1346:A:O3'  | 32:1a:1347:G:H4'  | 2.14                     | 0.48              |
| 48:1q:81:ARG:HD2  | 48:1q:83:ASP:OD1  | 2.14                     | 0.48              |
| 1:2A:236:C:H2'    | 1:2A:237:C:H6     | 1.78                     | 0.48              |
| 1:2A:1579:A:H2'   | 1:2A:1580:A:C8    | 2.48                     | 0.48              |
| 1:2A:1805:U:O2    | 3:2D:50:THR:HB    | 2.14                     | 0.48              |
| 1:2A:1849:G:H2'   | 1:2A:1850:G:H8    | 1.79                     | 0.48              |
| 2:2B:55:U:OP2     | 60:2B:307:HOH:O   | 2.20                     | 0.48              |
| 3:2D:108:PRO:HB3  | 3:2D:143:HIS:CE1  | 2.49                     | 0.48              |
| 4:2E:48:GLN:HB2   | 4:2E:80:GLU:HG3   | 1.95                     | 0.48              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 4:2E:50:GLY:O     | 4:2E:51:PHE:HB2    | 2.13                     | 0.48              |
| 4:2E:96:PHE:O     | 4:2E:175:VAL:HG11  | 2.14                     | 0.48              |
| 12:2Q:75:THR:HG21 | 12:2Q:87:LYS:NZ    | 2.29                     | 0.48              |
| 24:22:32:LEU:HD11 | 24:22:54:LYS:HG2   | 1.95                     | 0.48              |
| 32:2a:991:U:N3    | 32:2a:1212:U:O4'   | 2.47                     | 0.48              |
| 36:2e:43:LEU:O    | 36:2e:65:ASN:ND2   | 2.41                     | 0.48              |
| 40:2i:105:ASP:HB2 | 40:2i:107:ARG:HG3  | 1.95                     | 0.48              |
| 46:2o:6:GLU:OE1   | 46:2o:6:GLU:N      | 2.41                     | 0.48              |
| 50:2s:22:LEU:HD22 | 50:2s:27:GLU:HA    | 1.95                     | 0.48              |
| 1:1A:207:A:H2'    | 1:1A:208:C:O4'     | 2.14                     | 0.47              |
| 1:1A:667:U:O2     | 30:18:2:PRO:HD2    | 2.14                     | 0.47              |
| 1:1A:893:C:H2'    | 1:1A:894:C:C6      | 2.49                     | 0.47              |
| 1:1A:2386:C:H5'   | 60:1A:4460:HOH:O   | 2.13                     | 0.47              |
| 1:1A:2498:C:OP1   | 60:1A:4196:HOH:O   | 2.20                     | 0.47              |
| 1:1A:2611:U:C4    | 27:15:3:LYS:HG2    | 2.48                     | 0.47              |
| 9:1N:33:LEU:HD12  | 9:1N:38:HIS:CE1    | 2.48                     | 0.47              |
| 14:1S:43:GLU:OE2  | 22:10:49:LYS:HE3   | 2.14                     | 0.47              |
| 19:1X:34:ALA:O    | 19:1X:77:LYS:NZ    | 2.47                     | 0.47              |
| 21:1Z:146:ILE:HA  | 21:1Z:147:GLY:HA2  | 1.61                     | 0.47              |
| 32:1a:175:C:H2'   | 32:1a:176:C:C6     | 2.49                     | 0.47              |
| 32:1a:661:G:H1    | 32:1a:744:C:H42    | 1.62                     | 0.47              |
| 32:1a:1145:C:O2'  | 60:1a:1934:HOH:O   | 2.20                     | 0.47              |
| 32:1a:1279:A:H4'  | 32:1a:1281:U:H5    | 1.78                     | 0.47              |
| 37:1f:1:MET:HA    | 37:1f:67:MET:O     | 2.13                     | 0.47              |
| 38:1g:93:PRO:HA   | 38:1g:96:GLN:HB2   | 1.96                     | 0.47              |
| 1:2A:956:G:H2'    | 1:2A:957:A:H2'     | 1.96                     | 0.47              |
| 1:2A:1070:A:H2'   | 1:2A:1071:G:C8     | 2.48                     | 0.47              |
| 1:2A:1523:U:H2'   | 1:2A:1524:G:H8     | 1.79                     | 0.47              |
| 1:2A:2704:C:H2'   | 1:2A:2705:A:O4'    | 2.14                     | 0.47              |
| 1:1A:336:C:HO2'   | 20:1Y:35:TYR:HH    | 1.62                     | 0.47              |
| 1:1A:1709:U:H2'   | 1:1A:1710:C:C6     | 2.49                     | 0.47              |
| 6:1G:125:PHE:HB3  | 6:1G:166:ASP:OD1   | 2.14                     | 0.47              |
| 26:14:69:LYS:HD3  | 50:1s:20:LEU:HD13  | 1.95                     | 0.47              |
| 32:1a:250:A:H4'   | 32:1a:251:G:O5'    | 2.12                     | 0.47              |
| 32:1a:266:G:H2'   | 32:1a:266:G:N3     | 2.30                     | 0.47              |
| 32:1a:383:A:C5    | 32:1a:384:G:H1'    | 2.50                     | 0.47              |
| 33:1b:77:ALA:HA   | 33:1b:80:ILE:HG22  | 1.96                     | 0.47              |
| 35:1d:120:LEU:HB3 | 35:1d:126:ILE:HD11 | 1.96                     | 0.47              |
| 48:1q:45:HIS:HB3  | 48:1q:72:ARG:HB3   | 1.96                     | 0.47              |
| 1:2A:2115:G:H21   | 1:2A:2171:A:H61    | 1.61                     | 0.47              |
| 1:2A:2808:U:H5''  | 1:2A:2891:G:O6     | 2.14                     | 0.47              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 60:2A:5125:HOH:O  | 16:2U:2:PRO:HA     | 2.14                     | 0.47              |
| 2:2B:115:G:H2'    | 2:2B:116:G:O4'     | 2.14                     | 0.47              |
| 6:2G:44:GLY:O     | 6:2G:47:LYS:HE2    | 2.14                     | 0.47              |
| 32:2a:992:U:H5''  | 32:2a:993:G:C8     | 2.49                     | 0.47              |
| 32:2a:1256:A:N6   | 32:2a:1278:U:O2    | 2.48                     | 0.47              |
| 32:2a:1261:A:H5'  | 32:2a:1284:C:OP1   | 2.14                     | 0.47              |
| 33:2b:121:LEU:O   | 33:2b:125:PRO:HD2  | 2.14                     | 0.47              |
| 35:2d:79:PHE:HE1  | 35:2d:204:ILE:HD13 | 1.78                     | 0.47              |
| 41:2j:30:SER:OG   | 41:2j:81:THR:HG22  | 2.13                     | 0.47              |
| 1:1A:1099:G:OP2   | 60:1A:4199:HOH:O   | 2.20                     | 0.47              |
| 1:1A:1768:U:OP1   | 60:1A:4189:HOH:O   | 2.20                     | 0.47              |
| 1:1A:1800:C:H4'   | 60:1A:6402:HOH:O   | 2.13                     | 0.47              |
| 1:1A:2142:C:H2'   | 1:1A:2143:C:C6     | 2.50                     | 0.47              |
| 1:1A:2319:G:H22   | 14:1S:3:ARG:NH1    | 2.12                     | 0.47              |
| 8:1I:85:GLU:HG3   | 8:1I:86:THR:HG23   | 1.96                     | 0.47              |
| 32:1a:339:C:H2'   | 32:1a:340:U:C6     | 2.49                     | 0.47              |
| 32:1a:833:U:H2'   | 32:1a:834:C:C6     | 2.49                     | 0.47              |
| 32:1a:964:A:N3    | 32:1a:969:A:O2'    | 2.44                     | 0.47              |
| 36:1e:91:LEU:HB3  | 36:1e:118:ILE:HD11 | 1.96                     | 0.47              |
| 40:1i:17:VAL:HG11 | 40:1i:80:GLY:C     | 2.38                     | 0.47              |
| 1:2A:2130:U:H3    | 1:2A:2159:G:H1     | 1.61                     | 0.47              |
| 2:2B:103:G:H21    | 21:2Z:73:GLN:HE22  | 1.62                     | 0.47              |
| 4:2E:5:LEU:HD11   | 4:2E:79:ARG:HB2    | 1.96                     | 0.47              |
| 20:2Y:87:LYS:HB3  | 20:2Y:95:LYS:HD2   | 1.95                     | 0.47              |
| 21:2Z:163:LEU:HG  | 21:2Z:165:VAL:HG22 | 1.96                     | 0.47              |
| 32:2a:1123:A:H4'  | 41:2j:37:PRO:HD2   | 1.97                     | 0.47              |
| 42:2k:87:THR:O    | 42:2k:87:THR:OG1   | 2.27                     | 0.47              |
| 47:2p:74:LEU:HG   | 47:2p:79:VAL:HG21  | 1.96                     | 0.47              |
| 1:1A:2207:G:O2'   | 1:1A:2208:A:OP1    | 2.30                     | 0.47              |
| 2:1B:93:G:OP2     | 60:1B:305:HOH:O    | 2.20                     | 0.47              |
| 3:1D:242:ARG:HG3  | 3:1D:242:ARG:NH1   | 2.28                     | 0.47              |
| 8:1I:101:LEU:HD13 | 8:1I:107:VAL:HB    | 1.96                     | 0.47              |
| 18:1W:65:LEU:HD12 | 18:1W:68:ARG:HD2   | 1.97                     | 0.47              |
| 31:19:32:HIS:O    | 31:19:34:GLN:HG3   | 2.14                     | 0.47              |
| 32:1a:346:G:H3'   | 56:1a:1883:MPD:C5  | 2.45                     | 0.47              |
| 32:1a:825:G:O2'   | 39:1h:8:ASP:OD1    | 2.22                     | 0.47              |
| 32:1a:1241:G:H2'  | 32:1a:1242:C:C6    | 2.49                     | 0.47              |
| 34:1c:58:GLU:HB3  | 41:1j:92:THR:HG21  | 1.97                     | 0.47              |
| 35:1d:100:ARG:NH1 | 35:1d:137:SER:OG   | 2.46                     | 0.47              |
| 48:1q:45:HIS:O    | 48:1q:73:VAL:HG23  | 2.14                     | 0.47              |
| 53:1y:52:ALA:HB2  | 53:1y:77:LEU:HD21  | 1.97                     | 0.47              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:2A:263:C:H2'     | 1:2A:264:C:O4'    | 2.14                     | 0.47              |
| 1:2A:483:A:OP1     | 20:2Y:50:ARG:NH1  | 2.48                     | 0.47              |
| 1:2A:752:A:H4'     | 1:2A:753:C:O5'    | 2.14                     | 0.47              |
| 1:2A:1292:U:H2'    | 1:2A:1293:C:H6    | 1.79                     | 0.47              |
| 1:2A:1566:A:OP1    | 3:2D:211:ARG:NH1  | 2.48                     | 0.47              |
| 1:2A:1996:C:H4'    | 1:2A:1997:G:OP1   | 2.14                     | 0.47              |
| 1:2A:2130:U:H3'    | 1:2A:2130:U:H6    | 1.80                     | 0.47              |
| 11:2P:89:ALA:HA    | 11:2P:121:LYS:HD2 | 1.97                     | 0.47              |
| 18:2W:41:LYS:HE3   | 27:25:25:LEU:HD11 | 1.96                     | 0.47              |
| 32:2a:552:U:H4'    | 43:2l:87:GLY:HA2  | 1.95                     | 0.47              |
| 32:2a:866:C:H4'    | 32:2a:919:A:H5'   | 1.96                     | 0.47              |
| 32:2a:1452:C:H4'   | 32:2a:1457:G:C8   | 2.50                     | 0.47              |
| 45:2n:9:LYS:HA     | 45:2n:12:ARG:HD3  | 1.95                     | 0.47              |
| 1:1A:1932:A:H2'    | 1:1A:1933:G:O4'   | 2.14                     | 0.47              |
| 1:1A:2243:U:H2'    | 1:1A:2244:U:C6    | 2.49                     | 0.47              |
| 1:1A:2334:G:H5'    | 14:1S:9:ARG:HG2   | 1.97                     | 0.47              |
| 3:1D:63:ARG:O      | 60:1D:403:HOH:O   | 2.20                     | 0.47              |
| 5:1F:167:ALA:HB1   | 5:1F:173:VAL:HG11 | 1.95                     | 0.47              |
| 32:1a:1113:C:H42   | 32:1a:1187:G:H1   | 1.62                     | 0.47              |
| 32:1a:1277:C:O2'   | 32:1a:1279:A:H1'  | 2.13                     | 0.47              |
| 33:1b:192:SER:O    | 33:1b:194:PRO:HD3 | 2.14                     | 0.47              |
| 1:2A:784:A:C5      | 3:2D:229:VAL:HG11 | 2.49                     | 0.47              |
| 1:2A:1803:A:O2'    | 3:2D:259:THR:HG21 | 2.13                     | 0.47              |
| 1:2A:2537:U:H2'    | 1:2A:2538:C:C6    | 2.49                     | 0.47              |
| 1:2A:2658:C:H5''   | 7:2H:158:HIS:CD2  | 2.49                     | 0.47              |
| 4:2E:172:VAL:HG13  | 4:2E:182:LEU:HD11 | 1.96                     | 0.47              |
| 5:2F:116:ASP:OD1   | 5:2F:119:ARG:NH2  | 2.47                     | 0.47              |
| 6:2G:114:ILE:HG12  | 6:2G:140:ILE:HD12 | 1.96                     | 0.47              |
| 12:2Q:26:TYR:O     | 60:2Q:301:HOH:O   | 2.20                     | 0.47              |
| 23:21:83:GLU:HA    | 23:21:84:GLY:HA2  | 1.66                     | 0.47              |
| 26:24:57:GLU:HA    | 26:24:58:ARG:HA   | 1.64                     | 0.47              |
| 30:28:29:LYS:HG2   | 30:28:44:LYS:HB3  | 1.96                     | 0.47              |
| 32:2a:141:A:H1'    | 32:2a:182:U:O2    | 2.14                     | 0.47              |
| 32:2a:1034:G:H3'   | 32:2a:1035:A:H8   | 1.80                     | 0.47              |
| 53:2y:67:HIS:HB3   | 53:2y:73:ALA:HB2  | 1.97                     | 0.47              |
| 1:1A:1912:A:O2'    | 32:1a:1494:G:O2'  | 2.32                     | 0.47              |
| 1:1A:2723:C:OP1    | 13:1R:3:HIS:ND1   | 2.48                     | 0.47              |
| 1:1A:2823:A:OP1    | 4:1E:113:PHE:HB2  | 2.14                     | 0.47              |
| 8:1I:29:TYR:C      | 8:1I:32:PRO:HD2   | 2.39                     | 0.47              |
| 12:1Q:109:VAL:HG22 | 12:1Q:113:GLN:CD  | 2.39                     | 0.47              |
| 13:1R:104:ARG:NH2  | 60:1R:303:HOH:O   | 2.42                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 32:1a:41:G:H2'     | 32:1a:42:G:H8      | 1.79                     | 0.47              |
| 32:1a:166:G:H2'    | 32:1a:167:G:C8     | 2.50                     | 0.47              |
| 32:1a:1343:G:H2'   | 32:1a:1344:C:C6    | 2.49                     | 0.47              |
| 33:1b:55:PHE:HB3   | 33:1b:221:LEU:HD12 | 1.97                     | 0.47              |
| 33:1b:124:SER:HA   | 33:1b:125:PRO:HA   | 1.63                     | 0.47              |
| 33:1b:207:ALA:O    | 33:1b:211:ILE:HG13 | 2.14                     | 0.47              |
| 39:1h:86:ILE:HG21  | 39:1h:133:LEU:HD13 | 1.97                     | 0.47              |
| 1:2A:753:C:H2'     | 1:2A:754:C:C6      | 2.49                     | 0.47              |
| 1:2A:1094:U:OP1    | 1:2A:1096:A:N6     | 2.47                     | 0.47              |
| 1:2A:2109:U:H2'    | 1:2A:2110:G:C8     | 2.49                     | 0.47              |
| 1:2A:2113:U:H2'    | 1:2A:2114:A:O4'    | 2.14                     | 0.47              |
| 1:2A:2185:C:N4     | 1:2A:2186:G:O6     | 2.47                     | 0.47              |
| 12:2Q:59:ARG:NH1   | 12:2Q:60:ARG:HE    | 2.13                     | 0.47              |
| 32:2a:316:G:H4'    | 60:2a:3511:HOH:O   | 2.14                     | 0.47              |
| 32:2a:560:U:H4'    | 32:2a:561:U:O5'    | 2.14                     | 0.47              |
| 32:2a:683:G:O6     | 60:2a:3227:HOH:O   | 2.20                     | 0.47              |
| 32:2a:1000:U:H3    | 32:2a:1041:A:N6    | 2.12                     | 0.47              |
| 32:2a:1123:A:O3'   | 41:2j:36:GLY:HA3   | 2.14                     | 0.47              |
| 32:2a:1258:G:H8    | 32:2a:1258:G:OP2   | 1.97                     | 0.47              |
| 34:2c:180:ALA:HA   | 34:2c:206:GLU:HA   | 1.97                     | 0.47              |
| 38:2g:79:ARG:HA    | 38:2g:84:ASN:HA    | 1.96                     | 0.47              |
| 1:1A:744:G:N3      | 60:1A:4407:HOH:O   | 2.36                     | 0.47              |
| 1:1A:807:U:P       | 11:1P:36:LYS:HE2   | 2.55                     | 0.47              |
| 1:1A:1213:A:N3     | 1:1A:1238:G:O2'    | 2.42                     | 0.47              |
| 1:1A:1803:A:O2'    | 3:1D:259:THR:HG21  | 2.15                     | 0.47              |
| 1:1A:1904:G:O2'    | 1:1A:1928:A:N1     | 2.48                     | 0.47              |
| 1:1A:2065:C:H2'    | 1:1A:2066:C:C6     | 2.50                     | 0.47              |
| 1:1A:2189:U:H2'    | 1:1A:2190:G:H8     | 1.79                     | 0.47              |
| 1:1A:2591:C:H2'    | 1:1A:2592:G:C8     | 2.49                     | 0.47              |
| 1:1A:2615:U:OP2    | 60:1A:4195:HOH:O   | 2.20                     | 0.47              |
| 3:1D:71:ASP:HB3    | 3:1D:103:ARG:HH22  | 1.80                     | 0.47              |
| 6:1G:64:THR:HG21   | 6:1G:92:VAL:HG11   | 1.96                     | 0.47              |
| 20:1Y:6:HIS:H      | 20:1Y:6:HIS:CD2    | 2.33                     | 0.47              |
| 26:14:50:VAL:HG21  | 44:1m:64:TRP:C     | 2.39                     | 0.47              |
| 32:1a:45:U:H2'     | 32:1a:46:G:C8      | 2.50                     | 0.47              |
| 32:1a:534:U:O2'    | 60:1a:1938:HOH:O   | 2.21                     | 0.47              |
| 32:1a:936:C:H2'    | 32:1a:937:A:O4'    | 2.14                     | 0.47              |
| 32:1a:1073:U:H2'   | 32:1a:1074:G:C8    | 2.50                     | 0.47              |
| 32:1a:1401:G:C2    | 32:1a:1402:4OC:H1' | 2.50                     | 0.47              |
| 34:1c:138:VAL:HG13 | 34:1c:149:ALA:HB3  | 1.97                     | 0.47              |
| 37:1f:38:GLU:OE1   | 37:1f:64:GLN:NE2   | 2.46                     | 0.47              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 40:1i:89:ASN:O    | 40:1i:92:TYR:HB2   | 2.15                     | 0.47              |
| 43:1l:71:PRO:O    | 43:1l:102:ARG:HD3  | 2.15                     | 0.47              |
| 43:1l:109:GLY:HA3 | 43:1l:121:GLY:O    | 2.15                     | 0.47              |
| 46:1o:56:LEU:O    | 46:1o:60:VAL:HG23  | 2.14                     | 0.47              |
| 48:1q:67:LYS:C    | 48:1q:69:LYS:H     | 2.23                     | 0.47              |
| 52:1u:18:TYR:CE1  | 52:1u:24:ARG:HB3   | 2.50                     | 0.47              |
| 53:1y:85:LEU:O    | 53:1y:89:GLN:HG2   | 2.15                     | 0.47              |
| 1:2A:495:G:N3     | 18:2W:61:ASN:ND2   | 2.63                     | 0.47              |
| 1:2A:577:G:O2'    | 1:2A:1254:A:OP1    | 2.30                     | 0.47              |
| 1:2A:631:A:H2'    | 1:2A:632:A:O4'     | 2.15                     | 0.47              |
| 1:2A:910:A:N3     | 1:2A:2264:C:O2'    | 2.42                     | 0.47              |
| 1:2A:1153:C:OP2   | 60:2A:3918:HOH:O   | 2.20                     | 0.47              |
| 1:2A:1186:G:C2    | 1:2A:1187:G:H1'    | 2.49                     | 0.47              |
| 1:2A:2058:A:N7    | 60:2A:4090:HOH:O   | 2.36                     | 0.47              |
| 1:2A:2184:G:C2    | 1:2A:2185:C:H1'    | 2.50                     | 0.47              |
| 1:2A:2297:C:O2    | 1:2A:2333:A:N6     | 2.39                     | 0.47              |
| 1:2A:2723:C:OP2   | 4:2E:109:LYS:NZ    | 2.48                     | 0.47              |
| 2:2B:56:G:H5'     | 6:2G:27:ASN:ND2    | 2.29                     | 0.47              |
| 3:2D:76:PRO:HB2   | 3:2D:116:GLN:HE21  | 1.79                     | 0.47              |
| 6:2G:46:ALA:O     | 6:2G:51:ARG:HG3    | 2.14                     | 0.47              |
| 7:2H:164:TYR:HB2  | 7:2H:167:GLU:HB2   | 1.96                     | 0.47              |
| 11:2P:121:LYS:HG2 | 11:2P:122:PRO:HD2  | 1.97                     | 0.47              |
| 13:2R:104:ARG:HD2 | 13:2R:107:ASP:OD1  | 2.14                     | 0.47              |
| 19:2X:94:GLY:HA3  | 19:2X:95:LEU:C     | 2.39                     | 0.47              |
| 32:2a:500:G:N2    | 32:2a:546:G:H1'    | 2.30                     | 0.47              |
| 32:2a:1142:G:H2'  | 32:2a:1143:G:O4'   | 2.15                     | 0.47              |
| 33:2b:19:HIS:CG   | 33:2b:20:GLU:H     | 2.33                     | 0.47              |
| 37:2f:6:VAL:HG22  | 37:2f:90:VAL:HG22  | 1.97                     | 0.47              |
| 42:2k:82:VAL:HB   | 42:2k:108:ILE:HG12 | 1.97                     | 0.47              |
| 43:2l:47:LYS:HB2  | 43:2l:47:LYS:HE3   | 1.66                     | 0.47              |
| 49:2r:66:LEU:HG   | 49:2r:70:ILE:HD11  | 1.97                     | 0.47              |
| 50:2s:30:LEU:HD11 | 50:2s:50:ALA:HB2   | 1.96                     | 0.47              |
| 1:1A:1178:C:H2'   | 1:1A:1179:C:H6     | 1.79                     | 0.47              |
| 1:1A:1216:G:P     | 16:1U:12:ARG:HH21  | 2.37                     | 0.47              |
| 1:1A:1771:C:OP1   | 60:1A:4200:HOH:O   | 2.20                     | 0.47              |
| 1:1A:2086:U:H2'   | 1:1A:2087:G:C8     | 2.49                     | 0.47              |
| 1:1A:2121:G:N2    | 60:1A:4634:HOH:O   | 2.48                     | 0.47              |
| 7:1H:72:ILE:O     | 7:1H:76:VAL:HG23   | 2.15                     | 0.47              |
| 14:1S:10:ARG:O    | 14:1S:14:VAL:HG13  | 2.15                     | 0.47              |
| 22:10:43:THR:OG1  | 22:10:46:LYS:HG2   | 2.15                     | 0.47              |
| 26:14:53:GLU:O    | 26:14:56:VAL:HG12  | 2.15                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 32:1a:164:U:H2'    | 32:1a:165:C:C6     | 2.49                     | 0.47              |
| 32:1a:1179:A:O3'   | 40:1i:103:THR:HB   | 2.15                     | 0.47              |
| 33:1b:55:PHE:CD1   | 33:1b:58:ILE:HD12  | 2.49                     | 0.47              |
| 40:1i:116:LYS:HD2  | 40:1i:122:ALA:HA   | 1.97                     | 0.47              |
| 1:2A:1359:A:N3     | 1:2A:1359:A:H5'    | 2.29                     | 0.47              |
| 1:2A:1899:G:H2'    | 1:2A:1899:G:N3     | 2.30                     | 0.47              |
| 1:2A:2079:U:OP1    | 23:21:21:ARG:NH1   | 2.35                     | 0.47              |
| 6:2G:33:ARG:O      | 6:2G:161:THR:HG23  | 2.15                     | 0.47              |
| 7:2H:140:LYS:HB2   | 7:2H:140:LYS:HE3   | 1.78                     | 0.47              |
| 8:2I:14:ASP:O      | 8:2I:17:GLN:HB2    | 2.15                     | 0.47              |
| 21:2Z:182:LYS:O    | 21:2Z:186:GLU:N    | 2.46                     | 0.47              |
| 32:2a:96:U:H2'     | 32:2a:97:G:C8      | 2.49                     | 0.47              |
| 32:2a:950:U:H2'    | 32:2a:951:G:C8     | 2.50                     | 0.47              |
| 35:2d:88:VAL:HG22  | 36:2e:96:PRO:HB2   | 1.97                     | 0.47              |
| 40:2i:32:ASP:N     | 40:2i:35:GLU:OE1   | 2.41                     | 0.47              |
| 42:2k:46:GLY:HA2   | 42:2k:50:TYR:O     | 2.14                     | 0.47              |
| 42:2k:86:GLY:H     | 42:2k:112:THR:HG23 | 1.78                     | 0.47              |
| 1:1A:189:G:O6      | 1:1A:205:G:O2'     | 2.30                     | 0.47              |
| 1:1A:665:C:H2'     | 1:1A:666:G:H8      | 1.79                     | 0.47              |
| 1:1A:993:G:OP1     | 16:1U:50:ARG:NH2   | 2.47                     | 0.47              |
| 3:1D:146:GLU:HB2   | 3:1D:189:CYS:HB3   | 1.97                     | 0.47              |
| 4:1E:73:GLU:H      | 4:1E:73:GLU:CD     | 2.22                     | 0.47              |
| 5:1F:72:ARG:HE     | 5:1F:72:ARG:HB3    | 1.52                     | 0.47              |
| 6:1G:133:LEU:HD11  | 6:1G:157:ILE:HD12  | 1.97                     | 0.47              |
| 35:1d:163:GLU:O    | 35:1d:166:LYS:HG2  | 2.14                     | 0.47              |
| 1:2A:296:C:H2'     | 1:2A:297:C:C6      | 2.50                     | 0.47              |
| 1:2A:2073:C:H5''   | 3:2D:229:VAL:HG12  | 1.96                     | 0.47              |
| 1:2A:2152:G:H2'    | 1:2A:2153:G:H8     | 1.80                     | 0.47              |
| 26:24:40:HIS:O     | 26:24:44:THR:HG22  | 2.15                     | 0.47              |
| 32:2a:67:C:H2'     | 32:2a:68:G:C8      | 2.49                     | 0.47              |
| 32:2a:258:G:H2'    | 32:2a:259:G:C8     | 2.50                     | 0.47              |
| 32:2a:1442:G:H2'   | 32:2a:1442:G:N3    | 2.29                     | 0.47              |
| 40:2i:110:GLU:OE2  | 40:2i:113:LYS:NZ   | 2.47                     | 0.47              |
| 1:1A:385:C:O2      | 11:1P:71:VAL:HG21  | 2.15                     | 0.47              |
| 1:1A:2144:U:H2'    | 1:1A:2147:G:H1     | 1.80                     | 0.47              |
| 1:1A:2820:A:OP2    | 13:1R:2:ARG:NH2    | 2.48                     | 0.47              |
| 3:1D:30:GLU:OE2    | 60:1D:402:HOH:O    | 2.20                     | 0.47              |
| 10:1O:68:GLU:HB3   | 10:1O:78:ARG:HB2   | 1.96                     | 0.47              |
| 18:1W:25:ARG:NH2   | 18:1W:74:ALA:O     | 2.46                     | 0.47              |
| 18:1W:68:ARG:NH1   | 18:1W:111:HIS:HA   | 2.30                     | 0.47              |
| 33:1b:164:VAL:HG23 | 33:1b:186:ALA:HB2  | 1.95                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 33:1b:213:LEU:HD22 | 33:1b:214:ILE:HD13 | 1.96                     | 0.47              |
| 36:1e:69:VAL:HG12  | 36:1e:139:LEU:HB3  | 1.96                     | 0.47              |
| 39:1h:121:ASP:HB2  | 39:1h:125:ARG:NH2  | 2.30                     | 0.47              |
| 1:2A:153:C:H2'     | 1:2A:154:G:C8      | 2.50                     | 0.47              |
| 1:2A:530:G:H4'     | 1:2A:531:C:OP1     | 2.14                     | 0.47              |
| 1:2A:873:G:N2      | 1:2A:905:U:C2      | 2.83                     | 0.47              |
| 1:2A:1200:C:H1'    | 16:2U:2:PRO:HG3    | 1.95                     | 0.47              |
| 32:2a:922:G:N3     | 32:2a:1398:A:H2    | 2.13                     | 0.47              |
| 33:2b:121:LEU:HA   | 33:2b:125:PRO:HG2  | 1.97                     | 0.47              |
| 33:2b:134:GLU:HA   | 33:2b:137:ARG:HE   | 1.80                     | 0.47              |
| 33:2b:178:ARG:HB3  | 39:2h:72:PRO:HA    | 1.97                     | 0.47              |
| 39:2h:86:ILE:HD11  | 39:2h:136:GLU:HG2  | 1.96                     | 0.47              |
| 42:2k:85:ARG:HE    | 42:2k:111:ASP:HB3  | 1.80                     | 0.47              |
| 1:1A:2345:G:N3     | 1:1A:2381:C:H2'    | 2.30                     | 0.46              |
| 1:1A:2773:C:OP2    | 60:1A:4204:HOH:O   | 2.21                     | 0.46              |
| 6:1G:106:LEU:HA    | 6:1G:110:ALA:HB3   | 1.96                     | 0.46              |
| 12:1Q:36:ALA:HB2   | 12:1Q:103:MET:SD   | 2.56                     | 0.46              |
| 32:1a:839:U:H1'    | 32:1a:840:C:OP1    | 2.15                     | 0.46              |
| 32:1a:1370:G:O6    | 60:1a:1932:HOH:O   | 2.19                     | 0.46              |
| 34:1c:124:ILE:HD12 | 34:1c:196:LEU:HD13 | 1.97                     | 0.46              |
| 40:1i:10:ARG:HG2   | 40:1i:75:ASP:HB2   | 1.97                     | 0.46              |
| 46:1o:18:PHE:O     | 46:1o:20:GLY:N     | 2.48                     | 0.46              |
| 1:2A:272:G:N7      | 1:2A:421:U:H2'     | 2.30                     | 0.46              |
| 1:2A:848:G:H2'     | 1:2A:849:A:C8      | 2.50                     | 0.46              |
| 1:2A:2695:C:H2'    | 1:2A:2696:U:H6     | 1.81                     | 0.46              |
| 6:2G:38:VAL:HG22   | 6:2G:93:THR:HG23   | 1.97                     | 0.46              |
| 11:2P:68:GLN:HG3   | 60:2P:313:HOH:O    | 2.15                     | 0.46              |
| 11:2P:88:LEU:HD22  | 11:2P:95:VAL:HG21  | 1.96                     | 0.46              |
| 14:2S:34:HIS:HB2   | 14:2S:36:TYR:HE1   | 1.79                     | 0.46              |
| 14:2S:36:TYR:OH    | 14:2S:54:LEU:HD22  | 2.15                     | 0.46              |
| 32:2a:839:U:H5''   | 32:2a:840:C:C5     | 2.50                     | 0.46              |
| 32:2a:1347:G:N2    | 32:2a:1373:G:H2'   | 2.30                     | 0.46              |
| 1:1A:571:A:O2'     | 17:1V:78:LYS:HE2   | 2.15                     | 0.46              |
| 1:1A:1899:G:N3     | 1:1A:1899:G:H2'    | 2.30                     | 0.46              |
| 3:1D:26:LYS:HD3    | 3:1D:83:GLU:OE2    | 2.14                     | 0.46              |
| 20:1Y:23:ARG:HD3   | 60:1Y:312:HOH:O    | 2.15                     | 0.46              |
| 1:2A:107:C:H2'     | 1:2A:108:U:C6      | 2.49                     | 0.46              |
| 1:2A:811:U:H2'     | 11:2P:21:ARG:HA    | 1.96                     | 0.46              |
| 1:2A:1064:C:H3'    | 1:2A:1065:U:C5'    | 2.45                     | 0.46              |
| 1:2A:1290:C:H2'    | 1:2A:1291:C:H6     | 1.80                     | 0.46              |
| 1:2A:1441:G:H2'    | 1:2A:1442:G:H8     | 1.80                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:2A:1946:U:H2'    | 1:2A:1947:C:C6     | 2.50                     | 0.46              |
| 2:2B:11:C:OP2      | 2:2B:12:C:N4       | 2.37                     | 0.46              |
| 7:2H:13:LYS:HA     | 7:2H:14:GLY:HA2    | 1.73                     | 0.46              |
| 21:2Z:99:TYR:HB3   | 21:2Z:123:ASP:HB2  | 1.96                     | 0.46              |
| 23:21:64:ALA:HA    | 23:21:67:ILE:HG13  | 1.97                     | 0.46              |
| 32:2a:189(K):U:H2' | 32:2a:189(L):G:H8  | 1.77                     | 0.46              |
| 1:1A:733:G:OP1     | 60:1A:4197:HOH:O   | 2.20                     | 0.46              |
| 1:1A:1465:G:O2'    | 1:1A:1545:A:N1     | 2.43                     | 0.46              |
| 2:1B:33:G:C2       | 2:1B:50:G:C2       | 3.04                     | 0.46              |
| 7:1H:42:ARG:NH1    | 7:1H:53:GLU:OE1    | 2.49                     | 0.46              |
| 8:1I:61:ARG:HD3    | 8:1I:61:ARG:HA     | 1.59                     | 0.46              |
| 32:1a:487:A:H2'    | 32:1a:488:C:O4'    | 2.16                     | 0.46              |
| 32:1a:1032:G:H2'   | 32:1a:1033:G:O4'   | 2.14                     | 0.46              |
| 33:1b:88:ALA:HB2   | 33:1b:219:VAL:HG13 | 1.97                     | 0.46              |
| 34:1c:84:ILE:HA    | 34:1c:87:LEU:HD12  | 1.97                     | 0.46              |
| 37:1f:9:VAL:HB     | 37:1f:87:ARG:HB2   | 1.97                     | 0.46              |
| 1:2A:829:A:N7      | 1:2A:2248:C:H5'    | 2.31                     | 0.46              |
| 1:2A:840:C:OP2     | 1:2A:932:G:N2      | 2.45                     | 0.46              |
| 1:2A:858:U:OP2     | 22:20:77:ARG:NH2   | 2.46                     | 0.46              |
| 1:2A:1063:G:C8     | 1:2A:1065:U:H5     | 2.33                     | 0.46              |
| 1:2A:1118:C:H2'    | 1:2A:1119:C:O4'    | 2.15                     | 0.46              |
| 2:2B:59:A:H2'      | 2:2B:60:C:O4'      | 2.16                     | 0.46              |
| 60:2B:314:HOH:O    | 21:2Z:31:ARG:N     | 2.47                     | 0.46              |
| 10:2O:24:VAL:CG1   | 10:2O:33:ALA:HB2   | 2.44                     | 0.46              |
| 12:2Q:17:LEU:HD13  | 12:2Q:39:PRO:HB2   | 1.98                     | 0.46              |
| 23:21:53:VAL:HG22  | 23:21:74:VAL:HG13  | 1.98                     | 0.46              |
| 23:21:67:ILE:N     | 23:21:68:PRO:HD2   | 2.31                     | 0.46              |
| 27:25:20:ARG:HG2   | 27:25:23:HIS:CE1   | 2.50                     | 0.46              |
| 32:2a:179:A:H2'    | 32:2a:180:U:C6     | 2.49                     | 0.46              |
| 32:2a:224:C:H2'    | 32:2a:225:C:C6     | 2.50                     | 0.46              |
| 32:2a:841:U:H6     | 32:2a:841:U:P      | 2.38                     | 0.46              |
| 42:2k:99:GLN:NE2   | 42:2k:105:VAL:HG21 | 2.26                     | 0.46              |
| 53:2y:20:VAL:HG21  | 53:2y:41:LEU:HD21  | 1.98                     | 0.46              |
| 1:1A:2145:C:H5''   | 1:1A:2146:C:C5     | 2.50                     | 0.46              |
| 1:1A:2233:U:H2'    | 1:1A:2234:G:C8     | 2.50                     | 0.46              |
| 3:1D:113:VAL:HG12  | 60:1D:448:HOH:O    | 2.15                     | 0.46              |
| 10:1O:1:MET:HE3    | 10:1O:32:TYR:CZ    | 2.51                     | 0.46              |
| 16:1U:29:SER:C     | 16:1U:30:LYS:HD2   | 2.41                     | 0.46              |
| 17:1V:76:LYS:HB2   | 17:1V:81:TYR:HB3   | 1.97                     | 0.46              |
| 19:1X:31:HIS:CD2   | 19:1X:33:LYS:H     | 2.27                     | 0.46              |
| 32:1a:1492:A:H4'   | 32:1a:1493:A:N1    | 2.31                     | 0.46              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 42:1k:31:THR:HA   | 42:1k:42:TRP:HA    | 1.97                     | 0.46              |
| 1:2A:994:C:H2'    | 60:2A:5148:HOH:O   | 2.16                     | 0.46              |
| 1:2A:1783:A:H5'   | 1:2A:2608:G:H4'    | 1.97                     | 0.46              |
| 1:2A:2152:G:H2'   | 1:2A:2153:G:C8     | 2.50                     | 0.46              |
| 1:2A:2155:G:H3'   | 1:2A:2156:G:H8     | 1.81                     | 0.46              |
| 6:2G:60:LEU:HD23  | 6:2G:68:PRO:HG3    | 1.96                     | 0.46              |
| 18:2W:71:VAL:HG13 | 18:2W:105:VAL:HG13 | 1.96                     | 0.46              |
| 53:2y:48:PHE:HD2  | 53:2y:70:MET:HB2   | 1.80                     | 0.46              |
| 1:1A:1022:G:N7    | 9:1N:66:LYS:HE2    | 2.30                     | 0.46              |
| 1:1A:1379:A:OP2   | 60:1A:4203:HOH:O   | 2.21                     | 0.46              |
| 1:1A:1590:U:OP2   | 60:1A:4198:HOH:O   | 2.20                     | 0.46              |
| 1:1A:2119:A:O2'   | 1:1A:2120:G:H5'    | 2.15                     | 0.46              |
| 1:1A:2286:A:H4'   | 1:1A:2287:A:O4'    | 2.15                     | 0.46              |
| 32:1a:742:G:H4'   | 46:1o:58:MET:HE1   | 1.97                     | 0.46              |
| 32:1a:1002:G:C6   | 32:1a:1003:G:C2    | 3.04                     | 0.46              |
| 1:2A:536:A:H2'    | 1:2A:537:C:C6      | 2.51                     | 0.46              |
| 1:2A:671:C:N4     | 60:2A:4281:HOH:O   | 2.48                     | 0.46              |
| 1:2A:784:A:C6     | 3:2D:229:VAL:HG11  | 2.51                     | 0.46              |
| 1:2A:1364:G:OP2   | 23:21:3:LYS:HG3    | 2.16                     | 0.46              |
| 1:2A:1866:C:H2'   | 1:2A:1876:A:O4'    | 2.16                     | 0.46              |
| 2:2B:43:C:C5'     | 26:24:1:MET:HE2    | 2.45                     | 0.46              |
| 5:2F:31:HIS:HB2   | 11:2P:9:ASN:OD1    | 2.16                     | 0.46              |
| 10:2O:23:ARG:HD3  | 10:2O:24:VAL:H     | 1.81                     | 0.46              |
| 10:2O:107:ARG:CZ  | 15:2T:36:GLU:HG2   | 2.46                     | 0.46              |
| 32:2a:1114:C:H2'  | 32:2a:1115:C:C6    | 2.51                     | 0.46              |
| 37:2f:97:PHE:CZ   | 49:2r:61:LYS:HE3   | 2.50                     | 0.46              |
| 40:2i:23:ASN:HD21 | 40:2i:25:LYS:HE2   | 1.79                     | 0.46              |
| 41:2j:32:ALA:HB1  | 41:2j:33:GLN:CD    | 2.41                     | 0.46              |
| 1:1A:839:U:H1'    | 1:1A:1191:G:H1'    | 1.96                     | 0.46              |
| 1:1A:1935:G:H1'   | 1:1A:1964:G:N2     | 2.31                     | 0.46              |
| 1:1A:2693:A:H2'   | 1:1A:2694:G:H8     | 1.80                     | 0.46              |
| 4:1E:33:VAL:HG13  | 4:1E:89:ASP:C      | 2.40                     | 0.46              |
| 32:1a:258:G:O6    | 60:1a:1936:HOH:O   | 2.20                     | 0.46              |
| 32:1a:1043:C:H2'  | 32:1a:1044:A:O4'   | 2.15                     | 0.46              |
| 32:1a:1235:U:H2'  | 32:1a:1236:A:O4'   | 2.16                     | 0.46              |
| 34:1c:66:VAL:HG12 | 34:1c:68:VAL:HG23  | 1.98                     | 0.46              |
| 36:1e:16:THR:OG1  | 36:1e:17:ALA:N     | 2.46                     | 0.46              |
| 1:2A:594:U:H2'    | 1:2A:595:C:C6      | 2.51                     | 0.46              |
| 1:2A:1336:A:H2'   | 1:2A:1337:G:C8     | 2.50                     | 0.46              |
| 1:2A:1428:C:O2'   | 1:2A:1569:A:OP2    | 2.14                     | 0.46              |
| 1:2A:1902:C:H5'   | 3:2D:246:PRO:HD3   | 1.97                     | 0.46              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 6:2G:41:GLN:HB3   | 6:2G:43:LEU:HD13   | 1.98                     | 0.46              |
| 8:2I:48:GLU:HG3   | 8:2I:49:ALA:N      | 2.31                     | 0.46              |
| 32:2a:316:G:OP2   | 32:2a:351:G:O2'    | 2.32                     | 0.46              |
| 32:2a:438:G:H4'   | 35:2d:123:HIS:CD2  | 2.48                     | 0.46              |
| 32:2a:512:U:H2'   | 32:2a:513:C:C6     | 2.50                     | 0.46              |
| 32:2a:986:A:N3    | 50:2s:52:TYR:OH    | 2.48                     | 0.46              |
| 33:2b:111:ARG:HD2 | 33:2b:145:LEU:HD21 | 1.97                     | 0.46              |
| 40:2i:21:PRO:HA   | 40:2i:59:PHE:CD1   | 2.50                     | 0.46              |
| 1:1A:438:G:H2'    | 1:1A:440:G:C8      | 2.51                     | 0.46              |
| 1:1A:863:A:H2'    | 1:1A:864:G:C8      | 2.51                     | 0.46              |
| 1:1A:2190:G:H2'   | 1:1A:2191:G:O4'    | 2.15                     | 0.46              |
| 3:1D:232:PRO:HB3  | 3:1D:244:ARG:CZ    | 2.45                     | 0.46              |
| 32:1a:542:G:OP1   | 35:1d:10:ARG:NH2   | 2.49                     | 0.46              |
| 32:1a:927:G:O2'   | 32:1a:1503:A:N7    | 2.44                     | 0.46              |
| 32:1a:1095:U:OP1  | 32:1a:1108:G:N2    | 2.44                     | 0.46              |
| 32:1a:1101:A:H4'  | 32:1a:1102:A:O5'   | 2.16                     | 0.46              |
| 32:1a:1121:U:H2'  | 32:1a:1122:U:C6    | 2.50                     | 0.46              |
| 32:1a:1343:G:O2'  | 40:1i:121:ARG:HD2  | 2.15                     | 0.46              |
| 37:1f:96:PRO:HB3  | 49:1r:30:ASP:CG    | 2.40                     | 0.46              |
| 38:1g:54:THR:CB   | 38:1g:56:GLN:HE22  | 2.28                     | 0.46              |
| 43:1l:88:GLY:O    | 43:1l:99:HIS:HD2   | 1.99                     | 0.46              |
| 1:2A:9:U:O2'      | 1:2A:10:G:OP1      | 2.33                     | 0.46              |
| 1:2A:2165:G:H2'   | 1:2A:2166:G:O4'    | 2.16                     | 0.46              |
| 1:2A:2887:U:H2'   | 1:2A:2888:C:H6     | 1.80                     | 0.46              |
| 6:2G:16:ARG:O     | 6:2G:20:ILE:HG13   | 2.14                     | 0.46              |
| 13:2R:103:ARG:NH1 | 13:2R:108:GLY:O    | 2.46                     | 0.46              |
| 14:2S:36:TYR:N    | 14:2S:36:TYR:HD1   | 2.14                     | 0.46              |
| 32:2a:475:G:H2'   | 32:2a:476:G:C8     | 2.51                     | 0.46              |
| 32:2a:798:G:O6    | 60:2a:3228:HOH:O   | 2.20                     | 0.46              |
| 34:2c:97:LYS:O    | 34:2c:99:VAL:N     | 2.47                     | 0.46              |
| 35:2d:61:LYS:NZ   | 35:2d:72:GLU:OE1   | 2.45                     | 0.46              |
| 43:2l:71:PRO:HG2  | 43:2l:102:ARG:HG2  | 1.97                     | 0.46              |
| 3:1D:111:LEU:HD23 | 3:1D:111:LEU:HA    | 1.83                     | 0.46              |
| 4:1E:59:VAL:HB    | 4:1E:64:LYS:HE3    | 1.98                     | 0.46              |
| 10:1O:98:VAL:HG22 | 10:1O:118:ALA:HA   | 1.97                     | 0.46              |
| 32:1a:1003:G:C2   | 32:1a:1004:A:N3    | 2.84                     | 0.46              |
| 32:1a:1037:C:H2'  | 32:1a:1038:C:C6    | 2.51                     | 0.46              |
| 32:1a:1284:C:H3'  | 32:1a:1285:A:H8    | 1.80                     | 0.46              |
| 32:1a:1424:C:H2'  | 32:1a:1425:U:O4'   | 2.16                     | 0.46              |
| 33:1b:32:ILE:HD13 | 33:1b:40:HIS:CD2   | 2.51                     | 0.46              |
| 36:1e:6:PHE:CE1   | 36:1e:36:ASP:HB3   | 2.51                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 47:1p:6:LEU:HB3    | 47:1p:17:TYR:HB3   | 1.96                     | 0.46              |
| 1:2A:298:G:H5''    | 1:2A:299:A:OP1     | 2.15                     | 0.46              |
| 1:2A:821:A:H2'     | 1:2A:946:G:H5''    | 1.97                     | 0.46              |
| 1:2A:1068:G:H3'    | 1:2A:1096:A:OP2    | 2.16                     | 0.46              |
| 1:2A:1441:G:H2'    | 1:2A:1442:G:C8     | 2.51                     | 0.46              |
| 1:2A:2162:G:H4'    | 1:2A:2172:U:O2'    | 2.15                     | 0.46              |
| 1:2A:2626:C:H2'    | 1:2A:2627:G:O4'    | 2.16                     | 0.46              |
| 25:23:10:LYS:HB3   | 25:23:53:LEU:HA    | 1.98                     | 0.46              |
| 32:2a:619:U:C2     | 35:2d:135:LEU:HD21 | 2.51                     | 0.46              |
| 32:2a:693:G:H2'    | 32:2a:694:A:C8     | 2.51                     | 0.46              |
| 32:2a:1002:G:N3    | 32:2a:1003:G:H8    | 2.14                     | 0.46              |
| 32:2a:1490:C:H2'   | 32:2a:1491:G:C8    | 2.51                     | 0.46              |
| 36:2e:144:THR:H    | 36:2e:147:ASP:HB2  | 1.81                     | 0.46              |
| 37:2f:23:LYS:HG2   | 37:2f:61:LEU:HD21  | 1.98                     | 0.46              |
| 1:1A:26:G:C6       | 1:1A:27:G:N1       | 2.84                     | 0.46              |
| 1:1A:27:G:N2       | 1:1A:512:G:H1'     | 2.31                     | 0.46              |
| 1:1A:910:A:N3      | 1:1A:2264:C:O2'    | 2.47                     | 0.46              |
| 1:1A:2106:G:H2'    | 1:1A:2107:C:O4'    | 2.15                     | 0.46              |
| 1:1A:2567:G:H2'    | 1:1A:2568:C:C6     | 2.51                     | 0.46              |
| 5:1F:184:TYR:O     | 5:1F:188:ARG:HB2   | 2.16                     | 0.46              |
| 32:1a:452:A:H4'    | 47:1p:72:ARG:NH1   | 2.29                     | 0.46              |
| 32:1a:580:U:H2'    | 32:1a:581:G:O4'    | 2.15                     | 0.46              |
| 32:1a:604:G:C2     | 32:1a:635:G:C5     | 3.04                     | 0.46              |
| 32:1a:913:A:OP1    | 43:1l:46:LYS:NZ    | 2.47                     | 0.46              |
| 32:1a:966:M2G:O2'  | 40:1i:127:LYS:O    | 2.33                     | 0.46              |
| 32:1a:1133:G:H2'   | 32:1a:1134:G:C8    | 2.51                     | 0.46              |
| 32:1a:1313:U:P     | 50:1s:5:LEU:HB2    | 2.56                     | 0.46              |
| 32:1a:1486:G:H2'   | 32:1a:1487:G:O4'   | 2.16                     | 0.46              |
| 33:1b:201:ILE:HG21 | 33:1b:214:ILE:HG21 | 1.97                     | 0.46              |
| 35:1d:173:TRP:CE3  | 35:1d:174:LEU:HG   | 2.51                     | 0.46              |
| 46:1o:70:LEU:HD11  | 46:1o:77:ARG:HB3   | 1.98                     | 0.46              |
| 1:2A:729:G:C5      | 3:2D:208:LYS:HB2   | 2.51                     | 0.46              |
| 1:2A:1999:C:H4'    | 1:2A:2723:C:O2     | 2.16                     | 0.46              |
| 1:2A:2315:G:H2'    | 1:2A:2316:C:H6     | 1.81                     | 0.46              |
| 1:2A:2882:A:H5'    | 13:2R:96:ARG:HB2   | 1.98                     | 0.46              |
| 2:2B:28:C:H2'      | 2:2B:29:A:O4'      | 2.16                     | 0.46              |
| 4:2E:13:ARG:HD2    | 4:2E:20:ALA:HB1    | 1.97                     | 0.46              |
| 31:29:15:LYS:HB3   | 31:29:26:ILE:HG13  | 1.98                     | 0.46              |
| 32:2a:598:U:H2'    | 32:2a:599:C:C6     | 2.50                     | 0.46              |
| 32:2a:748:C:O2     | 32:2a:749:C:N4     | 2.49                     | 0.46              |
| 32:2a:1330:U:H4'   | 44:2m:23:TYR:CZ    | 2.51                     | 0.46              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 37:2f:33:TYR:HB2  | 37:2f:75:LEU:HD12  | 1.98                     | 0.46              |
| 44:2m:16:ASP:HB2  | 44:2m:27:LYS:NZ    | 2.31                     | 0.46              |
| 1:1A:224:G:H2'    | 1:1A:225:A:O4'     | 2.16                     | 0.46              |
| 1:1A:636:G:OP1    | 11:1P:132:LYS:HE2  | 2.15                     | 0.46              |
| 1:1A:796:C:H2'    | 1:1A:797:C:C6      | 2.50                     | 0.46              |
| 1:1A:1075:C:OP2   | 12:1Q:59:ARG:NE    | 2.43                     | 0.46              |
| 1:1A:2103:C:H2'   | 1:1A:2104:G:H5'    | 1.98                     | 0.46              |
| 1:1A:2134:A:O2'   | 1:1A:2159:G:N3     | 2.40                     | 0.46              |
| 1:1A:2506:U:OP1   | 4:1E:144:ARG:NH2   | 2.48                     | 0.46              |
| 8:1I:104:GLN:HE21 | 8:1I:105:HIS:CD2   | 2.33                     | 0.46              |
| 10:1O:70:LYS:HB3  | 10:1O:70:LYS:HE2   | 1.79                     | 0.46              |
| 11:1P:121:LYS:O   | 11:1P:123:LEU:N    | 2.45                     | 0.46              |
| 13:1R:36:THR:HG22 | 13:1R:37:THR:H     | 1.81                     | 0.46              |
| 21:1Z:80:ARG:HB3  | 21:1Z:82:ARG:HD3   | 1.97                     | 0.46              |
| 32:1a:1445:C:O2'  | 32:1a:1447:A:N6    | 2.39                     | 0.46              |
| 35:1d:190:ASP:OD1 | 35:1d:190:ASP:N    | 2.49                     | 0.46              |
| 40:1i:43:ALA:HA   | 40:1i:74:ILE:HD13  | 1.98                     | 0.46              |
| 1:2A:1405:U:H2'   | 1:2A:1406:U:C6     | 2.51                     | 0.46              |
| 1:2A:1932:A:H2'   | 1:2A:1933:G:O4'    | 2.16                     | 0.46              |
| 1:2A:2102:U:H2'   | 1:2A:2103:C:C6     | 2.51                     | 0.46              |
| 1:2A:2140:C:O2    | 1:2A:2152:G:N2     | 2.49                     | 0.46              |
| 1:2A:2278:A:O2'   | 21:2Z:199:LYS:HD3  | 2.16                     | 0.46              |
| 1:2A:2315:G:H2'   | 1:2A:2316:C:C6     | 2.51                     | 0.46              |
| 4:2E:50:GLY:HA3   | 4:2E:75:VAL:HG11   | 1.97                     | 0.46              |
| 9:2N:54:VAL:HB    | 9:2N:122:VAL:HG22  | 1.97                     | 0.46              |
| 11:2P:59:LEU:HD23 | 30:28:58:ILE:HD13  | 1.98                     | 0.46              |
| 16:2U:104:GLN:NE2 | 16:2U:105:VAL:HG23 | 2.27                     | 0.46              |
| 26:24:24:THR:OG1  | 26:24:25:TYR:N     | 2.43                     | 0.46              |
| 28:26:9:LEU:CD2   | 28:26:25:LYS:HG2   | 2.46                     | 0.46              |
| 32:2a:392:G:H2'   | 32:2a:393:A:C8     | 2.51                     | 0.46              |
| 32:2a:653:A:OP1   | 39:2h:56:LYS:NZ    | 2.36                     | 0.46              |
| 32:2a:1162:C:H42  | 32:2a:1174:G:H1    | 1.64                     | 0.46              |
| 34:2c:142:MET:HG3 | 34:2c:170:GLN:HB3  | 1.98                     | 0.46              |
| 35:2d:135:LEU:C   | 35:2d:137:SER:H    | 2.24                     | 0.46              |
| 36:2e:57:LYS:HG2  | 36:2e:61:TYR:CE2   | 2.51                     | 0.46              |
| 37:2f:96:PRO:HB3  | 49:2r:30:ASP:CG    | 2.40                     | 0.46              |
| 39:2h:11:THR:HG22 | 39:2h:15:ASN:ND2   | 2.31                     | 0.46              |
| 48:2q:64:PRO:HB3  | 48:2q:70:ARG:NH1   | 2.31                     | 0.46              |
| 1:1A:1756:G:H4'   | 1:1A:1758:G:O4'    | 2.16                     | 0.45              |
| 1:1A:1918:A:O2'   | 1:1A:1920:OMC:N4   | 2.50                     | 0.45              |
| 1:1A:2115:G:H2'   | 1:1A:2117:A:N6     | 2.31                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1A:2336:A:H61   | 22:10:43:THR:CG2  | 2.28                     | 0.45              |
| 11:1P:46:LYS:HE2  | 11:1P:46:LYS:HB3  | 1.72                     | 0.45              |
| 1:2A:1721:G:H2'   | 1:2A:1740:G:O6    | 2.15                     | 0.45              |
| 1:2A:2758:A:C2    | 1:2A:2759:G:H1'   | 2.51                     | 0.45              |
| 1:2A:2819:G:H2'   | 1:2A:2821:A:N7    | 2.31                     | 0.45              |
| 23:21:11:ARG:O    | 60:21:201:HOH:O   | 2.20                     | 0.45              |
| 32:2a:187:C:O2'   | 51:2t:89:ARG:HD3  | 2.16                     | 0.45              |
| 32:2a:540:G:H2'   | 32:2a:541:G:O4'   | 2.16                     | 0.45              |
| 32:2a:978:A:O2'   | 32:2a:1322:C:N3   | 2.47                     | 0.45              |
| 32:2a:1347:G:HO2' | 32:2a:1373:G:H1   | 1.64                     | 0.45              |
| 32:2a:1400:5MC:C2 | 53:2y:63:ALA:HA   | 2.52                     | 0.45              |
| 36:2e:122:GLU:OE1 | 36:2e:126:ARG:HD2 | 2.16                     | 0.45              |
| 41:2j:38:ILE:HD11 | 41:2j:71:LEU:HD22 | 1.99                     | 0.45              |
| 1:1A:278:A:O2'    | 1:1A:279:C:OP1    | 2.27                     | 0.45              |
| 1:1A:2246:G:H2'   | 1:1A:2247:A:C8    | 2.51                     | 0.45              |
| 1:1A:2304:G:O2'   | 6:1G:156:ASP:OD1  | 2.27                     | 0.45              |
| 2:1B:81:G:O6      | 57:1B:231:ARG:NH1 | 2.38                     | 0.45              |
| 3:1D:77:ALA:O     | 3:1D:116:GLN:HG3  | 2.16                     | 0.45              |
| 7:1H:11:VAL:HG13  | 7:1H:15:VAL:HG22  | 1.98                     | 0.45              |
| 9:1N:61:ARG:HA    | 9:1N:61:ARG:HD3   | 1.71                     | 0.45              |
| 14:1S:34:HIS:O    | 14:1S:97:ARG:NH2  | 2.50                     | 0.45              |
| 32:1a:1220:G:N2   | 50:1s:54:GLY:O    | 2.37                     | 0.45              |
| 34:1c:135:LYS:NZ  | 36:1e:53:LEU:HD11 | 2.31                     | 0.45              |
| 36:1e:82:VAL:HG21 | 36:1e:138:ALA:HA  | 1.98                     | 0.45              |
| 39:1h:21:LYS:O    | 39:1h:65:TYR:OH   | 2.25                     | 0.45              |
| 53:1y:49:VAL:HG22 | 53:1y:66:LYS:HG2  | 1.98                     | 0.45              |
| 1:2A:1167:U:O2    | 1:2A:1183:G:N2    | 2.49                     | 0.45              |
| 1:2A:2610:C:O2'   | 60:2A:3861:HOH:O  | 2.14                     | 0.45              |
| 6:2G:114:ILE:HD12 | 6:2G:117:PHE:CE1  | 2.51                     | 0.45              |
| 21:2Z:193:GLU:HG2 | 21:2Z:194:PRO:HD2 | 1.98                     | 0.45              |
| 32:2a:792:A:H4'   | 32:2a:793:U:O5'   | 2.16                     | 0.45              |
| 32:2a:850:U:H2'   | 32:2a:851:G:H5''  | 1.98                     | 0.45              |
| 1:1A:323:G:C8     | 5:1F:171:PRO:HG3  | 2.51                     | 0.45              |
| 1:1A:2062:A:OP1   | 60:1A:4192:HOH:O  | 2.20                     | 0.45              |
| 1:1A:2165:G:H2'   | 1:1A:2166:G:H8    | 1.80                     | 0.45              |
| 2:1B:90:A:C5      | 2:1B:91:C:H1'     | 2.51                     | 0.45              |
| 6:1G:12:TYR:HA    | 6:1G:16:ARG:HG3   | 1.98                     | 0.45              |
| 15:1T:55:ASN:N    | 15:1T:59:THR:HG22 | 2.12                     | 0.45              |
| 32:1a:238:G:OP1   | 48:1q:25:ARG:NH2  | 2.49                     | 0.45              |
| 32:1a:392:G:H5'   | 47:1p:12:LYS:HD3  | 1.98                     | 0.45              |
| 32:1a:438:G:O2'   | 32:1a:494:U:O4    | 2.33                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 32:1a:1060:C:H5''  | 41:1j:51:ARG:HG2   | 1.97                     | 0.45              |
| 32:1a:1162:C:N4    | 32:1a:1174:G:H1    | 2.15                     | 0.45              |
| 32:1a:1284:C:OP2   | 32:1a:1285:A:O2'   | 2.33                     | 0.45              |
| 33:1b:100:GLY:N    | 33:1b:176:GLU:OE2  | 2.45                     | 0.45              |
| 35:1d:111:ALA:HB1  | 35:1d:116:GLN:HB3  | 1.98                     | 0.45              |
| 44:1m:12:ASN:O     | 44:1m:44:ARG:HD2   | 2.16                     | 0.45              |
| 1:2A:579:G:H2'     | 1:2A:580:C:C6      | 2.52                     | 0.45              |
| 1:2A:746:A:HO2'    | 1:2A:2611:U:HO2'   | 1.63                     | 0.45              |
| 1:2A:1290:C:H2'    | 1:2A:1291:C:C6     | 2.51                     | 0.45              |
| 1:2A:1786:A:H1'    | 1:2A:1938:A:N6     | 2.32                     | 0.45              |
| 1:2A:2291:U:O2'    | 1:2A:2374:C:O2     | 2.35                     | 0.45              |
| 1:2A:2807:G:C2     | 1:2A:2808:U:H1'    | 2.51                     | 0.45              |
| 9:2N:38:HIS:CD2    | 9:2N:39:ARG:HG3    | 2.51                     | 0.45              |
| 12:2Q:111:GLU:O    | 12:2Q:115:MET:HG2  | 2.16                     | 0.45              |
| 13:2R:2:ARG:HG2    | 13:2R:5:LYS:HB2    | 1.98                     | 0.45              |
| 21:2Z:150:LEU:O    | 21:2Z:171:ILE:HG13 | 2.16                     | 0.45              |
| 22:20:70:GLN:HE21  | 22:20:72:ARG:HG2   | 1.80                     | 0.45              |
| 32:2a:8:A:N6       | 35:2d:209:ARG:HB2  | 2.31                     | 0.45              |
| 32:2a:932:C:H2'    | 32:2a:933:G:C8     | 2.51                     | 0.45              |
| 32:2a:1072:G:H2'   | 32:2a:1073:U:C6    | 2.52                     | 0.45              |
| 32:2a:1097:C:O2'   | 32:2a:1169:A:N3    | 2.47                     | 0.45              |
| 32:2a:1469:G:H2'   | 32:2a:1470:G:C8    | 2.51                     | 0.45              |
| 1:1A:2453:A:OP1    | 60:1A:4191:HOH:O   | 2.20                     | 0.45              |
| 5:1F:143:ALA:HB1   | 5:1F:148:LEU:HB2   | 1.98                     | 0.45              |
| 15:1T:1:MET:HE2    | 15:1T:3:ARG:HG3    | 1.97                     | 0.45              |
| 26:14:14:ILE:HG23  | 26:14:31:ILE:HB    | 1.98                     | 0.45              |
| 32:1a:1071:C:H2'   | 32:1a:1072:G:C8    | 2.50                     | 0.45              |
| 35:1d:105:VAL:HG13 | 35:1d:110:PHE:HB2  | 1.98                     | 0.45              |
| 35:1d:114:ARG:HA   | 35:1d:117:ALA:HB3  | 1.98                     | 0.45              |
| 1:2A:1053:C:H4'    | 1:2A:1054:A:OP1    | 2.17                     | 0.45              |
| 1:2A:1166:C:H2'    | 1:2A:1167:U:C6     | 2.51                     | 0.45              |
| 1:2A:1410:G:H2'    | 1:2A:1411:C:C6     | 2.51                     | 0.45              |
| 1:2A:1495:A:H2'    | 1:2A:1496:A:C8     | 2.51                     | 0.45              |
| 1:2A:2063:C:OP1    | 60:2A:3924:HOH:O   | 2.21                     | 0.45              |
| 10:2O:49:ARG:NH1   | 32:2a:1422:G:O3'   | 2.50                     | 0.45              |
| 19:2X:44:GLU:HG2   | 19:2X:49:VAL:O     | 2.15                     | 0.45              |
| 21:2Z:157:LEU:HD13 | 21:2Z:161:VAL:HG12 | 1.96                     | 0.45              |
| 32:2a:1226:C:H4'   | 50:2s:80:TYR:CZ    | 2.51                     | 0.45              |
| 33:2b:76:GLN:HG2   | 33:2b:77:ALA:N     | 2.31                     | 0.45              |
| 44:2m:108:ARG:HA   | 44:2m:108:ARG:HD3  | 1.78                     | 0.45              |
| 1:1A:1702:G:H2'    | 1:1A:1703:G:O4'    | 2.17                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:1A:2849:U:H4'    | 1:1A:2868:A:C2     | 2.51                     | 0.45              |
| 32:1a:1016:A:H2'   | 32:1a:1017:G:O4'   | 2.16                     | 0.45              |
| 32:1a:1092:A:H2'   | 32:1a:1093:A:C8    | 2.51                     | 0.45              |
| 32:1a:1228:C:OP1   | 44:1m:108:ARG:NH1  | 2.47                     | 0.45              |
| 33:1b:185:ILE:CG2  | 33:1b:199:TYR:HB2  | 2.44                     | 0.45              |
| 33:1b:222:ILE:O    | 33:1b:226:ARG:HB2  | 2.15                     | 0.45              |
| 35:1d:17:VAL:HG11  | 35:1d:197:PRO:HG3  | 1.98                     | 0.45              |
| 38:1g:113:GLU:HG3  | 38:1g:118:VAL:HG12 | 1.98                     | 0.45              |
| 47:1p:20:VAL:HG21  | 47:1p:32:TYR:CD2   | 2.52                     | 0.45              |
| 1:2A:76:C:O2'      | 24:22:62:THR:OG1   | 2.31                     | 0.45              |
| 1:2A:248:G:H5'     | 1:2A:250:G:N7      | 2.31                     | 0.45              |
| 1:2A:466:A:H5'     | 29:27:21:ARG:HH21  | 1.81                     | 0.45              |
| 1:2A:1493:C:N4     | 1:2A:2206:G:O2'    | 2.49                     | 0.45              |
| 1:2A:2150:U:H2'    | 1:2A:2151:G:C8     | 2.52                     | 0.45              |
| 60:2A:4932:HOH:O   | 5:2F:53:THR:HG21   | 2.17                     | 0.45              |
| 17:2V:24:LYS:HG3   | 17:2V:64:HIS:CD2   | 2.51                     | 0.45              |
| 21:2Z:108:PRO:HB3  | 21:2Z:144:LEU:HB2  | 1.99                     | 0.45              |
| 32:2a:189(F):U:C4  | 48:2q:72:ARG:NH1   | 2.85                     | 0.45              |
| 32:2a:473:G:OP2    | 47:2p:75:ARG:HD3   | 2.16                     | 0.45              |
| 32:2a:519:C:H2'    | 32:2a:520:A:O4'    | 2.16                     | 0.45              |
| 32:2a:1227:A:OP2   | 44:2m:111:LYS:HE2  | 2.17                     | 0.45              |
| 32:2a:1445:C:O2'   | 32:2a:1447:A:N6    | 2.49                     | 0.45              |
| 53:2y:65:GLY:N     | 53:2y:77:LEU:HB2   | 2.31                     | 0.45              |
| 1:1A:185:U:H2'     | 1:1A:186:G:H8      | 1.80                     | 0.45              |
| 1:1A:686:G:N2      | 1:1A:788:A:H61     | 2.15                     | 0.45              |
| 30:18:15:LYS:HB3   | 56:18:104:MPD:H31  | 1.99                     | 0.45              |
| 32:1a:922:G:C6     | 32:1a:923:A:C6     | 3.04                     | 0.45              |
| 32:1a:1036:G:H2'   | 32:1a:1036:G:N3    | 2.32                     | 0.45              |
| 32:1a:1207:2MG:H2' | 32:1a:1208:C:C6    | 2.52                     | 0.45              |
| 33:1b:16:HIS:HB2   | 33:1b:204:ASN:HB3  | 1.99                     | 0.45              |
| 44:1m:53:VAL:HG12  | 44:1m:57:ARG:HH12  | 1.82                     | 0.45              |
| 1:2A:568:U:H5'     | 1:2A:945:A:N6      | 2.32                     | 0.45              |
| 1:2A:2255:G:OP2    | 60:2A:3921:HOH:O   | 2.20                     | 0.45              |
| 21:2Z:40:ASP:OD2   | 21:2Z:42:VAL:HG13  | 2.16                     | 0.45              |
| 26:24:41:PRO:HG3   | 26:24:49:PHE:CD2   | 2.52                     | 0.45              |
| 26:24:48:ARG:HD2   | 26:24:52:THR:HA    | 1.98                     | 0.45              |
| 32:2a:1132:C:H2'   | 32:2a:1133:G:C8    | 2.51                     | 0.45              |
| 32:2a:1256:A:H61   | 32:2a:1278:U:C1'   | 2.29                     | 0.45              |
| 32:2a:1304:G:O2'   | 32:2a:1333:A:N6    | 2.46                     | 0.45              |
| 45:2n:27:CYS:SG    | 45:2n:29:ARG:HB2   | 2.57                     | 0.45              |
| 46:2o:4:THR:HG23   | 46:2o:7:GLU:HG3    | 1.97                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:1A:1359:A:N1     | 1:1A:1372:U:O4     | 2.50                     | 0.45              |
| 1:1A:1665:A:H4'    | 10:1O:67:LYS:HB2   | 1.98                     | 0.45              |
| 1:1A:2065:C:OP1    | 60:1A:4202:HOH:O   | 2.21                     | 0.45              |
| 1:1A:2183:C:H2'    | 1:1A:2184:G:C8     | 2.52                     | 0.45              |
| 1:1A:2189:U:H2'    | 1:1A:2190:G:C8     | 2.52                     | 0.45              |
| 1:1A:2766:G:H2'    | 1:1A:2766:G:N3     | 2.31                     | 0.45              |
| 6:1G:131:TYR:HE2   | 6:1G:133:LEU:HD23  | 1.82                     | 0.45              |
| 24:12:36:ARG:HD3   | 60:12:109:HOH:O    | 2.17                     | 0.45              |
| 32:1a:189(K):U:H2' | 32:1a:189(L):G:C8  | 2.52                     | 0.45              |
| 32:1a:632:A:H5'    | 32:1a:633:G:OP2    | 2.17                     | 0.45              |
| 32:1a:667:G:H4'    | 46:1o:51:HIS:ND1   | 2.31                     | 0.45              |
| 32:1a:1417:G:H2'   | 32:1a:1482:G:N2    | 2.32                     | 0.45              |
| 33:1b:157:ARG:HG2  | 33:1b:158:LEU:N    | 2.32                     | 0.45              |
| 34:1c:32:LEU:HD13  | 34:1c:59:ARG:HD3   | 1.97                     | 0.45              |
| 44:1m:14:ARG:HG3   | 44:1m:44:ARG:CZ    | 2.46                     | 0.45              |
| 1:2A:824:A:H1'     | 1:2A:2358:G:N7     | 2.32                     | 0.45              |
| 1:2A:1790:C:H5''   | 1:2A:1791:A:OP1    | 2.16                     | 0.45              |
| 1:2A:1991:U:H2'    | 1:2A:1992:G:H5''   | 1.98                     | 0.45              |
| 3:2D:71:ASP:OD2    | 3:2D:103:ARG:NH2   | 2.50                     | 0.45              |
| 7:2H:3:ARG:HE      | 7:2H:54:ARG:HH12   | 1.64                     | 0.45              |
| 9:2N:120:LEU:HD11  | 9:2N:122:VAL:HG23  | 1.99                     | 0.45              |
| 15:2T:54:ARG:HA    | 15:2T:59:THR:HG23  | 1.97                     | 0.45              |
| 16:2U:61:TRP:CH2   | 16:2U:93:LYS:HB2   | 2.51                     | 0.45              |
| 32:2a:415:A:H2'    | 32:2a:416:G:O4'    | 2.17                     | 0.45              |
| 32:2a:1146:A:H2'   | 32:2a:1147:C:O4'   | 2.17                     | 0.45              |
| 32:2a:1248:A:O2'   | 40:2i:70:LYS:NZ    | 2.46                     | 0.45              |
| 35:2d:63:LYS:HD2   | 35:2d:198:VAL:HG22 | 1.98                     | 0.45              |
| 38:2g:74:GLU:HG2   | 38:2g:91:VAL:HG22  | 1.99                     | 0.45              |
| 1:1A:818:G:H4'     | 1:1A:838:C:O3'     | 2.17                     | 0.45              |
| 1:1A:886:C:H2'     | 1:1A:887:A:H5''    | 1.99                     | 0.45              |
| 1:1A:2014:A:H2'    | 1:1A:2015:A:C8     | 2.51                     | 0.45              |
| 1:1A:2048:G:OP1    | 60:1A:4207:HOH:O   | 2.21                     | 0.45              |
| 2:1B:74:U:H2'      | 2:1B:75:G:O4'      | 2.17                     | 0.45              |
| 8:1I:84:GLY:O      | 8:1I:85:GLU:HB3    | 2.17                     | 0.45              |
| 21:1Z:152:ALA:HB1  | 21:1Z:163:LEU:HD21 | 1.99                     | 0.45              |
| 24:12:1:MET:HE2    | 24:12:6:VAL:HG22   | 1.99                     | 0.45              |
| 32:1a:1003:G:O2'   | 32:1a:1004:A:H4'   | 2.17                     | 0.45              |
| 33:1b:24:TRP:CH2   | 33:1b:26:PRO:HA    | 2.52                     | 0.45              |
| 33:1b:84:GLU:O     | 33:1b:219:VAL:HG21 | 2.16                     | 0.45              |
| 33:1b:231:GLU:HB3  | 33:1b:232:PRO:CD   | 2.46                     | 0.45              |
| 41:1j:5:ARG:NE     | 41:1j:73:ASP:OD1   | 2.38                     | 0.45              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 46:1o:5:LYS:O     | 46:1o:9:GLN:HG2    | 2.17                     | 0.45              |
| 47:1p:79:VAL:HG23 | 47:1p:80:PHE:CD1   | 2.51                     | 0.45              |
| 48:1q:58:GLU:O    | 48:1q:74:LEU:N     | 2.47                     | 0.45              |
| 1:2A:971:C:OP2    | 60:2A:3927:HOH:O   | 2.21                     | 0.45              |
| 1:2A:1025:G:C4    | 1:2A:1135:C:H1'    | 2.52                     | 0.45              |
| 1:2A:2304:G:H22   | 1:2A:2312:U:H3     | 1.65                     | 0.45              |
| 2:2B:78:A:H2'     | 2:2B:79:C:O4'      | 2.16                     | 0.45              |
| 32:2a:246:A:N1    | 32:2a:278:G:O2'    | 2.47                     | 0.45              |
| 32:2a:502:G:OP1   | 43:2l:118:SER:N    | 2.36                     | 0.45              |
| 32:2a:977:A:H2'   | 32:2a:978:A:H5''   | 1.99                     | 0.45              |
| 32:2a:1027:C:O2'  | 32:2a:1034:G:N2    | 2.49                     | 0.45              |
| 34:2c:131:ARG:NH2 | 36:2e:50:GLU:HG3   | 2.32                     | 0.45              |
| 35:2d:59:ARG:HD3  | 35:2d:59:ARG:HA    | 1.76                     | 0.45              |
| 1:1A:1651:G:N3    | 60:1A:4410:HOH:O   | 2.36                     | 0.45              |
| 1:1A:2031:A:C6    | 1:1A:2498:C:H1'    | 2.52                     | 0.45              |
| 1:1A:2502:G:N7    | 60:1A:4415:HOH:O   | 2.36                     | 0.45              |
| 1:1A:2662:A:H2'   | 1:1A:2663:G:O4'    | 2.17                     | 0.45              |
| 1:1A:2836:U:H2'   | 1:1A:2837:G:C8     | 2.52                     | 0.45              |
| 3:1D:206:LEU:HD22 | 3:1D:211:ARG:HG2   | 1.99                     | 0.45              |
| 10:1O:49:ARG:NH1  | 32:1a:1422:G:O3'   | 2.44                     | 0.45              |
| 32:1a:657:G:O2'   | 46:1o:23:GLY:HA2   | 2.17                     | 0.45              |
| 32:1a:1039:C:H2'  | 32:1a:1040:U:H6    | 1.82                     | 0.45              |
| 44:1m:20:THR:C    | 44:1m:22:ILE:H     | 2.25                     | 0.45              |
| 44:1m:114:ARG:NH1 | 60:1m:302:HOH:O    | 2.50                     | 0.45              |
| 53:1y:23:ARG:HD2  | 53:1y:23:ARG:HA    | 1.75                     | 0.45              |
| 1:2A:673:C:H5''   | 5:2F:81:PRO:HD2    | 1.98                     | 0.45              |
| 1:2A:2630:G:H2'   | 1:2A:2631:G:C8     | 2.52                     | 0.45              |
| 2:2B:56:G:P       | 6:2G:27:ASN:HD21   | 2.39                     | 0.45              |
| 5:2F:182:ASN:O    | 5:2F:186:ILE:HD12  | 2.17                     | 0.45              |
| 9:2N:16:ILE:HD13  | 9:2N:52:VAL:HG13   | 1.98                     | 0.45              |
| 17:2V:27:ALA:O    | 17:2V:64:HIS:HE1   | 2.00                     | 0.45              |
| 21:2Z:97:GLU:HB3  | 21:2Z:125:LEU:HD11 | 1.99                     | 0.45              |
| 32:2a:37:U:O2'    | 32:2a:500:G:H4'    | 2.17                     | 0.45              |
| 32:2a:132:C:H2'   | 32:2a:133:U:O4'    | 2.17                     | 0.45              |
| 32:2a:276:G:O3'   | 48:2q:68:ARG:NH1   | 2.49                     | 0.45              |
| 32:2a:839:U:H3'   | 32:2a:840:C:C5     | 2.52                     | 0.45              |
| 32:2a:1142:G:C2   | 32:2a:1143:G:H1'   | 2.52                     | 0.45              |
| 33:2b:55:PHE:O    | 33:2b:59:GLU:N     | 2.38                     | 0.45              |
| 35:2d:78:LEU:HD22 | 35:2d:96:LEU:HB3   | 1.99                     | 0.45              |
| 36:2e:78:HIS:CD2  | 36:2e:142:LEU:HD23 | 2.52                     | 0.45              |
| 40:2i:37:PHE:HB3  | 40:2i:43:ALA:HB2   | 1.99                     | 0.45              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:1A:847:U:OP2    | 60:1A:4201:HOH:O   | 2.21                     | 0.45              |
| 1:1A:1082:U:C4    | 1:1A:1086:A:N1     | 2.80                     | 0.45              |
| 1:1A:2009:G:OP1   | 18:1W:41:LYS:NZ    | 2.32                     | 0.45              |
| 4:1E:29:GLY:HA3   | 60:1E:408:HOH:O    | 2.16                     | 0.45              |
| 7:1H:3:ARG:NH1    | 7:1H:5:GLY:H       | 2.15                     | 0.45              |
| 9:1N:15:LEU:HB2   | 9:1N:135:PRO:HB2   | 1.99                     | 0.45              |
| 30:18:15:LYS:HB3  | 56:18:104:MPD:C5   | 2.45                     | 0.45              |
| 32:1a:688:G:H2'   | 32:1a:689:C:H6     | 1.82                     | 0.45              |
| 32:1a:978:A:O2'   | 32:1a:1322:C:N3    | 2.42                     | 0.45              |
| 32:1a:1504:G:OP1  | 32:1a:1507:A:H4'   | 2.17                     | 0.45              |
| 39:1h:37:ARG:NH1  | 39:1h:37:ARG:HB3   | 2.32                     | 0.45              |
| 41:1j:11:PHE:CE1  | 41:1j:67:THR:HG22  | 2.50                     | 0.45              |
| 44:1m:87:TYR:O    | 44:1m:91:ARG:HG2   | 2.17                     | 0.45              |
| 1:2A:911:A:H2'    | 12:2Q:9:TYR:OH     | 2.17                     | 0.45              |
| 1:2A:1491:G:H2'   | 1:2A:1492:G:H8     | 1.81                     | 0.45              |
| 1:2A:2267:A:H5''  | 1:2A:2268:A:H5'    | 1.99                     | 0.45              |
| 1:2A:2533:A:OP1   | 1:2A:2665:A:O2'    | 2.29                     | 0.45              |
| 4:2E:60:ASN:OD1   | 4:2E:63:LEU:HG     | 2.17                     | 0.45              |
| 4:2E:144:ARG:HB3  | 4:2E:145:LYS:H     | 1.59                     | 0.45              |
| 6:2G:138:GLN:HE22 | 6:2G:153:ARG:NH2   | 2.14                     | 0.45              |
| 16:2U:17:ILE:HG13 | 16:2U:32:PHE:HE1   | 1.82                     | 0.45              |
| 32:2a:343:U:H2'   | 32:2a:345:C:C5     | 2.52                     | 0.45              |
| 32:2a:410:G:C2    | 32:2a:429:U:C2     | 3.05                     | 0.45              |
| 32:2a:544:G:OP1   | 35:2d:62:GLN:NE2   | 2.44                     | 0.45              |
| 32:2a:1014:A:C2   | 32:2a:1219:U:H1'   | 2.52                     | 0.45              |
| 32:2a:1159:U:O4'  | 32:2a:1182:G:N2    | 2.50                     | 0.45              |
| 32:2a:1512:U:H2'  | 32:2a:1513:A:C8    | 2.52                     | 0.45              |
| 33:2b:57:PHE:HE2  | 33:2b:185:ILE:HD11 | 1.82                     | 0.45              |
| 36:2e:43:LEU:HD22 | 36:2e:136:MET:HG3  | 1.99                     | 0.45              |
| 41:2j:8:LEU:HB3   | 41:2j:16:LEU:HD22  | 1.98                     | 0.45              |
| 44:2m:23:TYR:HB2  | 44:2m:71:ARG:HH21  | 1.82                     | 0.45              |
| 1:1A:13:A:N1      | 1:1A:525:U:H2'     | 2.32                     | 0.44              |
| 1:1A:29:U:H2'     | 1:1A:30:G:C8       | 2.52                     | 0.44              |
| 1:1A:244:A:C2     | 1:1A:255:A:C4      | 3.05                     | 0.44              |
| 1:1A:747:U:O2     | 1:1A:2014:A:H1'    | 2.17                     | 0.44              |
| 1:1A:748:G:C8     | 18:1W:89:ALA:HB1   | 2.53                     | 0.44              |
| 1:1A:1080:C:H2'   | 1:1A:1081:U:H6     | 1.82                     | 0.44              |
| 1:1A:1805:U:O2    | 3:1D:50:THR:HB     | 2.17                     | 0.44              |
| 5:1F:129:PHE:CD2  | 5:1F:163:VAL:HG21  | 2.52                     | 0.44              |
| 22:10:25:ARG:HD3  | 22:10:29:GLN:NE2   | 2.32                     | 0.44              |
| 30:18:61:LEU:O    | 30:18:63:PRO:HD3   | 2.17                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 38:1g:44:TYR:HE2  | 40:1i:41:VAL:HG11 | 1.82                     | 0.44              |
| 39:1h:120:THR:H   | 39:1h:123:GLU:HB2 | 1.82                     | 0.44              |
| 1:2A:864:G:H1'    | 1:2A:914:C:H42    | 1.82                     | 0.44              |
| 1:2A:1131:G:O6    | 1:2A:2040:C:H1'   | 2.16                     | 0.44              |
| 1:2A:1319:G:C6    | 1:2A:1320:C:N4    | 2.85                     | 0.44              |
| 1:2A:2472:G:N1    | 1:2A:2477:C:OP1   | 2.47                     | 0.44              |
| 4:2E:9:VAL:HG22   | 4:2E:25:VAL:HB    | 1.98                     | 0.44              |
| 7:2H:136:ILE:H    | 7:2H:136:ILE:HG13 | 1.51                     | 0.44              |
| 10:2O:120:GLU:HB2 | 15:2T:68:TYR:HE2  | 1.83                     | 0.44              |
| 11:2P:148:LEU:HB2 | 11:2P:149:GLU:H   | 1.67                     | 0.44              |
| 32:2a:109:A:C6    | 32:2a:326:G:C6    | 3.05                     | 0.44              |
| 32:2a:580:U:H5''  | 46:2o:58:MET:HG2  | 1.99                     | 0.44              |
| 32:2a:837:G:H1    | 32:2a:849:C:H42   | 1.63                     | 0.44              |
| 32:2a:986:A:H1'   | 50:2s:54:GLY:O    | 2.17                     | 0.44              |
| 32:2a:1135:U:H2'  | 32:2a:1137:C:N3   | 2.31                     | 0.44              |
| 37:2f:2:ARG:CZ    | 37:2f:69:GLU:HG2  | 2.48                     | 0.44              |
| 40:2i:17:VAL:HG11 | 40:2i:80:GLY:C    | 2.42                     | 0.44              |
| 1:1A:621:A:OP2    | 11:1P:108:LYS:NZ  | 2.50                     | 0.44              |
| 1:1A:1371:G:H2'   | 1:1A:1372:U:H5    | 1.83                     | 0.44              |
| 1:1A:1866:C:H2'   | 1:1A:1876:A:O4'   | 2.18                     | 0.44              |
| 1:1A:2371:G:H1'   | 28:16:39:TYR:CE1  | 2.53                     | 0.44              |
| 8:1I:72:LEU:C     | 8:1I:74:ASN:N     | 2.76                     | 0.44              |
| 30:18:56:GLU:HG2  | 60:18:225:HOH:O   | 2.17                     | 0.44              |
| 32:1a:174:C:H2'   | 32:1a:175:C:H6    | 1.82                     | 0.44              |
| 32:1a:977:A:H2'   | 32:1a:978:A:H5''  | 1.99                     | 0.44              |
| 32:1a:1021:G:C2   | 32:1a:1022:G:H1'  | 2.53                     | 0.44              |
| 32:1a:1492:A:H4'  | 32:1a:1493:A:C6   | 2.53                     | 0.44              |
| 39:1h:16:ALA:HB1  | 39:1h:21:LYS:HB2  | 1.99                     | 0.44              |
| 1:2A:919:G:N2     | 1:2A:2269:A:OP2   | 2.47                     | 0.44              |
| 1:2A:2115:G:N2    | 1:2A:2117:A:H62   | 2.15                     | 0.44              |
| 1:2A:2185:C:C6    | 1:2A:2185:C:H3'   | 2.52                     | 0.44              |
| 5:2F:184:TYR:CD2  | 5:2F:188:ARG:HD2  | 2.52                     | 0.44              |
| 6:2G:108:ASN:HA   | 26:24:37:SER:HB3  | 1.99                     | 0.44              |
| 6:2G:111:LEU:HB2  | 6:2G:112:PRO:HD3  | 1.98                     | 0.44              |
| 8:2I:116:LEU:HD11 | 8:2I:120:ILE:HD11 | 1.98                     | 0.44              |
| 12:2Q:64:ILE:HD12 | 21:2Z:178:GLU:CD  | 2.42                     | 0.44              |
| 17:2V:21:ARG:NH2  | 17:2V:91:TYR:OH   | 2.50                     | 0.44              |
| 32:2a:489:C:H2'   | 32:2a:490:G:C8    | 2.51                     | 0.44              |
| 32:2a:499:A:H4'   | 32:2a:500:G:H5'   | 1.99                     | 0.44              |
| 32:2a:1323:G:H4'  | 32:2a:1363:C:C2   | 2.52                     | 0.44              |
| 34:2c:58:GLU:HB3  | 41:2j:92:THR:HG21 | 1.99                     | 0.44              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 35:2d:62:GLN:OE1  | 35:2d:65:ARG:NH1   | 2.50                     | 0.44              |
| 1:1A:2001:A:H2'   | 1:1A:2002:G:C8     | 2.52                     | 0.44              |
| 1:1A:2615:U:H2'   | 1:1A:2616:C:H6     | 1.82                     | 0.44              |
| 3:1D:133:LEU:HD23 | 3:1D:133:LEU:HA    | 1.85                     | 0.44              |
| 3:1D:142:VAL:HG13 | 3:1D:191:ALA:HB1   | 2.00                     | 0.44              |
| 5:1F:39:TRP:CH2   | 5:1F:106:ARG:HD3   | 2.52                     | 0.44              |
| 5:1F:183:VAL:HG13 | 60:1F:449:HOH:O    | 2.18                     | 0.44              |
| 21:1Z:129:SER:HB3 | 21:1Z:132:ASN:HB2  | 1.98                     | 0.44              |
| 23:11:8:SER:HB3   | 23:11:66:HIS:CD2   | 2.52                     | 0.44              |
| 24:12:41:ILE:HG13 | 24:12:43:GLN:HG3   | 1.99                     | 0.44              |
| 32:1a:433:C:H2'   | 32:1a:434:U:H6     | 1.82                     | 0.44              |
| 32:1a:762:C:H2'   | 32:1a:763:G:C8     | 2.51                     | 0.44              |
| 32:1a:997:U:H3    | 32:1a:1044:A:H61   | 1.65                     | 0.44              |
| 32:1a:1251:A:H2'  | 32:1a:1252:A:C8    | 2.52                     | 0.44              |
| 32:1a:1518:MA6:C9 | 32:1a:1519:MA6:H92 | 2.46                     | 0.44              |
| 33:1b:217:ARG:HA  | 33:1b:220:ASP:HB2  | 1.99                     | 0.44              |
| 34:1c:52:LEU:HD12 | 34:1c:53:ALA:H     | 1.82                     | 0.44              |
| 35:1d:166:LYS:HB2 | 35:1d:168:ARG:HH12 | 1.82                     | 0.44              |
| 45:1n:27:CYS:SG   | 45:1n:29:ARG:HB2   | 2.56                     | 0.44              |
| 1:2A:251:A:H2'    | 1:2A:252:G:O4'     | 2.18                     | 0.44              |
| 1:2A:630:G:N2     | 1:2A:633:A:OP2     | 2.44                     | 0.44              |
| 1:2A:774:A:H2'    | 1:2A:774:A:N3      | 2.32                     | 0.44              |
| 1:2A:1528:A:OP2   | 60:2A:3930:HOH:O   | 2.21                     | 0.44              |
| 1:2A:2104:G:N2    | 1:2A:2105:C:C4     | 2.85                     | 0.44              |
| 1:2A:2292:C:OP1   | 14:2S:17:ARG:NH2   | 2.41                     | 0.44              |
| 1:2A:2497:A:H5''  | 60:2A:4364:HOH:O   | 2.17                     | 0.44              |
| 51:2t:13:LEU:O    | 51:2t:17:ARG:HG3   | 2.17                     | 0.44              |
| 1:1A:271(P):C:H2' | 1:1A:271(Q):G:O4'  | 2.18                     | 0.44              |
| 1:1A:2186:G:C2    | 1:1A:2187:G:C8     | 3.05                     | 0.44              |
| 1:1A:2649:U:H2'   | 1:1A:2650:U:C6     | 2.52                     | 0.44              |
| 4:1E:13:ARG:HD2   | 4:1E:20:ALA:HB1    | 1.99                     | 0.44              |
| 6:1G:16:ARG:HB2   | 6:1G:17:PRO:HD3    | 2.00                     | 0.44              |
| 30:18:30:ARG:HD3  | 60:18:217:HOH:O    | 2.18                     | 0.44              |
| 32:1a:433:C:H2'   | 32:1a:434:U:C6     | 2.52                     | 0.44              |
| 35:1d:4:TYR:C     | 35:1d:6:GLY:H      | 2.25                     | 0.44              |
| 35:1d:85:LYS:HD2  | 35:1d:85:LYS:HA    | 1.68                     | 0.44              |
| 45:1n:37:PHE:CE1  | 45:1n:53:LEU:HD13  | 2.51                     | 0.44              |
| 47:1p:5:ARG:NH2   | 47:1p:24:ALA:HA    | 2.33                     | 0.44              |
| 1:2A:1019:U:H2'   | 1:2A:1020:A:C8     | 2.52                     | 0.44              |
| 1:2A:1109:C:H3'   | 1:2A:1110:G:C8     | 2.53                     | 0.44              |
| 1:2A:1607:C:H5''  | 1:2A:1608:A:H5'    | 2.00                     | 0.44              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:2A:2164:C:H3'    | 1:2A:2165:G:H8    | 1.81                     | 0.44              |
| 1:2A:2206:G:H5''   | 1:2A:2207:G:N7    | 2.32                     | 0.44              |
| 60:2A:4629:HOH:O   | 27:25:15:ARG:HG2  | 2.16                     | 0.44              |
| 8:2I:66:GLU:HA     | 8:2I:69:LYS:NZ    | 2.33                     | 0.44              |
| 28:26:6:ARG:NH1    | 28:26:26:ASN:HB2  | 2.33                     | 0.44              |
| 32:2a:300:A:H2'    | 32:2a:301:G:O4'   | 2.17                     | 0.44              |
| 32:2a:1314:C:H2'   | 32:2a:1315:U:C6   | 2.52                     | 0.44              |
| 33:2b:187:LEU:HD21 | 33:2b:205:ASP:HA  | 1.99                     | 0.44              |
| 35:2d:71:SER:OG    | 35:2d:74:GLN:HG3  | 2.17                     | 0.44              |
| 38:2g:46:ALA:O     | 38:2g:50:ILE:HG23 | 2.18                     | 0.44              |
| 38:2g:111:ARG:NH1  | 38:2g:113:GLU:OE2 | 2.35                     | 0.44              |
| 41:2j:13:HIS:HA    | 41:2j:16:LEU:HB2  | 1.99                     | 0.44              |
| 43:2l:10:LEU:HB3   | 48:2q:32:TYR:CE2  | 2.53                     | 0.44              |
| 43:2l:97:ARG:HB2   | 43:2l:98:TYR:CE2  | 2.52                     | 0.44              |
| 49:2r:56:THR:HB    | 49:2r:58:LEU:HD13 | 2.00                     | 0.44              |
| 1:1A:197:A:N6      | 1:1A:2430:A:H2'   | 2.32                     | 0.44              |
| 1:1A:583:G:OP2     | 16:1U:10:ARG:NH1  | 2.46                     | 0.44              |
| 1:1A:2320:A:H2'    | 1:1A:2320:A:N3    | 2.32                     | 0.44              |
| 5:1F:65:TRP:CZ2    | 5:1F:75:HIS:HD2   | 2.35                     | 0.44              |
| 11:1P:112:LEU:HD13 | 11:1P:127:ALA:HB2 | 1.98                     | 0.44              |
| 18:1W:68:ARG:HH12  | 18:1W:111:HIS:HA  | 1.82                     | 0.44              |
| 32:1a:418:C:H2'    | 32:1a:419:C:H6    | 1.82                     | 0.44              |
| 32:1a:753:A:OP1    | 46:1o:69:TYR:OH   | 2.33                     | 0.44              |
| 32:1a:1058:G:OP1   | 34:1c:199:LYS:HE3 | 2.17                     | 0.44              |
| 34:1c:9:GLY:HA2    | 34:1c:12:LEU:HG   | 1.99                     | 0.44              |
| 35:1d:50:ARG:HH22  | 36:1e:10:MET:HE3  | 1.82                     | 0.44              |
| 35:1d:170:VAL:HG12 | 35:1d:171:GLY:H   | 1.82                     | 0.44              |
| 41:1j:31:GLY:HA2   | 41:1j:32:ALA:HA   | 1.71                     | 0.44              |
| 47:1p:74:LEU:HB3   | 47:1p:79:VAL:HG21 | 1.98                     | 0.44              |
| 50:1s:37:ARG:H     | 50:1s:37:ARG:HG3  | 1.55                     | 0.44              |
| 1:2A:686:G:N2      | 60:2A:3815:HOH:O  | 2.34                     | 0.44              |
| 1:2A:1263:U:C4     | 1:2A:1264:G:C6    | 3.06                     | 0.44              |
| 1:2A:1467:C:C5     | 1:2A:1546:C:H2'   | 2.51                     | 0.44              |
| 1:2A:1477:A:H2'    | 1:2A:1478:G:O4'   | 2.18                     | 0.44              |
| 1:2A:1697:G:OP2    | 1:2A:1698:A:O2'   | 2.31                     | 0.44              |
| 1:2A:2097:C:H2'    | 1:2A:2098:U:C6    | 2.52                     | 0.44              |
| 1:2A:2784:C:H1'    | 4:2E:37:ARG:HH12  | 1.83                     | 0.44              |
| 10:2O:58:VAL:HG21  | 10:2O:86:ILE:HD13 | 2.00                     | 0.44              |
| 11:2P:85:LEU:HA    | 11:2P:88:LEU:HD12 | 2.00                     | 0.44              |
| 15:2T:16:ARG:HD3   | 15:2T:19:LEU:HG   | 1.98                     | 0.44              |
| 25:23:52:HIS:CD2   | 25:23:53:LEU:HG   | 2.52                     | 0.44              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 32:2a:114:U:H2'   | 32:2a:115:G:C8     | 2.52                     | 0.44              |
| 32:2a:604:G:C6    | 32:2a:605:U:C4     | 3.06                     | 0.44              |
| 32:2a:1503:A:OP1  | 32:2a:1531:A:O2'   | 2.26                     | 0.44              |
| 32:2a:1503:A:H5'  | 32:2a:1531:A:H1'   | 1.99                     | 0.44              |
| 33:2b:146:GLN:O   | 33:2b:150:SER:HB2  | 2.17                     | 0.44              |
| 36:2e:108:ALA:O   | 36:2e:112:LEU:HB2  | 2.18                     | 0.44              |
| 37:2f:30:LEU:HD23 | 37:2f:75:LEU:HD11  | 2.00                     | 0.44              |
| 40:2i:4:TYR:CE1   | 40:2i:88:TYR:HA    | 2.52                     | 0.44              |
| 45:2n:26:ARG:HD3  | 45:2n:43:CYS:HB3   | 2.00                     | 0.44              |
| 47:2p:1:MET:HE3   | 47:2p:3:LYS:HD2    | 1.99                     | 0.44              |
| 53:2y:23:ARG:HA   | 53:2y:23:ARG:HD3   | 1.69                     | 0.44              |
| 1:1A:903:C:H2'    | 1:1A:904:C:H6      | 1.82                     | 0.44              |
| 1:1A:2869:G:H2'   | 1:1A:2870:C:O4'    | 2.18                     | 0.44              |
| 4:1E:101:ARG:NH1  | 4:1E:169:ASN:O     | 2.50                     | 0.44              |
| 7:1H:13:LYS:HA    | 7:1H:14:GLY:HA2    | 1.66                     | 0.44              |
| 7:1H:159:GLU:HG3  | 7:1H:169:VAL:HG11  | 1.99                     | 0.44              |
| 10:1O:9:GLU:O     | 10:1O:83:ALA:HA    | 2.18                     | 0.44              |
| 18:1W:39:THR:O    | 60:1W:301:HOH:O    | 2.21                     | 0.44              |
| 21:1Z:155:LEU:HB3 | 21:1Z:157:LEU:HD21 | 2.00                     | 0.44              |
| 32:1a:221:C:H2'   | 32:1a:222:U:H6     | 1.83                     | 0.44              |
| 32:1a:1187:G:H2'  | 32:1a:1188:A:C8    | 2.53                     | 0.44              |
| 33:1b:163:PHE:HA  | 33:1b:185:ILE:O    | 2.18                     | 0.44              |
| 36:1e:43:LEU:HB2  | 36:1e:136:MET:HE2  | 1.99                     | 0.44              |
| 36:1e:66:MET:HE3  | 36:1e:66:MET:HB3   | 1.80                     | 0.44              |
| 40:1i:84:ALA:O    | 40:1i:87:GLN:HG2   | 2.17                     | 0.44              |
| 44:1m:4:ILE:HA    | 44:1m:5:ALA:HA     | 1.71                     | 0.44              |
| 44:1m:81:LEU:HD11 | 44:1m:88:ARG:HH12  | 1.82                     | 0.44              |
| 47:1p:28:ARG:C    | 47:1p:30:GLY:H     | 2.24                     | 0.44              |
| 1:2A:236:C:H2'    | 1:2A:237:C:C6      | 2.53                     | 0.44              |
| 1:2A:388:G:O2'    | 1:2A:389:G:N7      | 2.49                     | 0.44              |
| 1:2A:668:G:H5'    | 1:2A:669:G:OP2     | 2.18                     | 0.44              |
| 1:2A:1202:C:H42   | 1:2A:1243:G:H1     | 1.65                     | 0.44              |
| 1:2A:1287:A:OP1   | 60:2A:3929:HOH:O   | 2.21                     | 0.44              |
| 1:2A:1485:G:H2'   | 1:2A:1486:A:C8     | 2.53                     | 0.44              |
| 1:2A:1978:A:H2'   | 1:2A:1979:C:O4'    | 2.17                     | 0.44              |
| 3:2D:148:GLU:HB2  | 3:2D:151:LYS:HD2   | 1.99                     | 0.44              |
| 5:2F:126:VAL:HG21 | 5:2F:129:PHE:CZ    | 2.52                     | 0.44              |
| 6:2G:161:THR:HG22 | 6:2G:163:ALA:H     | 1.83                     | 0.44              |
| 8:2I:84:GLY:O     | 8:2I:85:GLU:HB2    | 2.16                     | 0.44              |
| 23:21:83:GLU:H    | 23:21:83:GLU:CD    | 2.26                     | 0.44              |
| 32:2a:1130:A:H2'  | 32:2a:1131:G:H8    | 1.82                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 33:2b:57:PHE:CE2   | 33:2b:185:ILE:HD11 | 2.53                     | 0.44              |
| 35:2d:70:ILE:HG12  | 35:2d:74:GLN:HB2   | 2.00                     | 0.44              |
| 44:2m:14:ARG:CZ    | 44:2m:42:ALA:HA    | 2.48                     | 0.44              |
| 1:1A:340:A:H2'     | 1:1A:341:G:O4'     | 2.17                     | 0.44              |
| 1:1A:784:A:C5      | 3:1D:229:VAL:HG21  | 2.52                     | 0.44              |
| 1:1A:1224:C:O2     | 60:1A:4175:HOH:O   | 2.17                     | 0.44              |
| 1:1A:1514:U:H2'    | 1:1A:1515:G:C8     | 2.52                     | 0.44              |
| 1:1A:2137:C:H42    | 1:1A:2154:G:H1     | 1.65                     | 0.44              |
| 6:1G:16:ARG:O      | 6:1G:20:ILE:HG13   | 2.17                     | 0.44              |
| 6:1G:139:LEU:H     | 6:1G:139:LEU:HG    | 1.58                     | 0.44              |
| 26:14:18:CYS:HB3   | 26:14:39:CYS:HB3   | 1.99                     | 0.44              |
| 32:1a:156:G:H5'    | 32:1a:157:G:OP2    | 2.18                     | 0.44              |
| 32:1a:1059:C:O2'   | 41:1j:53:PRO:HD3   | 2.18                     | 0.44              |
| 43:1l:70:ILE:HD13  | 43:1l:77:LEU:HD12  | 2.00                     | 0.44              |
| 1:2A:1636:C:H2'    | 1:2A:1637:A:C8     | 2.53                     | 0.44              |
| 1:2A:2389:G:H5''   | 1:2A:2390:U:O4'    | 2.17                     | 0.44              |
| 3:2D:158:ALA:O     | 3:2D:161:THR:OG1   | 2.33                     | 0.44              |
| 4:2E:181:LEU:HD12  | 4:2E:181:LEU:HA    | 1.70                     | 0.44              |
| 5:2F:140:LEU:HD13  | 5:2F:170:LEU:HD21  | 2.00                     | 0.44              |
| 8:2I:79:ILE:HG22   | 8:2I:81:VAL:HG22   | 2.00                     | 0.44              |
| 21:2Z:72:ARG:HB2   | 21:2Z:89:PHE:HB2   | 2.00                     | 0.44              |
| 21:2Z:182:LYS:O    | 21:2Z:186:GLU:HB2  | 2.18                     | 0.44              |
| 32:2a:8:A:C6       | 35:2d:209:ARG:HB2  | 2.52                     | 0.44              |
| 32:2a:1148:U:H2'   | 32:2a:1149:C:O4'   | 2.18                     | 0.44              |
| 40:2i:79:LEU:HD22  | 40:2i:104:ARG:HB3  | 1.99                     | 0.44              |
| 41:2j:44:VAL:HG13  | 41:2j:66:ARG:HG2   | 1.99                     | 0.44              |
| 1:1A:7:G:H2'       | 1:1A:8:A:O4'       | 2.17                     | 0.44              |
| 1:1A:414:C:H2'     | 1:1A:415:A:C8      | 2.52                     | 0.44              |
| 1:1A:1045:A:H1'    | 1:1A:1047:G:N3     | 2.32                     | 0.44              |
| 1:1A:2235:G:H2'    | 1:1A:2236:C:C6     | 2.53                     | 0.44              |
| 1:1A:2305:A:H5''   | 6:1G:134:GLY:HA3   | 2.00                     | 0.44              |
| 3:1D:118:VAL:HG22  | 3:1D:119:ALA:H     | 1.83                     | 0.44              |
| 4:1E:28:ALA:HB3    | 4:1E:93:VAL:CG1    | 2.48                     | 0.44              |
| 4:1E:168:MET:HE2   | 4:1E:203:LYS:HG2   | 2.00                     | 0.44              |
| 13:1R:71:GLN:NE2   | 60:1R:307:HOH:O    | 2.50                     | 0.44              |
| 32:1a:9:G:H2'      | 32:1a:10:A:C8      | 2.52                     | 0.44              |
| 32:1a:456:C:H2'    | 32:1a:457:C:H6     | 1.81                     | 0.44              |
| 32:1a:951:G:OP1    | 60:1a:1940:HOH:O   | 2.21                     | 0.44              |
| 33:1b:158:LEU:HD21 | 33:1b:180:LEU:HD22 | 2.00                     | 0.44              |
| 35:1d:178:VAL:C    | 35:1d:180:GLY:H    | 2.24                     | 0.44              |
| 40:1i:3:GLN:HE21   | 40:1i:20:ARG:NE    | 2.14                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 47:1p:53:VAL:HG22  | 47:1p:79:VAL:HG12  | 1.99                     | 0.44              |
| 1:2A:76:C:O3'      | 24:22:59:ARG:HG3   | 2.18                     | 0.44              |
| 1:2A:196:A:N3      | 1:2A:196:A:H2'     | 2.33                     | 0.44              |
| 1:2A:444:C:H5''    | 60:2A:4034:HOH:O   | 2.18                     | 0.44              |
| 1:2A:871:U:H2'     | 1:2A:872:A:C8      | 2.53                     | 0.44              |
| 1:2A:1452:A:OP2    | 60:2A:3932:HOH:O   | 2.21                     | 0.44              |
| 5:2F:187:VAL:HG12  | 11:2P:3:LEU:HD12   | 1.99                     | 0.44              |
| 24:22:1:MET:N      | 24:22:52:ASP:OD2   | 2.38                     | 0.44              |
| 40:2i:6:GLY:HA3    | 40:2i:80:GLY:O     | 2.17                     | 0.44              |
| 41:2j:49:VAL:HG11  | 45:2n:45:ARG:HD2   | 2.00                     | 0.44              |
| 51:2t:24:LEU:HD12  | 51:2t:24:LEU:HA    | 1.84                     | 0.44              |
| 1:1A:61:G:H5'      | 24:12:50:ILE:HG21  | 2.00                     | 0.44              |
| 1:1A:579:G:H2'     | 1:1A:580:C:C6      | 2.53                     | 0.44              |
| 1:1A:862:G:H2'     | 1:1A:863:A:O4'     | 2.18                     | 0.44              |
| 1:1A:1996:C:H4'    | 1:1A:1997:G:OP1    | 2.17                     | 0.44              |
| 1:1A:2134:A:N6     | 1:1A:2157:G:H4'    | 2.27                     | 0.44              |
| 4:1E:2:LYS:HG3     | 4:1E:200:GLU:HB2   | 1.98                     | 0.44              |
| 4:1E:78:LEU:O      | 4:1E:79:ARG:NH1    | 2.47                     | 0.44              |
| 32:1a:141:A:H2'    | 32:1a:142:G:C8     | 2.53                     | 0.44              |
| 32:1a:688:G:H5'    | 42:1k:46:GLY:C     | 2.42                     | 0.44              |
| 32:1a:922:G:H4'    | 36:1e:20:GLN:HA    | 2.00                     | 0.44              |
| 32:1a:1086:U:H3    | 32:1a:1099:G:H22   | 1.65                     | 0.44              |
| 33:1b:35:GLU:HB3   | 33:1b:40:HIS:HA    | 2.00                     | 0.44              |
| 34:1c:131:ARG:HH21 | 34:1c:135:LYS:NZ   | 2.16                     | 0.44              |
| 52:1u:14:TRP:HE3   | 52:1u:15:ARG:HG2   | 1.83                     | 0.44              |
| 1:2A:1009:A:OP2    | 9:2N:37:LYS:NZ     | 2.34                     | 0.44              |
| 1:2A:1044:G:H5'    | 1:2A:1045:A:OP1    | 2.18                     | 0.44              |
| 1:2A:1711:C:H2'    | 1:2A:1712:C:H6     | 1.83                     | 0.44              |
| 1:2A:1817:G:OP1    | 3:2D:88:ARG:NH2    | 2.45                     | 0.44              |
| 1:2A:2408:U:H2'    | 1:2A:2409:G:C8     | 2.53                     | 0.44              |
| 1:2A:2849:U:OP2    | 15:2T:95:ARG:NH1   | 2.49                     | 0.44              |
| 2:2B:64:C:H2'      | 2:2B:65:C:C6       | 2.52                     | 0.44              |
| 6:2G:40:ASN:O      | 6:2G:155:MET:HB2   | 2.17                     | 0.44              |
| 7:2H:149:ARG:HD3   | 7:2H:164:TYR:HD2   | 1.83                     | 0.44              |
| 13:2R:44:LEU:HD22  | 13:2R:48:VAL:HG23  | 1.99                     | 0.44              |
| 17:2V:62:LEU:HD21  | 17:2V:95:LEU:HB2   | 1.99                     | 0.44              |
| 32:2a:437:U:C5'    | 35:2d:155:LEU:HD11 | 2.47                     | 0.44              |
| 32:2a:707:C:H2'    | 32:2a:708:C:H6     | 1.83                     | 0.44              |
| 32:2a:936:C:H2'    | 32:2a:937:A:O4'    | 2.18                     | 0.44              |
| 32:2a:994:A:N7     | 32:2a:1216:G:H4'   | 2.33                     | 0.44              |
| 32:2a:1144:G:N2    | 32:2a:1146:A:H62   | 2.16                     | 0.44              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 36:2e:11:ILE:HD12 | 36:2e:31:LEU:HD13  | 2.00                     | 0.44              |
| 42:2k:56:GLY:O    | 42:2k:89:ALA:HB3   | 2.18                     | 0.44              |
| 1:1A:7:G:H2'      | 1:1A:8:A:H8        | 1.83                     | 0.43              |
| 1:1A:903:C:H2'    | 1:1A:904:C:C6      | 2.53                     | 0.43              |
| 1:1A:2180:U:H2'   | 1:1A:2181:G:O4'    | 2.18                     | 0.43              |
| 1:1A:2307:G:H5'   | 1:1A:2308:G:C2     | 2.53                     | 0.43              |
| 5:1F:129:PHE:HB3  | 5:1F:132:VAL:HG13  | 2.00                     | 0.43              |
| 7:1H:121:ILE:HD13 | 7:1H:121:ILE:HA    | 1.85                     | 0.43              |
| 18:1W:79:GLY:C    | 18:1W:100:THR:HG22 | 2.43                     | 0.43              |
| 23:11:23:LYS:HB3  | 23:11:29:GLY:HA3   | 1.99                     | 0.43              |
| 26:14:57:GLU:CB   | 26:14:58:ARG:HA    | 2.42                     | 0.43              |
| 31:19:16:VAL:HG22 | 31:19:25:VAL:HG22  | 2.00                     | 0.43              |
| 32:1a:193:C:O3'   | 51:1t:61:SER:OG    | 2.33                     | 0.43              |
| 32:1a:270:A:H2'   | 32:1a:271:C:C6     | 2.53                     | 0.43              |
| 32:1a:1060:C:C5   | 34:1c:2:GLY:HA3    | 2.53                     | 0.43              |
| 32:1a:1109:C:H2'  | 32:1a:1110:A:O4'   | 2.18                     | 0.43              |
| 33:1b:7:VAL:HG21  | 33:1b:221:LEU:HG   | 2.00                     | 0.43              |
| 37:1f:97:PHE:HB2  | 49:1r:32:ARG:HD2   | 1.98                     | 0.43              |
| 40:1i:77:ILE:O    | 40:1i:81:ILE:HG23  | 2.18                     | 0.43              |
| 44:1m:20:THR:HA   | 44:1m:25:ILE:HG22  | 1.98                     | 0.43              |
| 49:1r:43:PHE:C    | 49:1r:51:LEU:HD12  | 2.43                     | 0.43              |
| 53:1y:5:ILE:HG23  | 53:1y:39:ILE:HB    | 1.99                     | 0.43              |
| 1:2A:108:U:H2'    | 1:2A:109:G:C8      | 2.53                     | 0.43              |
| 1:2A:770:G:OP2    | 60:2A:3933:HOH:O   | 2.21                     | 0.43              |
| 1:2A:1196:C:H2'   | 1:2A:1197:G:H8     | 1.83                     | 0.43              |
| 1:2A:2286:A:H4'   | 1:2A:2287:A:O4'    | 2.18                     | 0.43              |
| 8:2I:127:VAL:HA   | 8:2I:141:LYS:HA    | 1.99                     | 0.43              |
| 10:2O:60:ALA:HB1  | 10:2O:84:ALA:HB1   | 2.00                     | 0.43              |
| 10:2O:87:ILE:HD12 | 10:2O:91:LEU:HA    | 2.00                     | 0.43              |
| 32:2a:1074:G:C2   | 32:2a:1075:C:C2    | 3.06                     | 0.43              |
| 32:2a:1194:U:H4'  | 36:2e:22:GLY:HA2   | 2.00                     | 0.43              |
| 32:2a:1277:C:H4'  | 32:2a:1281:U:C5    | 2.53                     | 0.43              |
| 34:2c:191:THR:OG1 | 34:2c:194:GLY:O    | 2.34                     | 0.43              |
| 40:2i:111:ARG:HG3 | 45:2n:61:TRP:NE1   | 2.33                     | 0.43              |
| 1:1A:171:G:O2'    | 1:1A:172:C:H5'     | 2.19                     | 0.43              |
| 1:1A:242:G:C8     | 30:18:5:LYS:HG2    | 2.53                     | 0.43              |
| 1:1A:614(C):A:C4  | 5:1F:180:GLY:HA3   | 2.52                     | 0.43              |
| 1:1A:1245:G:OP1   | 11:1P:13:ASN:ND2   | 2.51                     | 0.43              |
| 14:1S:59:LYS:H    | 14:1S:59:LYS:HG3   | 1.59                     | 0.43              |
| 14:1S:95:HIS:CG   | 14:1S:96:GLY:N     | 2.86                     | 0.43              |
| 20:1Y:55:TYR:CE1  | 20:1Y:61:ILE:HG21  | 2.53                     | 0.43              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 32:1a:600:C:H2'   | 32:1a:601:C:C6     | 2.50                     | 0.43              |
| 32:1a:674:G:H21   | 42:1k:116:HIS:HB2  | 1.83                     | 0.43              |
| 32:1a:985:C:H2'   | 32:1a:986:A:C8     | 2.53                     | 0.43              |
| 32:1a:1283:G:H2'  | 32:1a:1284:C:C6    | 2.53                     | 0.43              |
| 42:1k:82:VAL:HB   | 42:1k:108:ILE:HG12 | 1.99                     | 0.43              |
| 45:1n:37:PHE:HZ   | 45:1n:56:VAL:HG21  | 1.83                     | 0.43              |
| 1:2A:251:A:C5     | 1:2A:252:G:H1'     | 2.53                     | 0.43              |
| 1:2A:672:C:OP1    | 60:2A:3920:HOH:O   | 2.20                     | 0.43              |
| 1:2A:1830:C:OP2   | 60:2A:3931:HOH:O   | 2.21                     | 0.43              |
| 8:2I:62:LYS:HG2   | 8:2I:133:HIS:NE2   | 2.33                     | 0.43              |
| 14:2S:26:LEU:HD22 | 14:2S:87:PHE:CD1   | 2.53                     | 0.43              |
| 16:2U:11:ARG:O    | 16:2U:15:LYS:HG3   | 2.18                     | 0.43              |
| 18:2W:82:LEU:HD22 | 18:2W:84:ARG:HH22  | 1.83                     | 0.43              |
| 32:2a:54:C:N4     | 32:2a:353:A:OP2    | 2.41                     | 0.43              |
| 32:2a:420:U:H1'   | 32:2a:424:G:N2     | 2.33                     | 0.43              |
| 32:2a:625:G:H4'   | 47:2p:16:HIS:CD2   | 2.53                     | 0.43              |
| 32:2a:743:U:H2'   | 32:2a:744:C:C6     | 2.53                     | 0.43              |
| 32:2a:1371:G:H5'' | 40:2i:68:GLY:HA2   | 2.00                     | 0.43              |
| 44:2m:15:VAL:HG11 | 44:2m:48:LEU:HD21  | 2.00                     | 0.43              |
| 1:1A:456:C:H4'    | 60:1A:4772:HOH:O   | 2.18                     | 0.43              |
| 1:1A:483:A:H5''   | 20:1Y:50:ARG:HD3   | 2.00                     | 0.43              |
| 1:1A:795:C:H2'    | 1:1A:796:C:H6      | 1.83                     | 0.43              |
| 1:1A:1292:U:H2'   | 1:1A:1293:C:H6     | 1.83                     | 0.43              |
| 1:1A:2646:C:H2'   | 1:1A:2647:U:O4'    | 2.18                     | 0.43              |
| 1:1A:2844:G:O6    | 60:1A:4193:HOH:O   | 2.20                     | 0.43              |
| 7:1H:3:ARG:NH2    | 7:1H:65:HIS:HB3    | 2.33                     | 0.43              |
| 24:12:32:LEU:HD11 | 24:12:54:LYS:HG3   | 2.00                     | 0.43              |
| 32:1a:453:A:C6    | 32:1a:454:C:C4     | 3.06                     | 0.43              |
| 32:1a:503:C:H2'   | 32:1a:504:C:H6     | 1.84                     | 0.43              |
| 32:1a:1434:A:H2'  | 32:1a:1435:G:O4'   | 2.18                     | 0.43              |
| 38:1g:108:ALA:O   | 38:1g:119:ARG:HD2  | 2.18                     | 0.43              |
| 45:1n:37:PHE:HB3  | 45:1n:39:LEU:HD12  | 2.00                     | 0.43              |
| 53:1y:87:LYS:O    | 53:1y:91:LYS:HB2   | 2.18                     | 0.43              |
| 1:2A:813:U:H2'    | 1:2A:814:C:C6      | 2.54                     | 0.43              |
| 1:2A:2218:U:O4'   | 23:21:52:ARG:NH2   | 2.51                     | 0.43              |
| 3:2D:275:LYS:HD2  | 3:2D:275:LYS:HA    | 1.78                     | 0.43              |
| 4:2E:112:GLY:O    | 4:2E:159:HIS:HA    | 2.18                     | 0.43              |
| 8:2I:69:LYS:HB2   | 8:2I:69:LYS:HE2    | 1.67                     | 0.43              |
| 8:2I:93:THR:HA    | 60:2I:303:HOH:O    | 2.18                     | 0.43              |
| 9:2N:73:THR:HA    | 9:2N:83:LYS:O      | 2.18                     | 0.43              |
| 12:2Q:4:PRO:HG3   | 12:2Q:69:PHE:HE2   | 1.83                     | 0.43              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 20:2Y:11:ASP:O    | 20:2Y:27:VAL:HG23  | 2.18                     | 0.43              |
| 20:2Y:40:GLU:O    | 20:2Y:42:VAL:HG23  | 2.18                     | 0.43              |
| 21:2Z:67:LEU:HA   | 21:2Z:68:PRO:HD3   | 1.85                     | 0.43              |
| 21:2Z:98:MET:HE3  | 21:2Z:98:MET:HB2   | 1.91                     | 0.43              |
| 32:2a:256:U:H2'   | 32:2a:257:G:C8     | 2.53                     | 0.43              |
| 33:2b:97:TRP:HZ3  | 33:2b:172:ILE:HG22 | 1.82                     | 0.43              |
| 33:2b:178:ARG:NH1 | 39:2h:68:ARG:HH22  | 2.16                     | 0.43              |
| 34:2c:10:PHE:HD1  | 45:2n:58:LYS:HE2   | 1.84                     | 0.43              |
| 45:2n:32:SER:O    | 45:2n:40:CYS:HA    | 2.17                     | 0.43              |
| 52:2u:6:ARG:C     | 52:2u:8:THR:H      | 2.26                     | 0.43              |
| 1:1A:118:A:H3'    | 1:1A:119:A:C5'     | 2.48                     | 0.43              |
| 1:1A:220:G:O6     | 60:1A:4184:HOH:O   | 2.19                     | 0.43              |
| 1:1A:249:C:O2     | 30:18:12:LYS:NZ    | 2.40                     | 0.43              |
| 1:1A:1152:C:H4'   | 16:1U:77:SER:HA    | 2.00                     | 0.43              |
| 1:1A:2640:G:OP1   | 9:1N:97:ARG:NH2    | 2.49                     | 0.43              |
| 6:1G:114:ILE:HG12 | 6:1G:140:ILE:HG12  | 2.00                     | 0.43              |
| 10:1O:108:GLU:H   | 10:1O:108:GLU:HG3  | 1.62                     | 0.43              |
| 27:15:45:VAL:HG11 | 27:15:58:LEU:HD22  | 2.00                     | 0.43              |
| 29:17:9:ARG:NH1   | 29:17:47:ARG:HB2   | 2.33                     | 0.43              |
| 32:1a:100:C:H2'   | 32:1a:101:A:H8     | 1.77                     | 0.43              |
| 32:1a:109:A:C6    | 32:1a:326:G:C6     | 3.07                     | 0.43              |
| 32:1a:376:G:O3'   | 47:1p:5:ARG:NE     | 2.51                     | 0.43              |
| 32:1a:453:A:C5    | 32:1a:454:C:C4     | 3.07                     | 0.43              |
| 32:1a:474:G:H2'   | 32:1a:475:G:H8     | 1.81                     | 0.43              |
| 32:1a:742:G:OP2   | 46:1o:35:ARG:NH2   | 2.50                     | 0.43              |
| 41:1j:40:LEU:HB2  | 41:1j:69:ASN:HB2   | 2.00                     | 0.43              |
| 1:2A:363:G:H2'    | 1:2A:363(A):A:C8   | 2.52                     | 0.43              |
| 1:2A:705:A:H2'    | 1:2A:706:A:O4'     | 2.19                     | 0.43              |
| 1:2A:854:G:H2'    | 1:2A:855:G:C8      | 2.53                     | 0.43              |
| 1:2A:1096:A:C4    | 1:2A:1097:U:H5     | 2.36                     | 0.43              |
| 1:2A:1165:U:H2'   | 1:2A:1166:C:C6     | 2.52                     | 0.43              |
| 1:2A:1820:U:H4'   | 1:2A:1821:A:OP2    | 2.18                     | 0.43              |
| 1:2A:2001:A:H2'   | 1:2A:2002:G:C8     | 2.53                     | 0.43              |
| 1:2A:2345:G:N3    | 1:2A:2381:C:H2'    | 2.33                     | 0.43              |
| 1:2A:2410:G:C2    | 1:2A:2411:A:H1'    | 2.53                     | 0.43              |
| 1:2A:2869:G:H2'   | 1:2A:2870:C:O4'    | 2.19                     | 0.43              |
| 6:2G:165:THR:OG1  | 6:2G:168:GLU:HG3   | 2.18                     | 0.43              |
| 13:2R:82:GLU:O    | 13:2R:85:PRO:HD2   | 2.18                     | 0.43              |
| 32:2a:437:U:H5''  | 35:2d:155:LEU:HD11 | 2.00                     | 0.43              |
| 32:2a:570:G:H1'   | 32:2a:820:U:C4     | 2.54                     | 0.43              |
| 32:2a:1057:G:H2'  | 32:2a:1058:G:O4'   | 2.19                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 32:2a:1262:C:H2'  | 32:2a:1263:C:C6   | 2.53                     | 0.43              |
| 32:2a:1512:U:H2'  | 32:2a:1513:A:H8   | 1.82                     | 0.43              |
| 35:2d:173:TRP:CE2 | 35:2d:189:PRO:HG3 | 2.53                     | 0.43              |
| 38:2g:113:GLU:H   | 38:2g:113:GLU:HG2 | 1.45                     | 0.43              |
| 39:2h:9:MET:HG3   | 39:2h:26:VAL:HG11 | 2.00                     | 0.43              |
| 1:1A:330:A:O2'    | 1:1A:331:A:H8     | 2.01                     | 0.43              |
| 1:1A:549:G:H2'    | 1:1A:551:G:O4'    | 2.18                     | 0.43              |
| 1:1A:606:U:H4'    | 1:1A:658:C:H4'    | 1.99                     | 0.43              |
| 1:1A:1762:A:H2'   | 60:1A:7537:HOH:O  | 2.18                     | 0.43              |
| 1:1A:2114:A:O2'   | 1:1A:2168:G:OP1   | 2.35                     | 0.43              |
| 1:1A:2200:C:O2    | 1:1A:2226:C:N4    | 2.51                     | 0.43              |
| 8:1I:1:MET:HE2    | 8:1I:38:LEU:HD11  | 2.00                     | 0.43              |
| 11:1P:91:PHE:CE1  | 11:1P:99:LEU:HD22 | 2.54                     | 0.43              |
| 15:1T:79:HIS:NE2  | 60:1T:303:HOH:O   | 2.37                     | 0.43              |
| 24:12:65:ASN:OD1  | 24:12:69:ARG:NH1  | 2.48                     | 0.43              |
| 32:1a:1213:A:C8   | 32:1a:1215:G:C5   | 3.07                     | 0.43              |
| 32:1a:1261:A:H3'  | 32:1a:1262:C:C6   | 2.53                     | 0.43              |
| 32:1a:1376:U:P    | 38:1g:94:ARG:HH12 | 2.42                     | 0.43              |
| 33:1b:82:ARG:HG3  | 33:1b:92:TYR:CZ   | 2.54                     | 0.43              |
| 37:1f:26:ILE:O    | 37:1f:30:LEU:HG   | 2.18                     | 0.43              |
| 44:1m:95:GLY:O    | 44:1m:110:ARG:HB3 | 2.19                     | 0.43              |
| 1:2A:55:G:O2'     | 1:2A:127:A:N1     | 2.45                     | 0.43              |
| 1:2A:57:C:H2'     | 1:2A:58:G:O4'     | 2.18                     | 0.43              |
| 1:2A:1062:G:N3    | 1:2A:1063:G:C8    | 2.87                     | 0.43              |
| 1:2A:1359:A:N1    | 1:2A:1372:U:O4    | 2.51                     | 0.43              |
| 1:2A:2099:U:H3    | 1:2A:2190:G:H1    | 1.66                     | 0.43              |
| 1:2A:2539:C:H4'   | 31:29:3:VAL:HG21  | 2.00                     | 0.43              |
| 2:2B:24:G:H4'     | 2:2B:25:A:C8      | 2.54                     | 0.43              |
| 7:2H:88:LEU:HD13  | 7:2H:165:ALA:HA   | 2.01                     | 0.43              |
| 17:2V:19:LYS:HE2  | 17:2V:19:LYS:HB2  | 1.87                     | 0.43              |
| 32:2a:137:C:H2'   | 32:2a:138:G:H8    | 1.84                     | 0.43              |
| 32:2a:164:U:H2'   | 32:2a:165:C:H6    | 1.83                     | 0.43              |
| 32:2a:299:G:H2'   | 32:2a:300:A:C8    | 2.53                     | 0.43              |
| 32:2a:600:C:H2'   | 32:2a:601:C:H6    | 1.83                     | 0.43              |
| 32:2a:628:G:H2'   | 32:2a:629:G:C8    | 2.53                     | 0.43              |
| 32:2a:707:C:H2'   | 32:2a:708:C:C6    | 2.53                     | 0.43              |
| 32:2a:1107:C:C4   | 32:2a:1108:G:C8   | 3.07                     | 0.43              |
| 33:2b:82:ARG:HB2  | 33:2b:94:ASN:CG   | 2.43                     | 0.43              |
| 50:2s:40:ILE:HD12 | 50:2s:66:MET:O    | 2.18                     | 0.43              |
| 51:2t:13:LEU:HD23 | 51:2t:13:LEU:HA   | 1.85                     | 0.43              |
| 1:1A:7:G:H2'      | 1:1A:8:A:C8       | 2.54                     | 0.43              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:1A:64:A:O3'      | 19:1X:71:GLY:HA3  | 2.19                     | 0.43              |
| 1:1A:1430:C:H2'    | 1:1A:1431:U:C6    | 2.53                     | 0.43              |
| 1:1A:1754:C:H2'    | 1:1A:1755:A:O4'   | 2.18                     | 0.43              |
| 1:1A:1824:G:O3'    | 3:1D:249:PRO:HD3  | 2.19                     | 0.43              |
| 4:1E:49:LEU:HD12   | 4:1E:49:LEU:HA    | 1.65                     | 0.43              |
| 8:1I:109:ILE:HD12  | 8:1I:109:ILE:HA   | 1.85                     | 0.43              |
| 12:1Q:7:MET:HB2    | 12:1Q:7:MET:HE3   | 1.64                     | 0.43              |
| 32:1a:1024:G:H2'   | 32:1a:1024:G:N3   | 2.34                     | 0.43              |
| 32:1a:1184:G:H2'   | 32:1a:1185:G:H8   | 1.84                     | 0.43              |
| 32:1a:1206:G:C6    | 32:1a:1207:2MG:C5 | 3.07                     | 0.43              |
| 32:1a:1286:A:N6    | 32:1a:1355:G:OP1  | 2.45                     | 0.43              |
| 32:1a:1298:C:H4'   | 32:1a:1299:A:C4   | 2.53                     | 0.43              |
| 37:1f:69:GLU:CD    | 37:1f:69:GLU:H    | 2.26                     | 0.43              |
| 40:1i:66:ARG:HH21  | 40:1i:66:ARG:HB2  | 1.82                     | 0.43              |
| 1:2A:644:A:H4'     | 1:2A:645:C:C5     | 2.54                     | 0.43              |
| 1:2A:1593:G:H2'    | 1:2A:1594:G:H8    | 1.83                     | 0.43              |
| 1:2A:2313:C:H2'    | 1:2A:2314:C:C6    | 2.53                     | 0.43              |
| 1:2A:2336:A:H61    | 22:20:43:THR:CG2  | 2.32                     | 0.43              |
| 1:2A:2711:A:H5''   | 1:2A:2712:U:H5''  | 2.01                     | 0.43              |
| 1:2A:2816:C:O2     | 1:2A:2883:A:O2'   | 2.35                     | 0.43              |
| 1:2A:2881:C:H2'    | 1:2A:2882:A:O4'   | 2.19                     | 0.43              |
| 56:2A:3758:MPD:H12 | 56:2A:3758:MPD:H4 | 1.88                     | 0.43              |
| 4:2E:59:VAL:HG21   | 4:2E:74:PRO:HB3   | 2.00                     | 0.43              |
| 5:2F:155:LEU:HD23  | 5:2F:186:ILE:HG13 | 2.00                     | 0.43              |
| 11:2P:82:GLY:HA2   | 11:2P:113:LYS:O   | 2.19                     | 0.43              |
| 22:20:68:GLU:HB3   | 22:20:80:HIS:HB2  | 2.00                     | 0.43              |
| 24:22:10:LEU:HD21  | 24:22:59:ARG:HG2  | 2.01                     | 0.43              |
| 32:2a:586:C:O2'    | 32:2a:878:G:H4'   | 2.19                     | 0.43              |
| 32:2a:1181:G:O2'   | 32:2a:1182:G:N7   | 2.50                     | 0.43              |
| 32:2a:1255:G:O2'   | 32:2a:1258:G:O2'  | 2.29                     | 0.43              |
| 33:2b:24:TRP:CD1   | 33:2b:24:TRP:N    | 2.87                     | 0.43              |
| 34:2c:33:LEU:HA    | 34:2c:36:ASP:HB2  | 2.00                     | 0.43              |
| 35:2d:14:ARG:HA    | 35:2d:39:PRO:HB3  | 2.00                     | 0.43              |
| 45:2n:46:GLU:O     | 45:2n:50:LYS:HG2  | 2.19                     | 0.43              |
| 47:2p:28:ARG:HG3   | 47:2p:29:ASP:N    | 2.33                     | 0.43              |
| 1:1A:184:C:H2'     | 1:1A:185:U:H6     | 1.83                     | 0.43              |
| 1:1A:306:U:H2'     | 1:1A:307:G:O4'    | 2.19                     | 0.43              |
| 1:1A:1537:G:H2'    | 1:1A:1538:G:C8    | 2.50                     | 0.43              |
| 1:1A:1721:G:H5'    | 1:1A:1722:A:OP2   | 2.19                     | 0.43              |
| 1:1A:1932:A:OP2    | 60:1A:4213:HOH:O  | 2.21                     | 0.43              |
| 1:1A:2502:G:OP1    | 60:1A:4211:HOH:O  | 2.21                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 6:1G:34:LEU:HD12   | 6:1G:100:TRP:CZ3   | 2.54                     | 0.43              |
| 7:1H:88:LEU:HD23   | 7:1H:130:ARG:HG2   | 2.00                     | 0.43              |
| 7:1H:124:GLU:OE2   | 7:1H:132:ARG:HD2   | 2.18                     | 0.43              |
| 11:1P:100:LEU:HD12 | 11:1P:112:LEU:HD11 | 2.00                     | 0.43              |
| 17:1V:88:ARG:NH1   | 60:1V:308:HOH:O    | 2.47                     | 0.43              |
| 19:1X:35:THR:HG22  | 19:1X:38:GLU:HB3   | 2.01                     | 0.43              |
| 20:1Y:5:MET:HE2    | 20:1Y:32:PRO:HA    | 2.00                     | 0.43              |
| 28:16:6:ARG:NH1    | 28:16:26:ASN:HB2   | 2.33                     | 0.43              |
| 32:1a:114:U:O2'    | 32:1a:115:G:H5'    | 2.19                     | 0.43              |
| 32:1a:391:G:P      | 47:1p:28:ARG:HH12  | 2.42                     | 0.43              |
| 32:1a:472:A:H4'    | 47:1p:80:PHE:O     | 2.19                     | 0.43              |
| 32:1a:688:G:H2'    | 32:1a:689:C:C6     | 2.54                     | 0.43              |
| 32:1a:977:A:H1'    | 32:1a:982:U:O4     | 2.18                     | 0.43              |
| 32:1a:1446:U:O2'   | 32:1a:1447:A:H3'   | 2.18                     | 0.43              |
| 33:1b:98:LEU:O     | 33:1b:101:MET:HG3  | 2.18                     | 0.43              |
| 34:1c:148:GLY:HA3  | 34:1c:172:ARG:O    | 2.18                     | 0.43              |
| 36:1e:31:LEU:HD23  | 36:1e:31:LEU:HA    | 1.77                     | 0.43              |
| 40:1i:9:ARG:CB     | 40:1i:104:ARG:HE   | 2.31                     | 0.43              |
| 51:1t:58:LYS:HA    | 51:1t:58:LYS:HD2   | 1.81                     | 0.43              |
| 1:2A:93:G:H2'      | 1:2A:94:C:C6       | 2.54                     | 0.43              |
| 1:2A:192:C:O2'     | 1:2A:802:A:N3      | 2.50                     | 0.43              |
| 1:2A:224:G:H2'     | 1:2A:225:A:O4'     | 2.19                     | 0.43              |
| 1:2A:345:A:H1'     | 1:2A:346:A:N7      | 2.33                     | 0.43              |
| 1:2A:631:A:H1'     | 11:2P:66:GLY:HA2   | 2.00                     | 0.43              |
| 1:2A:993:G:H1'     | 17:2V:89:GLN:OE1   | 2.18                     | 0.43              |
| 1:2A:1073:A:H2'    | 1:2A:1074:G:H8     | 1.84                     | 0.43              |
| 1:2A:1962:5MC:N4   | 60:2A:4240:HOH:O   | 2.46                     | 0.43              |
| 4:2E:1:MET:O       | 4:2E:84:PHE:HB2    | 2.19                     | 0.43              |
| 4:2E:111:ARG:HA    | 13:2R:1:MET:SD     | 2.59                     | 0.43              |
| 11:2P:88:LEU:HD11  | 11:2P:114:ILE:HD12 | 2.00                     | 0.43              |
| 32:2a:189(D):C:H2' | 32:2a:189(E):U:O4' | 2.19                     | 0.43              |
| 32:2a:353:A:H5'    | 32:2a:353:A:H8     | 1.83                     | 0.43              |
| 32:2a:401:C:H1'    | 32:2a:622:A:H1'    | 2.00                     | 0.43              |
| 32:2a:1259:C:N4    | 32:2a:1260:C:O2    | 2.52                     | 0.43              |
| 35:2d:121:VAL:O    | 35:2d:134:ASP:HA   | 2.18                     | 0.43              |
| 38:2g:16:LEU:HD12  | 40:2i:41:VAL:HG12  | 1.99                     | 0.43              |
| 38:2g:62:PHE:HA    | 38:2g:124:LEU:HD22 | 2.01                     | 0.43              |
| 47:2p:48:TRP:HH2   | 47:2p:76:GLN:NE2   | 2.17                     | 0.43              |
| 48:2q:6:LEU:O      | 48:2q:58:GLU:HA    | 2.19                     | 0.43              |
| 1:1A:371:A:H5''    | 60:1A:5289:HOH:O   | 2.18                     | 0.43              |
| 1:1A:515:A:H2      | 1:1A:1260:G:N3     | 2.16                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:1A:1405:U:H2'    | 1:1A:1406:U:C6     | 2.54                     | 0.43              |
| 1:1A:2418:A:H2'    | 1:1A:2419:U:C6     | 2.54                     | 0.43              |
| 1:1A:2839:G:H5'    | 13:1R:46:GLY:HA2   | 2.01                     | 0.43              |
| 1:1A:2877:G:OP2    | 60:1A:4210:HOH:O   | 2.21                     | 0.43              |
| 3:1D:145:VAL:HG12  | 3:1D:146:GLU:O     | 2.19                     | 0.43              |
| 3:1D:147:LEU:HD13  | 3:1D:155:LEU:HD11  | 2.00                     | 0.43              |
| 13:1R:96:ARG:NH1   | 13:1R:117:VAL:HG22 | 2.34                     | 0.43              |
| 25:13:5:LYS:HG3    | 25:13:36:VAL:HG22  | 2.00                     | 0.43              |
| 25:13:31:LEU:HD23  | 25:13:31:LEU:HA    | 1.86                     | 0.43              |
| 32:1a:1223:C:P     | 50:1s:78:ARG:HH21  | 2.41                     | 0.43              |
| 32:1a:1305:G:H22   | 32:1a:1331:G:H1'   | 1.84                     | 0.43              |
| 33:1b:196:LEU:HD12 | 33:1b:196:LEU:HA   | 1.90                     | 0.43              |
| 33:1b:231:GLU:OE1  | 33:1b:231:GLU:HA   | 2.19                     | 0.43              |
| 44:1m:45:VAL:HG13  | 44:1m:48:LEU:HD12  | 2.00                     | 0.43              |
| 53:1y:64:SER:OG    | 53:1y:66:LYS:NZ    | 2.52                     | 0.43              |
| 1:2A:7:G:H2'       | 1:2A:8:A:O4'       | 2.19                     | 0.43              |
| 1:2A:218:A:N1      | 1:2A:235:U:H4'     | 2.34                     | 0.43              |
| 1:2A:667:U:O2      | 30:28:2:PRO:HD2    | 2.19                     | 0.43              |
| 1:2A:927:G:H2'     | 1:2A:928:G:O4'     | 2.18                     | 0.43              |
| 1:2A:990:A:N6      | 1:2A:1186:G:H1'    | 2.34                     | 0.43              |
| 1:2A:996:A:O3'     | 16:2U:91:ASP:HB2   | 2.19                     | 0.43              |
| 1:2A:2019:A:N7     | 27:25:9:LYS:HE2    | 2.32                     | 0.43              |
| 1:2A:2144:U:O3'    | 1:2A:2145:C:H2'    | 2.18                     | 0.43              |
| 1:2A:2287:A:O2'    | 1:2A:2289:G:N7     | 2.46                     | 0.43              |
| 1:2A:2303:G:O4'    | 6:2G:126:ASP:HA    | 2.19                     | 0.43              |
| 1:2A:2469:A:H2'    | 1:2A:2470:G:O4'    | 2.19                     | 0.43              |
| 7:2H:101:ARG:HG2   | 7:2H:117:PRO:HG2   | 2.01                     | 0.43              |
| 8:2I:69:LYS:HD3    | 8:2I:136:VAL:HG13  | 2.01                     | 0.43              |
| 8:2I:100:ALA:O     | 8:2I:104:GLN:N     | 2.46                     | 0.43              |
| 10:2O:12:ASP:C     | 10:2O:99:PHE:HE2   | 2.26                     | 0.43              |
| 32:2a:948:C:OP2    | 44:2m:108:ARG:HB2  | 2.18                     | 0.43              |
| 32:2a:1036:G:H3'   | 32:2a:1037:C:H6    | 1.83                     | 0.43              |
| 32:2a:1318:A:O2'   | 50:2s:37:ARG:HD2   | 2.19                     | 0.43              |
| 32:2a:1323:G:H4'   | 32:2a:1363:C:N3    | 2.33                     | 0.43              |
| 34:2c:180:ALA:HB1  | 34:2c:203:PHE:CE1  | 2.51                     | 0.43              |
| 44:2m:27:LYS:HD2   | 44:2m:27:LYS:HA    | 1.81                     | 0.43              |
| 1:1A:773:U:H5'     | 3:1D:47:GLY:HA3    | 2.01                     | 0.43              |
| 1:1A:948:G:OP2     | 60:1A:4209:HOH:O   | 2.21                     | 0.43              |
| 1:1A:2422:A:H2'    | 60:1A:7536:HOH:O   | 2.19                     | 0.43              |
| 60:1A:4503:HOH:O   | 27:15:55:ARG:NH2   | 2.44                     | 0.43              |
| 7:1H:13:LYS:HB3    | 7:1H:13:LYS:HE2    | 1.78                     | 0.43              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 11:1P:68:GLN:HG3  | 60:1P:302:HOH:O    | 2.18                     | 0.43              |
| 15:1T:15:VAL:HG12 | 15:1T:16:ARG:N     | 2.34                     | 0.43              |
| 19:1X:41:ASN:O    | 19:1X:45:THR:HG23  | 2.19                     | 0.43              |
| 32:1a:280:C:N3    | 48:1q:39:SER:OG    | 2.51                     | 0.43              |
| 32:1a:651:C:H2'   | 32:1a:652:U:C6     | 2.54                     | 0.43              |
| 32:1a:690:G:C6    | 32:1a:691:G:C6     | 3.07                     | 0.43              |
| 32:1a:731:G:OP1   | 32:1a:766:A:H1'    | 2.18                     | 0.43              |
| 32:1a:831:U:H2'   | 32:1a:832:C:C6     | 2.54                     | 0.43              |
| 32:1a:867:G:O2'   | 32:1a:873:A:N1     | 2.51                     | 0.43              |
| 32:1a:1263:C:H2'  | 32:1a:1264:C:H6    | 1.84                     | 0.43              |
| 36:1e:8:GLU:HG2   | 36:1e:34:VAL:HG23  | 1.99                     | 0.43              |
| 36:1e:51:VAL:O    | 36:1e:55:VAL:HG23  | 2.19                     | 0.43              |
| 1:2A:662:G:H5''   | 11:2P:16:ARG:HG2   | 2.01                     | 0.43              |
| 1:2A:776:G:H4'    | 1:2A:777:A:O5'     | 2.18                     | 0.43              |
| 1:2A:853:G:N7     | 60:2A:4099:HOH:O   | 2.36                     | 0.43              |
| 1:2A:2111:C:N4    | 1:2A:2147:G:H22    | 2.13                     | 0.43              |
| 1:2A:2560:C:OP2   | 60:2A:3936:HOH:O   | 2.21                     | 0.43              |
| 1:2A:2746:U:N3    | 1:2A:2756:U:O4     | 2.47                     | 0.43              |
| 12:2Q:1:MET:HE2   | 12:2Q:1:MET:HB3    | 1.89                     | 0.43              |
| 16:2U:106:PHE:O   | 16:2U:110:VAL:HG23 | 2.19                     | 0.43              |
| 22:20:46:LYS:N    | 22:20:77:ARG:O     | 2.51                     | 0.43              |
| 32:2a:35:G:C5     | 32:2a:36:C:C4      | 3.06                     | 0.43              |
| 32:2a:947:G:H1    | 32:2a:1234:C:H42   | 1.65                     | 0.43              |
| 32:2a:1091:U:H2'  | 32:2a:1093:A:OP2   | 2.19                     | 0.43              |
| 38:2g:16:LEU:H    | 38:2g:16:LEU:HG    | 1.41                     | 0.43              |
| 42:2k:22:HIS:HB3  | 42:2k:29:ILE:HB    | 2.00                     | 0.43              |
| 49:2r:21:LYS:HE3  | 49:2r:54:ARG:O     | 2.19                     | 0.43              |
| 1:1A:458:G:O2'    | 29:17:39:ARG:HD3   | 2.18                     | 0.43              |
| 1:1A:1275:A:N1    | 1:1A:1295:C:O2'    | 2.48                     | 0.43              |
| 1:1A:1688:U:H1'   | 1:1A:1701:A:C6     | 2.54                     | 0.43              |
| 1:1A:2115:G:H22   | 1:1A:2119:A:P      | 2.42                     | 0.43              |
| 1:1A:2682:U:O2'   | 15:1T:58:ASN:ND2   | 2.51                     | 0.43              |
| 3:1D:221:VAL:CG2  | 3:1D:226:MET:HE2   | 2.49                     | 0.43              |
| 5:1F:135:LYS:HB2  | 5:1F:138:GLU:CD    | 2.44                     | 0.43              |
| 30:18:61:LEU:C    | 30:18:63:PRO:HD3   | 2.43                     | 0.43              |
| 32:1a:137:C:H2'   | 32:1a:138:G:H8     | 1.84                     | 0.43              |
| 32:1a:232:G:H1'   | 32:1a:262:A:N1     | 2.34                     | 0.43              |
| 33:1b:98:LEU:HB2  | 33:1b:101:MET:HE3  | 2.01                     | 0.43              |
| 35:1d:22:LYS:O    | 35:1d:113:SER:HB3  | 2.19                     | 0.43              |
| 37:1f:15:ASP:OD1  | 37:1f:18:GLN:N     | 2.27                     | 0.43              |
| 40:1i:49:PRO:HB3  | 40:1i:82:ALA:HB2   | 2.01                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 49:1r:31:LEU:HD12  | 49:1r:31:LEU:HA    | 1.86                     | 0.43              |
| 50:1s:70:LYS:HB2   | 50:1s:73:GLU:HG3   | 2.01                     | 0.43              |
| 1:2A:220:G:O2'     | 1:2A:233:A:N3      | 2.47                     | 0.43              |
| 1:2A:686:G:H2'     | 1:2A:788:A:N1      | 2.34                     | 0.43              |
| 1:2A:1091:G:N2     | 1:2A:1100:C:O2     | 2.50                     | 0.43              |
| 1:2A:2377:A:H2'    | 1:2A:2378:A:C8     | 2.54                     | 0.43              |
| 4:2E:52:LEU:HD13   | 4:2E:76:ARG:HD3    | 2.00                     | 0.43              |
| 22:20:45:PHE:HE1   | 22:20:77:ARG:HE    | 1.67                     | 0.43              |
| 28:26:28:ARG:HE    | 28:26:28:ARG:HB2   | 1.56                     | 0.43              |
| 32:2a:715:A:H2'    | 32:2a:716:A:C8     | 2.53                     | 0.43              |
| 32:2a:858:G:O6     | 32:2a:869:G:H3'    | 2.19                     | 0.43              |
| 36:2e:88:LYS:HD3   | 36:2e:123:LEU:HD12 | 2.01                     | 0.43              |
| 37:2f:9:VAL:HB     | 37:2f:87:ARG:HB2   | 2.01                     | 0.43              |
| 38:2g:54:THR:O     | 38:2g:56:GLN:N     | 2.51                     | 0.43              |
| 42:2k:85:ARG:HG2   | 42:2k:111:ASP:O    | 2.19                     | 0.43              |
| 1:1A:118:A:H3'     | 1:1A:119:A:H5''    | 2.00                     | 0.42              |
| 1:1A:1439:A:H2'    | 1:1A:1440:G:O4'    | 2.19                     | 0.42              |
| 1:1A:1963:U:H4'    | 1:1A:1964:G:OP1    | 2.18                     | 0.42              |
| 1:1A:2695:C:H2'    | 1:1A:2696:U:C6     | 2.54                     | 0.42              |
| 6:1G:20:ILE:O      | 6:1G:24:GLY:N      | 2.45                     | 0.42              |
| 6:1G:50:ALA:HB1    | 6:1G:52:ILE:HG12   | 2.02                     | 0.42              |
| 21:1Z:92:SER:O     | 21:1Z:130:PRO:HG2  | 2.19                     | 0.42              |
| 32:1a:430:A:OP1    | 35:1d:9:CYS:HB2    | 2.19                     | 0.42              |
| 32:1a:984:C:N4     | 32:1a:1221:G:H1    | 2.17                     | 0.42              |
| 32:1a:1228:C:P     | 44:1m:108:ARG:HH22 | 2.41                     | 0.42              |
| 33:1b:215:LEU:HD23 | 33:1b:215:LEU:HA   | 1.84                     | 0.42              |
| 33:1b:223:ILE:H    | 33:1b:223:ILE:HG13 | 1.73                     | 0.42              |
| 36:1e:48:ALA:HB3   | 36:1e:54:ALA:HB2   | 2.01                     | 0.42              |
| 39:1h:87:SER:HA    | 39:1h:93:VAL:HG23  | 2.01                     | 0.42              |
| 1:2A:184:C:H2'     | 1:2A:185:U:H6      | 1.83                     | 0.42              |
| 1:2A:290:G:H2'     | 1:2A:291:C:O4'     | 2.17                     | 0.42              |
| 1:2A:482:A:P       | 20:2Y:50:ARG:HH22  | 2.42                     | 0.42              |
| 1:2A:1011:G:OP1    | 16:2U:77:SER:OG    | 2.29                     | 0.42              |
| 1:2A:1047:G:H2'    | 1:2A:1110:G:H22    | 1.83                     | 0.42              |
| 1:2A:2151:G:C6     | 1:2A:2152:G:C6     | 3.07                     | 0.42              |
| 1:2A:2186:G:N1     | 1:2A:2187:G:C6     | 2.87                     | 0.42              |
| 8:2I:72:LEU:HB3    | 8:2I:140:LEU:HD12  | 2.00                     | 0.42              |
| 11:2P:86:LYS:HE3   | 11:2P:86:LYS:HB2   | 1.73                     | 0.42              |
| 25:23:37:LEU:HB3   | 25:23:43:ILE:HG21  | 2.01                     | 0.42              |
| 32:2a:78:G:H2'     | 32:2a:79:G:H5'     | 2.00                     | 0.42              |
| 32:2a:312:C:H2'    | 32:2a:313:A:O4'    | 2.19                     | 0.42              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 32:2a:404:U:H2'   | 32:2a:405:U:C6     | 2.54                     | 0.42              |
| 32:2a:545:C:OP1   | 35:2d:61:LYS:NZ    | 2.50                     | 0.42              |
| 32:2a:730:G:C5    | 32:2a:731:G:H1'    | 2.54                     | 0.42              |
| 32:2a:1401:G:C2   | 32:2a:1402:4OC:H1' | 2.54                     | 0.42              |
| 33:2b:178:ARG:NH2 | 39:2h:68:ARG:HH22  | 2.17                     | 0.42              |
| 38:2g:68:ASN:ND2  | 38:2g:128:ALA:HA   | 2.32                     | 0.42              |
| 43:2l:53:ARG:HD2  | 43:2l:93:LEU:HD11  | 2.00                     | 0.42              |
| 46:2o:35:ARG:O    | 46:2o:39:LEU:HB2   | 2.19                     | 0.42              |
| 47:2p:34:GLU:OE1  | 47:2p:55:ARG:NH2   | 2.46                     | 0.42              |
| 47:2p:34:GLU:CD   | 47:2p:55:ARG:HH21  | 2.27                     | 0.42              |
| 48:2q:62:SER:CB   | 48:2q:72:ARG:HH11  | 2.32                     | 0.42              |
| 49:2r:21:LYS:HA   | 49:2r:21:LYS:HD3   | 1.89                     | 0.42              |
| 1:1A:956:G:H2'    | 1:1A:957:A:H2'     | 2.01                     | 0.42              |
| 1:1A:1173:G:N2    | 1:1A:1177:A:OP1    | 2.52                     | 0.42              |
| 1:1A:1398:C:OP1   | 19:1X:53:LYS:NZ    | 2.49                     | 0.42              |
| 1:1A:2150:U:H2'   | 1:1A:2151:G:H8     | 1.84                     | 0.42              |
| 1:1A:2168:G:C2    | 1:1A:2171:A:C8     | 3.08                     | 0.42              |
| 2:1B:90:A:N7      | 2:1B:91:C:H1'      | 2.34                     | 0.42              |
| 3:1D:244:ARG:HB2  | 3:1D:245:PRO:HD2   | 2.01                     | 0.42              |
| 4:1E:79:ARG:HA    | 4:1E:79:ARG:HD3    | 1.83                     | 0.42              |
| 6:1G:96:ARG:N     | 6:1G:99:MET:HE2    | 2.33                     | 0.42              |
| 7:1H:86:GLU:OE2   | 7:1H:132:ARG:NH1   | 2.51                     | 0.42              |
| 14:1S:11:LYS:O    | 14:1S:15:ARG:HG3   | 2.19                     | 0.42              |
| 22:10:53:MET:HA   | 22:10:58:THR:O     | 2.19                     | 0.42              |
| 23:11:95:LEU:O    | 23:11:98:LEU:HB2   | 2.18                     | 0.42              |
| 32:1a:1201:A:H4'  | 32:1a:1202:G:O5'   | 2.19                     | 0.42              |
| 32:1a:1226:C:O2'  | 44:1m:111:LYS:NZ   | 2.53                     | 0.42              |
| 33:1b:21:ARG:HA   | 33:1b:39:ILE:HA    | 2.00                     | 0.42              |
| 33:1b:208:ILE:H   | 33:1b:208:ILE:HG12 | 1.62                     | 0.42              |
| 37:1f:68:PRO:HG2  | 37:1f:71:ARG:HD2   | 2.01                     | 0.42              |
| 38:1g:89:MET:SD   | 38:1g:155:ARG:HB2  | 2.59                     | 0.42              |
| 46:1o:39:LEU:HD23 | 46:1o:39:LEU:HA    | 1.85                     | 0.42              |
| 1:2A:438:G:H2'    | 1:2A:440:G:H8      | 1.85                     | 0.42              |
| 1:2A:637:A:H2'    | 11:2P:117:GLU:OE2  | 2.19                     | 0.42              |
| 1:2A:820:A:N3     | 1:2A:943:U:H4'     | 2.34                     | 0.42              |
| 1:2A:1417:C:H2'   | 1:2A:1418:G:O4'    | 2.18                     | 0.42              |
| 1:2A:2161:C:O2'   | 1:2A:2173:A:O2'    | 2.36                     | 0.42              |
| 1:2A:2224:G:H4'   | 1:2A:2226:C:C2     | 2.54                     | 0.42              |
| 1:2A:2461:C:H2'   | 1:2A:2462:U:C6     | 2.54                     | 0.42              |
| 3:2D:124:PRO:HG2  | 3:2D:129:ASN:HD21  | 1.83                     | 0.42              |
| 32:2a:535:A:H3'   | 32:2a:536:C:H5     | 1.84                     | 0.42              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 32:2a:1515:C:H2'  | 32:2a:1516:G:H8    | 1.82                     | 0.42              |
| 33:2b:104:ASN:O   | 33:2b:108:ILE:HG12 | 2.19                     | 0.42              |
| 44:2m:4:ILE:HG13  | 44:2m:57:ARG:HA    | 2.01                     | 0.42              |
| 47:2p:60:LEU:HD12 | 47:2p:60:LEU:HA    | 1.85                     | 0.42              |
| 50:2s:3:ARG:NH1   | 50:2s:7:LYS:HE2    | 2.34                     | 0.42              |
| 1:1A:55:G:O2'     | 1:1A:127:A:N1      | 2.51                     | 0.42              |
| 1:1A:557:U:OP1    | 60:1A:4215:HOH:O   | 2.21                     | 0.42              |
| 1:1A:719:C:H2'    | 1:1A:720:C:C6      | 2.55                     | 0.42              |
| 1:1A:1071:G:H1'   | 1:1A:1089:G:C8     | 2.54                     | 0.42              |
| 1:1A:2830:G:H4'   | 60:1A:5631:HOH:O   | 2.18                     | 0.42              |
| 3:1D:13:ARG:HA    | 3:1D:13:ARG:HD2    | 1.87                     | 0.42              |
| 7:1H:71:LEU:HD12  | 7:1H:71:LEU:HA     | 1.75                     | 0.42              |
| 10:1O:107:ARG:C   | 10:1O:109:LYS:H    | 2.27                     | 0.42              |
| 15:1T:4:GLY:O     | 15:1T:8:LYS:HG2    | 2.20                     | 0.42              |
| 24:12:10:LEU:HD23 | 24:12:10:LEU:HA    | 1.91                     | 0.42              |
| 30:18:4:MET:HE2   | 30:18:4:MET:HB3    | 1.87                     | 0.42              |
| 32:1a:141:A:H1'   | 32:1a:182:U:O2     | 2.19                     | 0.42              |
| 32:1a:328:C:H4'   | 32:1a:329:A:H5''   | 2.02                     | 0.42              |
| 32:1a:434:U:H2'   | 32:1a:435:C:C6     | 2.53                     | 0.42              |
| 32:1a:598:U:H4'   | 39:1h:94:TYR:CD2   | 2.54                     | 0.42              |
| 32:1a:1008:C:H2'  | 32:1a:1009:G:O4'   | 2.19                     | 0.42              |
| 32:1a:1090:U:H2'  | 32:1a:1091:U:H6    | 1.84                     | 0.42              |
| 32:1a:1352:C:H2'  | 32:1a:1353:G:C8    | 2.54                     | 0.42              |
| 33:1b:70:PHE:O    | 33:1b:92:TYR:HA    | 2.19                     | 0.42              |
| 35:1d:163:GLU:C   | 35:1d:165:MET:H    | 2.26                     | 0.42              |
| 36:1e:45:PHE:CD2  | 36:1e:47:LYS:HE2   | 2.55                     | 0.42              |
| 39:1h:11:THR:HG23 | 39:1h:14:ARG:HH21  | 1.83                     | 0.42              |
| 43:1l:11:VAL:HG11 | 48:1q:36:ILE:HG21  | 2.01                     | 0.42              |
| 44:1m:78:ILE:HG22 | 44:1m:82:MET:HE2   | 2.01                     | 0.42              |
| 48:1q:14:LYS:HB2  | 48:1q:14:LYS:HE2   | 1.70                     | 0.42              |
| 49:1r:51:LEU:HD23 | 49:1r:52:PRO:HD2   | 2.01                     | 0.42              |
| 1:2A:1022:G:N7    | 9:2N:66:LYS:HE2    | 2.34                     | 0.42              |
| 1:2A:1267:U:H2'   | 1:2A:1268:A:H8     | 1.84                     | 0.42              |
| 1:2A:2571:C:H5''  | 1:2A:2572:A:H5''   | 2.01                     | 0.42              |
| 12:2Q:2:LEU:O     | 12:2Q:70:PRO:HG2   | 2.20                     | 0.42              |
| 14:2S:66:ALA:HA   | 14:2S:69:VAL:HG12  | 2.01                     | 0.42              |
| 20:2Y:88:LYS:HA   | 20:2Y:88:LYS:HD2   | 1.93                     | 0.42              |
| 28:26:50:ARG:HG2  | 28:26:51:GLU:H     | 1.84                     | 0.42              |
| 32:2a:695:A:OP2   | 42:2k:53:SER:N     | 2.53                     | 0.42              |
| 32:2a:737:A:H2'   | 32:2a:738:C:H6     | 1.82                     | 0.42              |
| 32:2a:932:C:H2'   | 32:2a:933:G:H8     | 1.83                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 32:2a:1465:C:H2'   | 32:2a:1466:C:O4'   | 2.19                     | 0.42              |
| 33:2b:158:LEU:HD12 | 33:2b:158:LEU:HA   | 1.90                     | 0.42              |
| 1:1A:864:G:O2'     | 1:1A:865:C:H5'     | 2.19                     | 0.42              |
| 1:1A:1496:A:N7     | 60:1A:4417:HOH:O   | 2.37                     | 0.42              |
| 60:1A:4405:HOH:O   | 16:1U:15:LYS:NZ    | 2.45                     | 0.42              |
| 32:1a:44:G:C2      | 32:1a:45:U:H1'     | 2.55                     | 0.42              |
| 32:1a:265:G:H5'    | 48:1q:64:PRO:O     | 2.19                     | 0.42              |
| 32:1a:1429:C:H2'   | 32:1a:1430:C:C6    | 2.54                     | 0.42              |
| 39:1h:28:ALA:HA    | 39:1h:59:LEU:HG    | 2.02                     | 0.42              |
| 39:1h:121:ASP:OD1  | 39:1h:121:ASP:N    | 2.53                     | 0.42              |
| 44:1m:51:ALA:O     | 44:1m:55:ARG:HG3   | 2.20                     | 0.42              |
| 50:1s:52:TYR:HB2   | 50:1s:57:HIS:CE1   | 2.53                     | 0.42              |
| 51:1t:49:ALA:O     | 51:1t:53:LEU:HG    | 2.19                     | 0.42              |
| 1:2A:271(E):U:H2'  | 1:2A:271(F):C:C6   | 2.54                     | 0.42              |
| 1:2A:372:G:H8      | 23:21:65:SER:O     | 2.02                     | 0.42              |
| 1:2A:900:A:H2'     | 1:2A:901:A:O4'     | 2.20                     | 0.42              |
| 1:2A:1038:C:H42    | 1:2A:1117:G:H1     | 1.66                     | 0.42              |
| 1:2A:1357:U:H2'    | 1:2A:1358:G:O4'    | 2.19                     | 0.42              |
| 1:2A:2133:G:C2     | 1:2A:2157:G:H2'    | 2.54                     | 0.42              |
| 1:2A:2233:U:H2'    | 1:2A:2234:G:C8     | 2.54                     | 0.42              |
| 1:2A:2466:C:H5''   | 31:29:6:SER:HB2    | 2.00                     | 0.42              |
| 3:2D:24:ILE:HG23   | 3:2D:83:GLU:HA     | 2.02                     | 0.42              |
| 5:2F:40:GLN:HE22   | 5:2F:182:ASN:HB2   | 1.84                     | 0.42              |
| 10:2O:15:GLY:HA2   | 10:2O:47:ILE:HD11  | 2.01                     | 0.42              |
| 12:2Q:37:LEU:HD12  | 12:2Q:128:LYS:HB3  | 2.02                     | 0.42              |
| 17:2V:37:VAL:O     | 17:2V:52:VAL:HG22  | 2.18                     | 0.42              |
| 19:2X:72:LYS:HG2   | 19:2X:73:ARG:O     | 2.19                     | 0.42              |
| 23:21:62:VAL:HG22  | 23:21:63:ALA:O     | 2.20                     | 0.42              |
| 32:2a:381:C:H2'    | 32:2a:382:A:O4'    | 2.19                     | 0.42              |
| 32:2a:827:U:H5''   | 32:2a:828:A:OP2    | 2.19                     | 0.42              |
| 32:2a:1179:A:H2'   | 32:2a:1180:A:O4'   | 2.20                     | 0.42              |
| 32:2a:1236:A:O2'   | 32:2a:1304:G:H4'   | 2.19                     | 0.42              |
| 35:2d:61:LYS:HA    | 35:2d:203:VAL:HG22 | 2.00                     | 0.42              |
| 36:2e:6:PHE:HB2    | 36:2e:34:VAL:HG22  | 2.02                     | 0.42              |
| 44:2m:60:VAL:HG23  | 44:2m:64:TRP:HZ3   | 1.85                     | 0.42              |
| 47:2p:1:MET:HE2    | 47:2p:1:MET:H1     | 1.84                     | 0.42              |
| 48:2q:50:LYS:HE3   | 48:2q:51:TYR:HE2   | 1.84                     | 0.42              |
| 50:2s:44:MET:O     | 50:2s:47:HIS:HB2   | 2.19                     | 0.42              |
| 1:1A:228:A:H2'     | 1:1A:230:U:H1'     | 2.02                     | 0.42              |
| 1:1A:436:C:H2'     | 1:1A:437:G:C8      | 2.55                     | 0.42              |
| 1:1A:1045:A:OP1    | 1:1A:1045:A:H4'    | 2.18                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:1B:91:C:OP1      | 12:1Q:16:ARG:NH1   | 2.51                     | 0.42              |
| 3:1D:146:GLU:HG2   | 3:1D:152:GLY:C     | 2.45                     | 0.42              |
| 11:1P:95:VAL:HG22  | 11:1P:125:VAL:HB   | 2.02                     | 0.42              |
| 17:1V:16:PRO:HA    | 17:1V:96:ILE:HG22  | 2.01                     | 0.42              |
| 28:16:9:LEU:HA     | 28:16:54:ILE:HB    | 2.01                     | 0.42              |
| 32:1a:277:C:H5''   | 48:1q:68:ARG:HH21  | 1.84                     | 0.42              |
| 32:1a:438:G:H5'    | 35:1d:123:HIS:HD2  | 1.84                     | 0.42              |
| 33:1b:80:ILE:HD13  | 33:1b:211:ILE:HB   | 2.00                     | 0.42              |
| 35:1d:57:ARG:HE    | 35:1d:205:GLU:HB3  | 1.84                     | 0.42              |
| 53:1y:70:MET:HE2   | 53:1y:70:MET:HB3   | 1.81                     | 0.42              |
| 1:2A:300:A:H2'     | 1:2A:334:C:H1'     | 2.01                     | 0.42              |
| 1:2A:1065:U:H4'    | 1:2A:1066:U:H5'    | 2.00                     | 0.42              |
| 1:2A:1091:G:H2'    | 1:2A:1091:G:N3     | 2.34                     | 0.42              |
| 1:2A:1340:U:OP1    | 19:2X:16:LYS:NZ    | 2.40                     | 0.42              |
| 1:2A:1826:G:H4'    | 3:2D:242:ARG:CZ    | 2.50                     | 0.42              |
| 1:2A:2030:A:H4'    | 1:2A:2031:A:C8     | 2.54                     | 0.42              |
| 1:2A:2157:G:H8     | 1:2A:2157:G:O5'    | 2.02                     | 0.42              |
| 1:2A:2595:G:OP2    | 60:2A:3922:HOH:O   | 2.21                     | 0.42              |
| 3:2D:77:ALA:HA     | 3:2D:97:TYR:HA     | 2.01                     | 0.42              |
| 3:2D:218:ARG:HB3   | 3:2D:219:PRO:HD2   | 2.00                     | 0.42              |
| 4:2E:170:LEU:HD23  | 4:2E:184:VAL:HG11  | 2.02                     | 0.42              |
| 14:2S:15:ARG:HB3   | 14:2S:19:LYS:HE2   | 2.00                     | 0.42              |
| 21:2Z:23:LYS:HB3   | 21:2Z:38:TYR:CD1   | 2.55                     | 0.42              |
| 25:23:8:LEU:O      | 25:23:32:GLN:N     | 2.42                     | 0.42              |
| 32:2a:254:G:OP1    | 48:2q:66:SER:OG    | 2.29                     | 0.42              |
| 32:2a:539:A:H2'    | 32:2a:540:G:C8     | 2.55                     | 0.42              |
| 32:2a:583:A:H2'    | 32:2a:584:G:O4'    | 2.19                     | 0.42              |
| 33:2b:170:GLU:HB3  | 33:2b:173:ALA:HB3  | 2.02                     | 0.42              |
| 42:2k:83:ILE:HG23  | 42:2k:109:VAL:HG13 | 2.01                     | 0.42              |
| 43:2l:110:VAL:HG23 | 43:2l:120:TYR:HB3  | 2.01                     | 0.42              |
| 51:2t:17:ARG:O     | 51:2t:21:LYS:HG3   | 2.19                     | 0.42              |
| 1:1A:391:G:H1'     | 1:1A:411:G:O4'     | 2.20                     | 0.42              |
| 1:1A:443:A:N7      | 5:1F:45:ARG:HG2    | 2.34                     | 0.42              |
| 1:1A:2100:G:C6     | 1:1A:2190:G:C6     | 3.08                     | 0.42              |
| 4:1E:21:VAL:O      | 4:1E:23:VAL:HG13   | 2.20                     | 0.42              |
| 5:1F:53:THR:CG2    | 5:1F:55:GLY:H      | 2.32                     | 0.42              |
| 7:1H:126:PRO:HB2   | 7:1H:127:GLU:H     | 1.65                     | 0.42              |
| 8:1I:9:LEU:HD21    | 8:1I:35:LEU:HD13   | 2.00                     | 0.42              |
| 12:1Q:64:ILE:HG13  | 21:1Z:178:GLU:HG3  | 2.01                     | 0.42              |
| 15:1T:36:GLU:HG2   | 32:1a:346:G:OP1    | 2.19                     | 0.42              |
| 21:1Z:182:LYS:HB3  | 21:1Z:182:LYS:HE2  | 1.77                     | 0.42              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 32:1a:58:C:O2'    | 32:1a:388:G:N7     | 2.45                     | 0.42              |
| 32:1a:841:U:C5    | 32:1a:848:C:H1'    | 2.54                     | 0.42              |
| 32:1a:1003:G:H8   | 32:1a:1003:G:O5'   | 2.02                     | 0.42              |
| 32:1a:1168:A:H3'  | 32:1a:1169:A:H8    | 1.85                     | 0.42              |
| 32:1a:1293:G:H2'  | 32:1a:1294:G:C8    | 2.53                     | 0.42              |
| 35:1d:10:ARG:HB2  | 35:1d:40:PRO:HG3   | 2.01                     | 0.42              |
| 35:1d:122:ARG:HD2 | 35:1d:122:ARG:HA   | 1.72                     | 0.42              |
| 39:1h:77:GLU:HG2  | 39:1h:78:GLN:N     | 2.35                     | 0.42              |
| 1:2A:674:G:P      | 60:2A:4048:HOH:O   | 2.78                     | 0.42              |
| 1:2A:1087:G:H2'   | 1:2A:1088:A:H5'    | 2.01                     | 0.42              |
| 1:2A:1364:G:N7    | 23:21:3:LYS:HD2    | 2.35                     | 0.42              |
| 1:2A:2130:U:O2'   | 1:2A:2133:G:H4'    | 2.19                     | 0.42              |
| 7:2H:90:LYS:HD3   | 7:2H:159:GLU:HG2   | 2.02                     | 0.42              |
| 8:2I:50:ARG:O     | 8:2I:54:GLN:NE2    | 2.53                     | 0.42              |
| 8:2I:73:GLU:C     | 8:2I:75:LEU:H      | 2.28                     | 0.42              |
| 32:2a:41:G:H2'    | 32:2a:42:G:C8      | 2.54                     | 0.42              |
| 32:2a:441:A:H3'   | 32:2a:442:C:H6     | 1.83                     | 0.42              |
| 35:2d:20:TYR:N    | 35:2d:20:TYR:CD2   | 2.88                     | 0.42              |
| 39:2h:104:ARG:HD3 | 39:2h:104:ARG:HA   | 1.77                     | 0.42              |
| 1:1A:524:U:H2'    | 1:1A:525:U:C6      | 2.55                     | 0.42              |
| 1:1A:811:U:H2'    | 11:1P:21:ARG:HA    | 2.02                     | 0.42              |
| 1:1A:820:A:H1'    | 1:1A:943:U:H1'     | 2.01                     | 0.42              |
| 1:1A:1143:A:OP2   | 60:1A:4205:HOH:O   | 2.21                     | 0.42              |
| 1:1A:2661:G:H2'   | 1:1A:2662:A:C8     | 2.54                     | 0.42              |
| 9:1N:138:LEU:HD23 | 9:1N:138:LEU:HA    | 1.76                     | 0.42              |
| 16:1U:59:ARG:O    | 16:1U:63:VAL:HG23  | 2.20                     | 0.42              |
| 16:1U:81:HIS:CE1  | 16:1U:85:LYS:HD3   | 2.54                     | 0.42              |
| 20:1Y:9:LYS:HA    | 20:1Y:10:GLY:HA2   | 1.66                     | 0.42              |
| 29:17:39:ARG:NE   | 60:17:202:HOH:O    | 2.50                     | 0.42              |
| 32:1a:656:C:C2'   | 46:1o:28:GLN:HE22  | 2.32                     | 0.42              |
| 32:1a:1367:C:H5'  | 41:1j:60:ARG:NH1   | 2.34                     | 0.42              |
| 33:1b:166:ASP:HB3 | 33:1b:169:LYS:HB3  | 2.01                     | 0.42              |
| 36:1e:12:LEU:HB3  | 36:1e:31:LEU:HB2   | 2.00                     | 0.42              |
| 39:1h:86:ILE:HG13 | 39:1h:133:LEU:HD22 | 2.02                     | 0.42              |
| 48:1q:10:VAL:HG22 | 48:1q:21:VAL:HG22  | 2.01                     | 0.42              |
| 1:2A:30:G:H2'     | 1:2A:31:C:C6       | 2.54                     | 0.42              |
| 1:2A:370:G:OP2    | 1:2A:370:G:H8      | 2.03                     | 0.42              |
| 1:2A:859:G:N2     | 1:2A:917:A:OP2     | 2.31                     | 0.42              |
| 1:2A:954:G:C5     | 1:2A:955:C:C5      | 3.08                     | 0.42              |
| 1:2A:1005:C:H2'   | 1:2A:1006:C:H6     | 1.83                     | 0.42              |
| 1:2A:1015:G:O2'   | 1:2A:1016:G:H5'    | 2.20                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:2A:1325:G:OP1    | 1:2A:1647:G:O2'    | 2.26                     | 0.42              |
| 1:2A:1783:A:OP2    | 60:2A:3939:HOH:O   | 2.22                     | 0.42              |
| 1:2A:2467:C:H4'    | 12:2Q:123:HIS:CD2  | 2.54                     | 0.42              |
| 1:2A:2817:G:OP1    | 13:2R:99:LYS:NZ    | 2.51                     | 0.42              |
| 5:2F:155:LEU:HB2   | 5:2F:189:THR:HG21  | 2.02                     | 0.42              |
| 14:2S:77:ALA:HB1   | 14:2S:82:ILE:HB    | 2.02                     | 0.42              |
| 32:2a:756:C:H2'    | 32:2a:757:U:O4'    | 2.20                     | 0.42              |
| 32:2a:1027:C:H2'   | 32:2a:1028:C:N3    | 2.35                     | 0.42              |
| 32:2a:1068:G:H8    | 32:2a:1068:G:OP2   | 2.01                     | 0.42              |
| 32:2a:1074:G:O2'   | 32:2a:1101:A:N1    | 2.45                     | 0.42              |
| 33:2b:69:LEU:HB3   | 33:2b:162:ILE:HG22 | 2.01                     | 0.42              |
| 34:2c:39:ILE:O     | 34:2c:43:LEU:HG    | 2.20                     | 0.42              |
| 36:2e:12:LEU:HD13  | 36:2e:129:ILE:HG13 | 2.01                     | 0.42              |
| 50:2s:52:TYR:HB2   | 50:2s:57:HIS:CE1   | 2.55                     | 0.42              |
| 51:2t:72:LEU:HD23  | 51:2t:72:LEU:HA    | 1.83                     | 0.42              |
| 1:1A:12:U:O2       | 1:1A:12:U:H2'      | 2.19                     | 0.42              |
| 1:1A:72:U:OP2      | 24:12:29:LYS:NZ    | 2.51                     | 0.42              |
| 1:1A:289:A:H2'     | 1:1A:290:G:O4'     | 2.19                     | 0.42              |
| 1:1A:1054:A:H5'    | 1:1A:1055:G:OP2    | 2.20                     | 0.42              |
| 1:1A:1798:U:H5'    | 3:1D:259:THR:CG2   | 2.38                     | 0.42              |
| 1:1A:2014:A:OP1    | 60:1A:4220:HOH:O   | 2.22                     | 0.42              |
| 1:1A:2139:C:O5'    | 1:1A:2139:C:H6     | 2.02                     | 0.42              |
| 5:1F:11:VAL:HA     | 5:1F:125:LEU:O     | 2.20                     | 0.42              |
| 5:1F:132:VAL:HA    | 5:1F:138:GLU:HB3   | 2.01                     | 0.42              |
| 6:1G:38:VAL:HG22   | 6:1G:93:THR:HG23   | 2.00                     | 0.42              |
| 7:1H:152:ARG:HD3   | 7:1H:152:ARG:HA    | 1.74                     | 0.42              |
| 8:1I:140:LEU:HD23  | 8:1I:140:LEU:HA    | 1.76                     | 0.42              |
| 12:1Q:109:VAL:HG22 | 12:1Q:113:GLN:OE1  | 2.19                     | 0.42              |
| 16:1U:39:LEU:HD23  | 16:1U:39:LEU:HA    | 1.88                     | 0.42              |
| 32:1a:8:A:H5'      | 36:1e:101:ILE:HG22 | 2.00                     | 0.42              |
| 32:1a:263:A:OP2    | 51:1t:79:ARG:NH1   | 2.53                     | 0.42              |
| 32:1a:971:G:OP1    | 32:1a:972:C:H5''   | 2.19                     | 0.42              |
| 32:1a:983:A:H2     | 32:1a:984:C:C6     | 2.38                     | 0.42              |
| 33:1b:95:GLN:HB3   | 33:1b:96:ARG:H     | 1.67                     | 0.42              |
| 37:1f:14:LEU:HD13  | 37:1f:18:GLN:HB3   | 2.01                     | 0.42              |
| 37:1f:44:GLY:HA2   | 37:1f:59:TYR:CZ    | 2.55                     | 0.42              |
| 49:1r:42:ARG:HD3   | 49:1r:42:ARG:HA    | 1.71                     | 0.42              |
| 53:1y:61:LEU:HD11  | 53:1y:85:LEU:HB2   | 2.01                     | 0.42              |
| 1:2A:335:C:H4'     | 20:2Y:73:ARG:NH1   | 2.35                     | 0.42              |
| 1:2A:702:G:C2      | 1:2A:731:C:C2      | 3.07                     | 0.42              |
| 1:2A:719:C:H2'     | 1:2A:720:C:C6      | 2.55                     | 0.42              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:2A:1016:G:C4     | 1:2A:1017:G:C8    | 3.08                     | 0.42              |
| 1:2A:1025:G:O2'    | 60:2A:3826:HOH:O  | 2.16                     | 0.42              |
| 1:2A:1153:C:H2'    | 1:2A:1154:G:O4'   | 2.19                     | 0.42              |
| 1:2A:2203:U:H2'    | 1:2A:2205:C:C6    | 2.55                     | 0.42              |
| 1:2A:2336:A:H61    | 22:20:43:THR:HG22 | 1.84                     | 0.42              |
| 1:2A:2641:G:OP1    | 9:2N:83:LYS:HD2   | 2.19                     | 0.42              |
| 4:2E:143:ASN:HD22  | 4:2E:147:PRO:CD   | 2.33                     | 0.42              |
| 5:2F:129:PHE:CD2   | 5:2F:163:VAL:HG21 | 2.54                     | 0.42              |
| 7:2H:30:LYS:HE3    | 7:2H:30:LYS:HB3   | 1.92                     | 0.42              |
| 8:2I:104:GLN:OE1   | 8:2I:105:HIS:CG   | 2.72                     | 0.42              |
| 11:2P:97:PRO:HD3   | 11:2P:126:VAL:O   | 2.20                     | 0.42              |
| 32:2a:1005:A:N6    | 32:2a:1024:G:O2'  | 2.53                     | 0.42              |
| 32:2a:1010:G:H2'   | 32:2a:1011:G:H8   | 1.84                     | 0.42              |
| 32:2a:1490:C:H2'   | 32:2a:1491:G:H8   | 1.84                     | 0.42              |
| 33:2b:15:VAL:HB    | 33:2b:209:ARG:HB3 | 2.01                     | 0.42              |
| 33:2b:98:LEU:HB2   | 33:2b:101:MET:HG3 | 2.02                     | 0.42              |
| 44:2m:90:LEU:HD23  | 44:2m:93:ARG:HH21 | 1.84                     | 0.42              |
| 50:2s:50:ALA:HB1   | 50:2s:57:HIS:HB3  | 2.02                     | 0.42              |
| 1:1A:234:C:H2'     | 1:1A:235:U:H6     | 1.84                     | 0.42              |
| 1:1A:827:U:OP1     | 60:1A:4219:HOH:O  | 2.22                     | 0.42              |
| 1:1A:1054:A:C6     | 1:1A:1106:G:C6    | 3.08                     | 0.42              |
| 1:1A:1607:C:N4     | 1:1A:1622:G:OP2   | 2.39                     | 0.42              |
| 1:1A:1771:C:O2'    | 60:1A:4172:HOH:O  | 2.17                     | 0.42              |
| 1:1A:1865:G:N2     | 1:1A:1877:A:OP2   | 2.52                     | 0.42              |
| 14:1S:110:LEU:HD12 | 14:1S:110:LEU:HA  | 1.77                     | 0.42              |
| 15:1T:96:ARG:HG2   | 60:1T:305:HOH:O   | 2.20                     | 0.42              |
| 17:1V:19:LYS:HA    | 17:1V:94:LEU:O    | 2.20                     | 0.42              |
| 19:1X:57:LEU:HD11  | 19:1X:78:LYS:HE2  | 2.02                     | 0.42              |
| 32:1a:137:C:H2'    | 32:1a:138:G:C8    | 2.55                     | 0.42              |
| 32:1a:601:C:H2'    | 32:1a:602:A:C8    | 2.55                     | 0.42              |
| 32:1a:1237:C:H3'   | 32:1a:1336:C:H41  | 1.85                     | 0.42              |
| 32:1a:1345:U:OP2   | 60:1a:1939:HOH:O  | 2.21                     | 0.42              |
| 35:1d:81:GLU:O     | 35:1d:85:LYS:HB2  | 2.20                     | 0.42              |
| 50:1s:40:ILE:HA    | 50:1s:44:MET:SD   | 2.60                     | 0.42              |
| 1:2A:271(A):A:N1   | 1:2A:272(D):G:O2' | 2.40                     | 0.42              |
| 1:2A:493:G:H2'     | 1:2A:494:G:O4'    | 2.20                     | 0.42              |
| 1:2A:1258:C:OP2    | 60:2A:3937:HOH:O  | 2.22                     | 0.42              |
| 1:2A:2022:U:OP2    | 27:25:15:ARG:NH2  | 2.53                     | 0.42              |
| 1:2A:2250:G:O2'    | 1:2A:2496:C:OP1   | 2.29                     | 0.42              |
| 1:2A:2782:G:OP2    | 60:2A:3942:HOH:O  | 2.22                     | 0.42              |
| 1:2A:2830:G:O2'    | 1:2A:2883:A:N1    | 2.48                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:2B:24:G:H4'      | 2:2B:25:A:N7       | 2.34                     | 0.42              |
| 15:2T:16:ARG:NH2   | 15:2T:83:ILE:O     | 2.53                     | 0.42              |
| 18:2W:72:LYS:N     | 18:2W:106:ILE:O    | 2.52                     | 0.42              |
| 20:2Y:13:VAL:HG11  | 20:2Y:72:VAL:HG13  | 2.02                     | 0.42              |
| 32:2a:1329:A:H5''  | 44:2m:26:GLY:N     | 2.34                     | 0.42              |
| 34:2c:128:PHE:HD1  | 34:2c:129:ALA:H    | 1.67                     | 0.42              |
| 36:2e:33:VAL:HA    | 36:2e:42:GLY:O     | 2.20                     | 0.42              |
| 1:1A:330:A:O2'     | 1:1A:331:A:C8      | 2.72                     | 0.42              |
| 1:1A:686:G:H8      | 29:17:6:GLN:O      | 2.02                     | 0.42              |
| 1:1A:719:C:O5'     | 1:1A:719:C:H6      | 2.03                     | 0.42              |
| 1:1A:855:G:N2      | 60:1A:4231:HOH:O   | 2.23                     | 0.42              |
| 1:1A:857:C:N4      | 1:1A:858:U:O4      | 2.53                     | 0.42              |
| 1:1A:870:A:C2      | 1:1A:908:C:C2      | 3.08                     | 0.42              |
| 1:1A:1557:C:H5''   | 1:1A:1558:A:OP2    | 2.19                     | 0.42              |
| 1:1A:1634:A:H5''   | 60:1A:4598:HOH:O   | 2.20                     | 0.42              |
| 1:1A:2356:C:H2'    | 1:1A:2357:U:O4'    | 2.20                     | 0.42              |
| 1:1A:2858:C:OP2    | 60:1A:4206:HOH:O   | 2.21                     | 0.42              |
| 7:1H:40:GLU:OE2    | 7:1H:60:ARG:NH1    | 2.48                     | 0.42              |
| 8:1I:6:LEU:HG      | 8:1I:36:ALA:HA     | 2.00                     | 0.42              |
| 8:1I:77:LEU:HD12   | 8:1I:77:LEU:HA     | 1.86                     | 0.42              |
| 20:1Y:90:LEU:HB3   | 20:1Y:92:ASN:HD22  | 1.85                     | 0.42              |
| 32:1a:59:A:H3'     | 32:1a:331:G:H22    | 1.84                     | 0.42              |
| 32:1a:768:A:H4'    | 32:1a:1523:G:N2    | 2.35                     | 0.42              |
| 32:1a:1106:G:C6    | 32:1a:1107:C:C4    | 3.08                     | 0.42              |
| 32:1a:1120:G:N2    | 32:1a:1154:G:H1'   | 2.35                     | 0.42              |
| 32:1a:1328:C:OP1   | 52:1u:21:TYR:OH    | 2.31                     | 0.42              |
| 36:1e:72:GLN:O     | 36:1e:75:THR:HG22  | 2.19                     | 0.42              |
| 36:1e:77:PRO:HD2   | 36:1e:142:LEU:HD22 | 2.01                     | 0.42              |
| 1:2A:615:G:O2'     | 5:2F:205:ARG:NH1   | 2.53                     | 0.42              |
| 1:2A:2505:G:N7     | 27:25:3:LYS:NZ     | 2.67                     | 0.42              |
| 3:2D:95:LEU:HD11   | 3:2D:105:ILE:HG12  | 2.02                     | 0.42              |
| 14:2S:25:ARG:HG3   | 14:2S:88:ASP:HB2   | 2.02                     | 0.42              |
| 32:2a:114:U:O2'    | 32:2a:115:G:H5'    | 2.19                     | 0.42              |
| 32:2a:420:U:H2'    | 32:2a:422:C:C4     | 2.54                     | 0.42              |
| 32:2a:708:C:H2'    | 32:2a:709:G:H8     | 1.85                     | 0.42              |
| 32:2a:728:A:H2'    | 32:2a:729:A:C8     | 2.55                     | 0.42              |
| 33:2b:24:TRP:CD1   | 33:2b:24:TRP:H     | 2.36                     | 0.42              |
| 34:2c:131:ARG:HH22 | 36:2e:50:GLU:HG3   | 1.85                     | 0.42              |
| 39:2h:26:VAL:HG22  | 39:2h:59:LEU:HB2   | 2.01                     | 0.42              |
| 1:1A:25:U:H5'      | 18:1W:79:GLY:HA2   | 2.02                     | 0.41              |
| 1:1A:2115:G:N3     | 1:1A:2117:A:N6     | 2.68                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1A:2319:G:N2    | 14:1S:3:ARG:HA    | 2.35                     | 0.41              |
| 1:1A:2492:U:H2'   | 1:1A:2493:U:H6    | 1.85                     | 0.41              |
| 1:1A:2751:G:H4'   | 7:1H:4:ILE:HD11   | 2.02                     | 0.41              |
| 25:13:4:LEU:O     | 25:13:36:VAL:HA   | 2.20                     | 0.41              |
| 32:1a:192:U:H4'   | 51:1t:57:ARG:HD3  | 2.02                     | 0.41              |
| 32:1a:325:A:OP2   | 51:1t:70:SER:HB3  | 2.20                     | 0.41              |
| 32:1a:1122:U:H2'  | 32:1a:1123:A:O4'  | 2.20                     | 0.41              |
| 32:1a:1239:A:H62  | 32:1a:1299:A:N6   | 2.17                     | 0.41              |
| 32:1a:1316:G:N1   | 32:1a:1319:A:OP2  | 2.48                     | 0.41              |
| 32:1a:1458:G:OP1  | 51:1t:35:THR:OG1  | 2.31                     | 0.41              |
| 35:1d:70:ILE:HD11 | 35:1d:74:GLN:HB3  | 2.02                     | 0.41              |
| 38:1g:26:PHE:CE2  | 38:1g:30:ILE:HD11 | 2.55                     | 0.41              |
| 47:1p:60:LEU:HD12 | 47:1p:60:LEU:HA   | 1.78                     | 0.41              |
| 1:2A:583:G:OP2    | 16:2U:10:ARG:HD2  | 2.21                     | 0.41              |
| 1:2A:922:U:H2'    | 1:2A:923:C:C6     | 2.55                     | 0.41              |
| 1:2A:1221(A):C:C2 | 1:2A:1229:G:C2    | 3.08                     | 0.41              |
| 1:2A:1364:G:P     | 23:21:3:LYS:HG3   | 2.60                     | 0.41              |
| 1:2A:2171:A:H4'   | 1:2A:2172:U:OP1   | 2.18                     | 0.41              |
| 1:2A:2361:A:OP1   | 30:28:27:THR:HG23 | 2.20                     | 0.41              |
| 1:2A:2472:G:N2    | 1:2A:2477:C:OP1   | 2.47                     | 0.41              |
| 1:2A:2705:A:H2'   | 1:2A:2706:G:O4'   | 2.20                     | 0.41              |
| 1:2A:2712:U:H1'   | 1:2A:2712(A):A:C8 | 2.55                     | 0.41              |
| 6:2G:98:ARG:HA    | 6:2G:101:ILE:HD12 | 2.02                     | 0.41              |
| 10:2O:43:VAL:HG23 | 10:2O:56:ASP:O    | 2.20                     | 0.41              |
| 32:2a:46:G:HO2'   | 32:2a:365:U:H1'   | 1.84                     | 0.41              |
| 32:2a:229:U:H5''  | 47:2p:33:ILE:HD13 | 2.02                     | 0.41              |
| 32:2a:251:G:C6    | 32:2a:266:G:O6    | 2.73                     | 0.41              |
| 32:2a:582:U:C2    | 32:2a:760:G:C6    | 3.08                     | 0.41              |
| 32:2a:1011:G:H2'  | 32:2a:1012:U:O4'  | 2.20                     | 0.41              |
| 33:2b:82:ARG:HB2  | 33:2b:94:ASN:OD1  | 2.20                     | 0.41              |
| 44:2m:15:VAL:O    | 44:2m:19:LEU:HD22 | 2.21                     | 0.41              |
| 47:2p:55:ARG:HD2  | 47:2p:55:ARG:HA   | 1.90                     | 0.41              |
| 1:1A:888:C:H4'    | 1:1A:889:C:OP1    | 2.20                     | 0.41              |
| 1:1A:909:A:H2'    | 1:1A:912:C:C5     | 2.55                     | 0.41              |
| 1:1A:1649:G:O2'   | 13:1R:107:ASP:OD2 | 2.30                     | 0.41              |
| 2:1B:29:A:H2'     | 2:1B:30:C:O4'     | 2.20                     | 0.41              |
| 4:1E:44:TYR:HB2   | 60:1E:415:HOH:O   | 2.19                     | 0.41              |
| 6:1G:47:LYS:H     | 6:1G:47:LYS:HG2   | 1.60                     | 0.41              |
| 8:1I:104:GLN:HB2  | 8:1I:105:HIS:CD2  | 2.49                     | 0.41              |
| 8:1I:121:LYS:HD2  | 8:1I:121:LYS:HA   | 1.76                     | 0.41              |
| 22:10:32:ARG:H    | 22:10:35:ASN:ND2  | 2.18                     | 0.41              |

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| Atom-1              | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|-------------------|--------------------------|-------------------|
| 27:15:40:LYS:NZ     | 27:15:44:THR:O    | 2.54                     | 0.41              |
| 32:1a:103:C:O2'     | 32:1a:172:A:N1    | 2.51                     | 0.41              |
| 32:1a:171:A:H2'     | 32:1a:172:A:C8    | 2.55                     | 0.41              |
| 32:1a:222:U:H2'     | 32:1a:223:U:H6    | 1.86                     | 0.41              |
| 32:1a:814:A:N7      | 32:1a:816:A:C4    | 2.88                     | 0.41              |
| 32:1a:1243:C:H2'    | 32:1a:1244:C:C6   | 2.55                     | 0.41              |
| 37:1f:69:GLU:O      | 37:1f:72:VAL:HG12 | 2.20                     | 0.41              |
| 1:2A:586:A:N1       | 1:2A:809:G:O2'    | 2.47                     | 0.41              |
| 1:2A:1084:A:H3'     | 1:2A:1085:A:C4'   | 2.50                     | 0.41              |
| 1:2A:1668:A:O2'     | 1:2A:1674:G:N7    | 2.48                     | 0.41              |
| 1:2A:2104:G:O6      | 1:2A:2186:G:C5    | 2.73                     | 0.41              |
| 1:2A:2118:U:H3'     | 1:2A:2119:A:H5''  | 2.02                     | 0.41              |
| 1:2A:2478:A:OP2     | 31:29:2:LYS:NZ    | 2.48                     | 0.41              |
| 1:2A:2481:G:O2'     | 60:2A:3940:HOH:O  | 2.22                     | 0.41              |
| 1:2A:2711:A:OP1     | 1:2A:2712:U:H3'   | 2.19                     | 0.41              |
| 10:2O:70:LYS:HB3    | 10:2O:70:LYS:HE2  | 1.84                     | 0.41              |
| 16:2U:29:SER:C      | 16:2U:30:LYS:HD2  | 2.46                     | 0.41              |
| 19:2X:12:VAL:HG22   | 19:2X:29:TRP:CE2  | 2.55                     | 0.41              |
| 21:2Z:54:HIS:HB3    | 21:2Z:101:PRO:HD3 | 2.01                     | 0.41              |
| 32:2a:767:A:H3'     | 60:2a:3206:HOH:O  | 2.21                     | 0.41              |
| 32:2a:974:A:OP2     | 45:2n:29:ARG:NH2  | 2.53                     | 0.41              |
| 32:2a:1348:U:H2'    | 32:2a:1349:A:H8   | 1.84                     | 0.41              |
| 33:2b:16:HIS:CB     | 33:2b:210:SER:HB3 | 2.50                     | 0.41              |
| 33:2b:50:GLU:HB3    | 33:2b:200:ILE:O   | 2.19                     | 0.41              |
| 33:2b:54:THR:HG23   | 33:2b:199:TYR:HB3 | 2.01                     | 0.41              |
| 53:2y:27:LEU:HD21   | 53:2y:81:LEU:C    | 2.45                     | 0.41              |
| 1:1A:97:C:OP1       | 24:12:2:LYS:NZ    | 2.50                     | 0.41              |
| 1:1A:196:A:H2'      | 1:1A:196:A:N3     | 2.35                     | 0.41              |
| 1:1A:481:G:C4       | 1:1A:507:A:C2     | 3.07                     | 0.41              |
| 1:1A:1639:U:O2'     | 1:1A:1640:C:H5'   | 2.20                     | 0.41              |
| 1:1A:2120:G:C2      | 1:1A:2179:C:C2    | 3.09                     | 0.41              |
| 1:1A:2348:U:O4      | 1:1A:2382:G:C2    | 2.73                     | 0.41              |
| 2:1B:66:A:N6        | 2:1B:108:U:H2'    | 2.34                     | 0.41              |
| 16:1U:46:ALA:O      | 16:1U:50:ARG:HG2  | 2.19                     | 0.41              |
| 26:14:8:LYS:HB3     | 26:14:8:LYS:HE2   | 1.91                     | 0.41              |
| 26:14:55:ARG:N      | 26:14:56:VAL:HA   | 2.35                     | 0.41              |
| 26:14:59:PHE:O      | 26:14:62:ARG:HG2  | 2.19                     | 0.41              |
| 32:1a:585:G:N3      | 32:1a:879:C:H4'   | 2.35                     | 0.41              |
| 32:1a:691:G:H2'     | 32:1a:692:U:C6    | 2.55                     | 0.41              |
| 32:1a:1179:A:H2'    | 32:1a:1180:A:O4'  | 2.20                     | 0.41              |
| 32:1a:1207:2MG:HO2' | 32:1a:1208:C:P    | 2.43                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 32:1a:1250:A:H4'   | 40:1i:68:GLY:N     | 2.35                     | 0.41              |
| 38:1g:14:PRO:HB3   | 38:1g:19:GLY:C     | 2.45                     | 0.41              |
| 41:1j:16:LEU:HD21  | 41:1j:70:ARG:HG2   | 2.01                     | 0.41              |
| 46:1o:16:ALA:HB1   | 46:1o:21:ASP:HB3   | 2.02                     | 0.41              |
| 1:2A:1049:C:H1'    | 1:2A:1113:U:H4'    | 2.02                     | 0.41              |
| 1:2A:1069:A:H2'    | 1:2A:1073:A:N7     | 2.35                     | 0.41              |
| 1:2A:1113:U:H2'    | 1:2A:1114:G:C8     | 2.56                     | 0.41              |
| 1:2A:2118:U:C3'    | 1:2A:2119:A:H5''   | 2.50                     | 0.41              |
| 4:2E:14:ILE:HG13   | 4:2E:21:VAL:HG13   | 2.02                     | 0.41              |
| 11:2P:6:LEU:HA     | 11:2P:6:LEU:HD23   | 1.79                     | 0.41              |
| 27:25:16:ARG:HG2   | 27:25:17:ASP:OD1   | 2.20                     | 0.41              |
| 32:2a:1427:U:H2'   | 32:2a:1428:A:C8    | 2.54                     | 0.41              |
| 33:2b:167:PRO:HD3  | 33:2b:187:LEU:O    | 2.20                     | 0.41              |
| 35:2d:78:LEU:HD23  | 35:2d:78:LEU:HA    | 1.84                     | 0.41              |
| 42:2k:109:VAL:HG23 | 49:2r:86:VAL:HG13  | 2.03                     | 0.41              |
| 49:2r:52:PRO:HB2   | 49:2r:54:ARG:HG3   | 2.02                     | 0.41              |
| 1:1A:272(C):G:H2'  | 1:1A:272(D):G:O4'  | 2.20                     | 0.41              |
| 1:1A:776:G:H4'     | 1:1A:777:A:O5'     | 2.20                     | 0.41              |
| 1:1A:1198:U:H2'    | 1:1A:1199:U:C6     | 2.56                     | 0.41              |
| 1:1A:2543:G:H2'    | 1:1A:2544:G:O4'    | 2.19                     | 0.41              |
| 3:1D:16:MET:HE3    | 3:1D:16:MET:HB2    | 1.84                     | 0.41              |
| 5:1F:53:THR:HG22   | 5:1F:55:GLY:H      | 1.85                     | 0.41              |
| 6:1G:11:TYR:CZ     | 6:1G:16:ARG:HD3    | 2.56                     | 0.41              |
| 17:1V:60:GLU:OE1   | 17:1V:97:LYS:NZ    | 2.52                     | 0.41              |
| 20:1Y:96:ILE:HG13  | 20:1Y:98:VAL:HG13  | 2.03                     | 0.41              |
| 23:11:77:ALA:O     | 23:11:80:LEU:HB2   | 2.21                     | 0.41              |
| 32:1a:107:G:H2'    | 32:1a:108:G:O4'    | 2.20                     | 0.41              |
| 32:1a:998:G:H2'    | 32:1a:999:C:C6     | 2.55                     | 0.41              |
| 32:1a:1030(C):G:H8 | 32:1a:1030(D):A:N7 | 2.17                     | 0.41              |
| 32:1a:1187:G:OP1   | 40:1i:113:LYS:HE3  | 2.21                     | 0.41              |
| 32:1a:1311:G:H2'   | 32:1a:1312:G:O4'   | 2.20                     | 0.41              |
| 34:1c:22:TRP:HB3   | 34:1c:59:ARG:HB2   | 2.02                     | 0.41              |
| 35:1d:29:PRO:HA    | 35:1d:34:GLU:HG2   | 2.03                     | 0.41              |
| 38:1g:18:TYR:CE1   | 38:1g:59:LEU:HB2   | 2.55                     | 0.41              |
| 1:2A:839:U:H2'     | 1:2A:840:C:C6      | 2.54                     | 0.41              |
| 1:2A:861:A:N3      | 2:2B:79:C:O2'      | 2.51                     | 0.41              |
| 1:2A:1092:C:O2     | 1:2A:1092:C:H2'    | 2.20                     | 0.41              |
| 1:2A:2170:A:H8     | 1:2A:2170:A:O5'    | 2.04                     | 0.41              |
| 1:2A:2275:C:H6     | 1:2A:2275:C:H5'    | 1.86                     | 0.41              |
| 3:2D:275:LYS:HA    | 3:2D:276:LYS:C     | 2.45                     | 0.41              |
| 6:2G:138:GLN:OE1   | 6:2G:153:ARG:N     | 2.53                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:2H:26:VAL:O     | 7:2H:79:VAL:HG11  | 2.20                     | 0.41              |
| 8:2I:69:LYS:O     | 8:2I:73:GLU:N     | 2.51                     | 0.41              |
| 9:2N:1:MET:HE1    | 16:2U:94:ASN:ND2  | 2.36                     | 0.41              |
| 12:2Q:25:ASP:OD1  | 12:2Q:25:ASP:N    | 2.53                     | 0.41              |
| 16:2U:89:GLU:HG2  | 17:2V:50:PRO:HB3  | 2.03                     | 0.41              |
| 28:26:38:LYS:HE3  | 28:26:38:LYS:HB3  | 1.91                     | 0.41              |
| 30:28:50:LEU:HD23 | 30:28:50:LEU:HA   | 1.90                     | 0.41              |
| 32:2a:564:C:C4    | 48:2q:31:LEU:HD11 | 2.55                     | 0.41              |
| 33:2b:115:LEU:O   | 33:2b:119:GLU:N   | 2.32                     | 0.41              |
| 35:2d:145:GLU:HA  | 35:2d:184:LYS:HG2 | 2.02                     | 0.41              |
| 37:2f:91:VAL:HG12 | 37:2f:92:LYS:O    | 2.21                     | 0.41              |
| 1:1A:466:A:N3     | 1:1A:683:C:H1'    | 2.35                     | 0.41              |
| 1:1A:569:U:C4     | 1:1A:570:G:C6     | 3.08                     | 0.41              |
| 1:1A:1508:A:H5'   | 1:1A:1509(A):A:C8 | 2.56                     | 0.41              |
| 1:1A:2712:U:OP1   | 1:1A:2714:G:H4'   | 2.21                     | 0.41              |
| 5:1F:110:LEU:HD23 | 5:1F:110:LEU:HA   | 1.94                     | 0.41              |
| 6:1G:11:TYR:HB2   | 6:1G:176:LEU:HD21 | 2.03                     | 0.41              |
| 6:1G:76:SER:N     | 6:1G:84:LYS:HB2   | 2.35                     | 0.41              |
| 6:1G:114:ILE:HB   | 6:1G:117:PHE:HB2  | 2.01                     | 0.41              |
| 12:1Q:137:TYR:HB3 | 21:1Z:76:LEU:HD21 | 2.03                     | 0.41              |
| 29:17:3:ARG:HD3   | 29:17:3:ARG:HA    | 1.84                     | 0.41              |
| 32:1a:78:G:N2     | 32:1a:92:C:N3     | 2.69                     | 0.41              |
| 32:1a:620:C:H2'   | 32:1a:621:A:O4'   | 2.21                     | 0.41              |
| 32:1a:833:U:H2'   | 32:1a:834:C:H6    | 1.84                     | 0.41              |
| 32:1a:1155:G:H2'  | 32:1a:1156:G:O4'  | 2.21                     | 0.41              |
| 32:1a:1401:G:N7   | 53:1y:83:ARG:NH1  | 2.69                     | 0.41              |
| 32:1a:1499:A:O2'  | 32:1a:1520:G:H5'  | 2.20                     | 0.41              |
| 39:1h:83:ILE:HA   | 39:1h:136:GLU:O   | 2.20                     | 0.41              |
| 43:1l:34:ARG:O    | 43:1l:61:THR:HG23 | 2.19                     | 0.41              |
| 49:1r:86:VAL:HG12 | 49:1r:87:ARG:H    | 1.85                     | 0.41              |
| 50:1s:61:TYR:CE2  | 50:1s:63:THR:HG23 | 2.56                     | 0.41              |
| 1:2A:198:C:H2'    | 60:2A:4640:HOH:O  | 2.19                     | 0.41              |
| 1:2A:438:G:H2'    | 1:2A:440:G:C8     | 2.55                     | 0.41              |
| 1:2A:764:A:N1     | 1:2A:1789:A:O2'   | 2.48                     | 0.41              |
| 5:2F:28:ILE:HD12  | 5:2F:119:ARG:HH21 | 1.84                     | 0.41              |
| 11:2P:50:ARG:HD3  | 30:28:7:HIS:NE2   | 2.36                     | 0.41              |
| 32:2a:292:G:N7    | 32:2a:293:G:H1'   | 2.36                     | 0.41              |
| 32:2a:983:A:H3'   | 32:2a:983:A:N3    | 2.36                     | 0.41              |
| 32:2a:1008:C:H2'  | 32:2a:1009:G:H8   | 1.83                     | 0.41              |
| 36:2e:140:ARG:O   | 36:2e:143:ARG:NH1 | 2.51                     | 0.41              |
| 43:2l:82:VAL:O    | 43:2l:106:ASP:HB2 | 2.21                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 46:2o:32:LEU:HD11  | 46:2o:62:GLN:HB3   | 2.01                     | 0.41              |
| 46:2o:34:LEU:HA    | 46:2o:34:LEU:HD12  | 1.88                     | 0.41              |
| 50:2s:70:LYS:HB2   | 50:2s:73:GLU:HG3   | 2.02                     | 0.41              |
| 1:1A:721:C:H2'     | 1:1A:722:A:C8      | 2.55                     | 0.41              |
| 1:1A:868:U:H3'     | 60:1A:4708:HOH:O   | 2.19                     | 0.41              |
| 1:1A:922:U:H2'     | 1:1A:923:C:C6      | 2.56                     | 0.41              |
| 1:1A:2101:G:H2'    | 1:1A:2102:U:O4'    | 2.20                     | 0.41              |
| 1:1A:2262:U:H5     | 22:10:16:SER:HB3   | 1.84                     | 0.41              |
| 1:1A:2704:C:H2'    | 1:1A:2705:A:O4'    | 2.21                     | 0.41              |
| 3:1D:70:TRP:CE2    | 3:1D:150:LYS:HD2   | 2.55                     | 0.41              |
| 5:1F:53:THR:HB     | 5:1F:56:GLU:OE1    | 2.21                     | 0.41              |
| 7:1H:137:ASP:HB3   | 7:1H:140:LYS:HB3   | 2.01                     | 0.41              |
| 9:1N:9:VAL:HG22    | 60:1N:305:HOH:O    | 2.20                     | 0.41              |
| 9:1N:67:LEU:HD22   | 60:1N:321:HOH:O    | 2.20                     | 0.41              |
| 11:1P:90:ARG:NH1   | 11:1P:105:LEU:HD11 | 2.35                     | 0.41              |
| 12:1Q:31:ASP:HA    | 12:1Q:134:ARG:NH1  | 2.36                     | 0.41              |
| 32:1a:736:C:H2'    | 32:1a:737:A:C8     | 2.55                     | 0.41              |
| 47:1p:57:ARG:HH21  | 47:1p:79:VAL:C     | 2.28                     | 0.41              |
| 47:1p:75:ARG:HG3   | 47:1p:80:PHE:HD2   | 1.85                     | 0.41              |
| 51:1t:38:LYS:HG3   | 51:1t:39:LYS:N     | 2.36                     | 0.41              |
| 52:1u:3:LYS:HB3    | 52:1u:14:TRP:CD1   | 2.55                     | 0.41              |
| 1:2A:11:G:C2'      | 1:2A:12:U:H5'      | 2.49                     | 0.41              |
| 1:2A:27:G:N2       | 1:2A:512:G:H1'     | 2.35                     | 0.41              |
| 1:2A:969:U:O3'     | 25:23:14:GLY:HA2   | 2.21                     | 0.41              |
| 1:2A:1287:A:H8     | 13:2R:104:ARG:HD3  | 1.86                     | 0.41              |
| 1:2A:1772:G:O6     | 56:2A:3758:MPD:H31 | 2.20                     | 0.41              |
| 1:2A:2185:C:H3'    | 1:2A:2185:C:H6     | 1.86                     | 0.41              |
| 4:2E:11:MET:CG     | 4:2E:24:THR:HG22   | 2.44                     | 0.41              |
| 8:2I:9:LEU:HD21    | 8:2I:35:LEU:HD13   | 2.01                     | 0.41              |
| 12:2Q:8:LYS:HG3    | 21:2Z:197:ILE:HD12 | 2.03                     | 0.41              |
| 13:2R:67:LEU:HD12  | 13:2R:76:VAL:HG21  | 2.03                     | 0.41              |
| 14:2S:24:LEU:O     | 14:2S:85:VAL:HG22  | 2.21                     | 0.41              |
| 15:2T:57:PHE:HD1   | 15:2T:79:HIS:HD2   | 1.68                     | 0.41              |
| 20:2Y:23:ARG:HG2   | 20:2Y:42:VAL:HG22  | 2.02                     | 0.41              |
| 21:2Z:99:TYR:HA    | 21:2Z:124:ILE:O    | 2.20                     | 0.41              |
| 22:20:41:ARG:HA    | 60:20:204:HOH:O    | 2.21                     | 0.41              |
| 32:2a:721:G:H4'    | 32:2a:722:A:O4'    | 2.21                     | 0.41              |
| 32:2a:742:G:P      | 46:2o:35:ARG:HH22  | 2.44                     | 0.41              |
| 32:2a:857:C:H2'    | 32:2a:858:G:O4'    | 2.20                     | 0.41              |
| 32:2a:1071:C:H2'   | 32:2a:1072:G:C8    | 2.56                     | 0.41              |
| 33:2b:204:ASN:HD21 | 33:2b:207:ALA:HB3  | 1.86                     | 0.41              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 35:2d:43:HIS:ND1  | 35:2d:46:LYS:HD2 | 2.35                     | 0.41              |
| 37:2f:50:TYR:CE2  | 49:2r:77:GLY:HA2 | 2.56                     | 0.41              |
| 38:2g:22:LEU:HD23 | 38:2g:62:PHE:CZ  | 2.56                     | 0.41              |
| 42:2k:110:ASP:HB3 | 49:2r:85:LEU:HB3 | 2.03                     | 0.41              |
| 44:2m:82:MET:HE3  | 44:2m:92:HIS:HB3 | 2.01                     | 0.41              |
| 49:2r:53:ARG:HA   | 49:2r:56:THR:OG1 | 2.20                     | 0.41              |
| 51:2t:11:SER:O    | 51:2t:15:ARG:HB2 | 2.21                     | 0.41              |
| 1:1A:1028:A:N6    | 1:1A:1125:G:H2'  | 2.35                     | 0.41              |
| 1:1A:1268:A:C2    | 1:1A:2013:A:C4   | 3.09                     | 0.41              |
| 1:1A:1423:G:H2'   | 1:1A:1424:G:H8   | 1.86                     | 0.41              |
| 1:1A:1432:C:H2'   | 1:1A:1433:U:O4'  | 2.21                     | 0.41              |
| 1:1A:1712:C:H2'   | 1:1A:1713:U:O4'  | 2.21                     | 0.41              |
| 1:1A:2164:C:H5''  | 1:1A:2165:G:OP2  | 2.19                     | 0.41              |
| 1:1A:2292:C:OP1   | 14:1S:17:ARG:NH2 | 2.54                     | 0.41              |
| 1:1A:2331:G:O2'   | 1:1A:2336:A:N1   | 2.42                     | 0.41              |
| 57:1B:231:ARG:HG3 | 60:1B:321:HOH:O  | 2.20                     | 0.41              |
| 4:1E:181:LEU:HD11 | 15:1T:6:LEU:HD23 | 2.02                     | 0.41              |
| 21:1Z:40:ASP:HB3  | 21:1Z:43:GLU:HB2 | 2.02                     | 0.41              |
| 32:1a:501:C:H2'   | 32:1a:502:G:C8   | 2.56                     | 0.41              |
| 32:1a:597:G:H1'   | 32:1a:644:G:N2   | 2.36                     | 0.41              |
| 32:1a:768:A:H2'   | 32:1a:769:G:O4'  | 2.19                     | 0.41              |
| 32:1a:975:A:H4'   | 32:1a:976:G:C5'  | 2.47                     | 0.41              |
| 32:1a:1005:A:H5'' | 32:1a:1006:C:OP2 | 2.21                     | 0.41              |
| 32:1a:1226:C:O3'  | 44:1m:111:LYS:NZ | 2.54                     | 0.41              |
| 32:1a:1264:C:H2'  | 32:1a:1265:G:C8  | 2.55                     | 0.41              |
| 32:1a:1314:C:H2'  | 32:1a:1315:U:C6  | 2.55                     | 0.41              |
| 35:1d:19:LEU:O    | 35:1d:21:LEU:N   | 2.53                     | 0.41              |
| 38:1g:28:ASN:HA   | 38:1g:31:MET:HE2 | 2.02                     | 0.41              |
| 39:1h:6:ILE:O     | 39:1h:10:LEU:HG  | 2.20                     | 0.41              |
| 51:1t:74:LYS:HB3  | 51:1t:74:LYS:HE3 | 1.83                     | 0.41              |
| 1:2A:70:G:O2'     | 1:2A:113:G:O2'   | 2.30                     | 0.41              |
| 1:2A:657:U:H2'    | 1:2A:658:C:C6    | 2.56                     | 0.41              |
| 1:2A:1435:G:H2'   | 1:2A:1436:G:O4'  | 2.20                     | 0.41              |
| 1:2A:1973:G:H2'   | 1:2A:1974:C:C6   | 2.56                     | 0.41              |
| 1:2A:2219:G:H2'   | 1:2A:2220:G:H8   | 1.86                     | 0.41              |
| 1:2A:2320:A:H1'   | 1:2A:2321:G:C6   | 2.56                     | 0.41              |
| 1:2A:2390:U:O2'   | 1:2A:2391:G:H5'  | 2.19                     | 0.41              |
| 1:2A:2576:G:O2'   | 60:2A:3941:HOH:O | 2.22                     | 0.41              |
| 8:2I:145:VAL:HG12 | 8:2I:146:ALA:H   | 1.86                     | 0.41              |
| 14:2S:64:GLU:H    | 14:2S:64:GLU:HG3 | 1.51                     | 0.41              |
| 17:2V:4:ILE:HD12  | 17:2V:39:LEU:HB3 | 2.03                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 26:24:46:GLN:HB3   | 26:24:48:ARG:NH1   | 2.36                     | 0.41              |
| 29:27:24:THR:O     | 29:27:28:ARG:HG3   | 2.21                     | 0.41              |
| 32:2a:1235:U:H2'   | 32:2a:1236:A:O4'   | 2.19                     | 0.41              |
| 32:2a:1375:A:H4'   | 38:2g:29:LYS:NZ    | 2.36                     | 0.41              |
| 32:2a:1486:G:H2'   | 32:2a:1487:G:O4'   | 2.21                     | 0.41              |
| 32:2a:1509:C:H2'   | 32:2a:1510:U:O4'   | 2.21                     | 0.41              |
| 32:2a:1511:G:H2'   | 32:2a:1512:U:O4'   | 2.21                     | 0.41              |
| 33:2b:21:ARG:O     | 33:2b:23:ARG:N     | 2.45                     | 0.41              |
| 36:2e:92:LYS:HB3   | 36:2e:119:LEU:HB2  | 2.01                     | 0.41              |
| 44:2m:16:ASP:OD1   | 44:2m:16:ASP:N     | 2.53                     | 0.41              |
| 1:1A:191:A:H2'     | 1:1A:192:C:C6      | 2.56                     | 0.41              |
| 1:1A:895:U:H5'     | 1:1A:896:A:OP2     | 2.20                     | 0.41              |
| 1:1A:1341:U:O4'    | 19:1X:57:LEU:HD23  | 2.20                     | 0.41              |
| 1:1A:1400:G:H2'    | 1:1A:1401:G:C8     | 2.56                     | 0.41              |
| 1:1A:1593:G:H2'    | 1:1A:1594:G:C8     | 2.56                     | 0.41              |
| 4:1E:28:ALA:HB3    | 4:1E:93:VAL:HG12   | 2.03                     | 0.41              |
| 7:1H:41:MET:HE1    | 7:1H:54:ARG:HB3    | 2.02                     | 0.41              |
| 18:1W:3:ALA:HB3    | 18:1W:58:ALA:HB2   | 2.03                     | 0.41              |
| 19:1X:35:THR:HG23  | 19:1X:37:THR:H     | 1.85                     | 0.41              |
| 20:1Y:50:ARG:HG2   | 60:1Y:317:HOH:O    | 2.19                     | 0.41              |
| 32:1a:262:A:C6     | 32:1a:263:A:C6     | 3.09                     | 0.41              |
| 32:1a:491:G:H2'    | 32:1a:492:G:H8     | 1.85                     | 0.41              |
| 32:1a:953:G:C2     | 32:1a:954:G:H1'    | 2.56                     | 0.41              |
| 32:1a:992:U:H2'    | 32:1a:1043:C:H41   | 1.86                     | 0.41              |
| 32:1a:1070:U:OP1   | 36:1e:18:ARG:NH2   | 2.54                     | 0.41              |
| 32:1a:1239:A:H62   | 32:1a:1299:A:H61   | 1.69                     | 0.41              |
| 32:1a:1511:G:H2'   | 32:1a:1512:U:O4'   | 2.20                     | 0.41              |
| 35:1d:170:VAL:HG12 | 35:1d:171:GLY:N    | 2.36                     | 0.41              |
| 36:1e:78:HIS:CE1   | 36:1e:142:LEU:HD23 | 2.56                     | 0.41              |
| 39:1h:35:ILE:O     | 39:1h:39:LEU:HD22  | 2.21                     | 0.41              |
| 53:1y:32:THR:OG1   | 53:1y:57:PRO:HD2   | 2.20                     | 0.41              |
| 1:2A:271(M):G:H4'  | 1:2A:271(N):U:OP1  | 2.21                     | 0.41              |
| 1:2A:1028:A:N3     | 1:2A:2486:G:O2'    | 2.51                     | 0.41              |
| 1:2A:1041:C:N4     | 1:2A:1114:G:H1     | 2.04                     | 0.41              |
| 1:2A:1045:A:H5'    | 1:2A:1047:G:OP1    | 2.20                     | 0.41              |
| 1:2A:1448:G:H2'    | 1:2A:1449:A:C8     | 2.56                     | 0.41              |
| 1:2A:1676:A:H2'    | 1:2A:1677:A:O4'    | 2.20                     | 0.41              |
| 4:2E:9:VAL:HG13    | 4:2E:25:VAL:O      | 2.20                     | 0.41              |
| 6:2G:51:ARG:HE     | 6:2G:51:ARG:HB2    | 1.48                     | 0.41              |
| 32:2a:127:G:O2'    | 48:2q:2:PRO:O      | 2.39                     | 0.41              |
| 32:2a:161:A:H2'    | 32:2a:162:A:C8     | 2.55                     | 0.41              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 32:2a:502:G:OP1    | 43:2l:117:ARG:N   | 2.54                     | 0.41              |
| 32:2a:575:G:O2'    | 32:2a:821:G:H5'   | 2.21                     | 0.41              |
| 32:2a:1122:U:C4    | 32:2a:1123:A:N7   | 2.88                     | 0.41              |
| 34:2c:115:LEU:HD12 | 34:2c:115:LEU:HA  | 1.83                     | 0.41              |
| 35:2d:76:ARG:NH2   | 35:2d:80:GLU:OE1  | 2.54                     | 0.41              |
| 44:2m:82:MET:CE    | 44:2m:92:HIS:HB3  | 2.51                     | 0.41              |
| 1:1A:271(X):G:C2   | 1:1A:271(Y):U:O4  | 2.74                     | 0.41              |
| 1:1A:657:U:H2'     | 1:1A:658:C:C6     | 2.56                     | 0.41              |
| 1:1A:705:A:C2      | 1:1A:727:A:H1'    | 2.56                     | 0.41              |
| 1:1A:1166:C:O2'    | 60:1A:4166:HOH:O  | 2.17                     | 0.41              |
| 1:1A:1665:A:H1'    | 10:1O:1:MET:HG2   | 2.03                     | 0.41              |
| 1:1A:1790:C:H2'    | 1:1A:1791:A:C5    | 2.55                     | 0.41              |
| 1:1A:1930:G:O2'    | 1:1A:1968:G:O6    | 2.24                     | 0.41              |
| 1:1A:2142:C:N3     | 1:1A:2149:G:O6    | 2.54                     | 0.41              |
| 1:1A:2256:G:H2'    | 1:1A:2257:U:O4'   | 2.20                     | 0.41              |
| 1:1A:2287:A:C8     | 1:1A:2289:G:C8    | 3.09                     | 0.41              |
| 1:1A:2687:U:H2'    | 1:1A:2688:U:O4'   | 2.20                     | 0.41              |
| 1:1A:2786:U:O2'    | 4:1E:62:PRO:O     | 2.33                     | 0.41              |
| 1:1A:2849:U:OP2    | 15:1T:95:ARG:NH1  | 2.54                     | 0.41              |
| 1:1A:2872:G:O2'    | 1:1A:2873:A:H5'   | 2.20                     | 0.41              |
| 6:1G:43:LEU:C      | 6:1G:45:GLU:H     | 2.29                     | 0.41              |
| 8:1I:2:LYS:NZ      | 8:1I:20:ASP:OD2   | 2.53                     | 0.41              |
| 13:1R:28:LEU:HA    | 13:1R:28:LEU:HD12 | 1.87                     | 0.41              |
| 20:1Y:90:LEU:HD12  | 20:1Y:90:LEU:HA   | 1.84                     | 0.41              |
| 26:14:40:HIS:HB3   | 26:14:43:TYR:CD2  | 2.45                     | 0.41              |
| 32:1a:49:U:C2      | 32:1a:361:G:N2    | 2.89                     | 0.41              |
| 32:1a:321:A:C2     | 32:1a:333:G:C2    | 3.09                     | 0.41              |
| 32:1a:341:C:H2'    | 32:1a:342:C:C6    | 2.55                     | 0.41              |
| 32:1a:359:U:H2'    | 32:1a:360:A:C8    | 2.55                     | 0.41              |
| 32:1a:461:A:O2'    | 32:1a:471:G:N7    | 2.51                     | 0.41              |
| 32:1a:491:G:H2'    | 32:1a:492:G:C8    | 2.56                     | 0.41              |
| 32:1a:745:C:H2'    | 32:1a:746:A:C8    | 2.56                     | 0.41              |
| 32:1a:877:C:H5''   | 39:1h:88:LYS:HD3  | 2.02                     | 0.41              |
| 32:1a:933:G:C6     | 32:1a:1385:G:C6   | 3.09                     | 0.41              |
| 32:1a:952:U:C4     | 44:1m:104:ARG:HD3 | 2.55                     | 0.41              |
| 32:1a:955:U:O2'    | 50:1s:83:HIS:HD2  | 2.04                     | 0.41              |
| 32:1a:1149:C:H2'   | 32:1a:1150:U:C6   | 2.56                     | 0.41              |
| 34:1c:5:ILE:HG13   | 34:1c:6:HIS:N     | 2.36                     | 0.41              |
| 35:1d:107:ARG:HH21 | 35:1d:194:LEU:HG  | 1.86                     | 0.41              |
| 38:1g:75:VAL:HG13  | 38:1g:145:ALA:HA  | 2.01                     | 0.41              |
| 40:1i:6:GLY:HA3    | 40:1i:83:ARG:HB2  | 2.02                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 42:1k:108:ILE:HG22 | 49:1r:87:ARG:HD2   | 2.02                     | 0.41              |
| 44:1m:14:ARG:HG3   | 44:1m:44:ARG:NH1   | 2.36                     | 0.41              |
| 46:1o:84:LYS:HA    | 46:1o:84:LYS:HD2   | 1.85                     | 0.41              |
| 48:1q:60:ILE:HG12  | 48:1q:61:GLU:N     | 2.35                     | 0.41              |
| 48:1q:62:SER:CB    | 48:1q:72:ARG:HD3   | 2.50                     | 0.41              |
| 50:1s:62:ILE:HA    | 50:1s:66:MET:SD    | 2.61                     | 0.41              |
| 1:2A:411:G:C5      | 11:2P:72:PRO:HB3   | 2.55                     | 0.41              |
| 1:2A:570:G:H2'     | 1:2A:2030:A:C5     | 2.55                     | 0.41              |
| 1:2A:861:A:C2      | 1:2A:917:A:C4      | 3.09                     | 0.41              |
| 1:2A:1005:C:C2     | 1:2A:1143:A:C5     | 3.09                     | 0.41              |
| 1:2A:1075:C:O2     | 1:2A:1076:C:H2'    | 2.21                     | 0.41              |
| 1:2A:1196:C:H2'    | 1:2A:1197:G:C8     | 2.56                     | 0.41              |
| 1:2A:1430:C:H2'    | 1:2A:1431:U:C6     | 2.56                     | 0.41              |
| 1:2A:2168:G:H2'    | 1:2A:2170:A:OP2    | 2.21                     | 0.41              |
| 1:2A:2321:G:HO2'   | 1:2A:2322:A:P      | 2.42                     | 0.41              |
| 1:2A:2825:C:H2'    | 1:2A:2826:A:O4'    | 2.21                     | 0.41              |
| 1:2A:2852:G:P      | 13:2R:64:ARG:HH22  | 2.44                     | 0.41              |
| 1:2A:2895:U:H2'    | 1:2A:2896:C:O4'    | 2.21                     | 0.41              |
| 2:2B:30:C:H2'      | 2:2B:31:C:H5'      | 2.01                     | 0.41              |
| 5:2F:24:LEU:HD21   | 5:2F:114:VAL:HG12  | 2.02                     | 0.41              |
| 5:2F:138:GLU:O     | 5:2F:141:ALA:HB3   | 2.21                     | 0.41              |
| 6:2G:109:VAL:O     | 6:2G:113:ARG:HB2   | 2.20                     | 0.41              |
| 7:2H:67:LEU:O      | 7:2H:71:LEU:HB2    | 2.21                     | 0.41              |
| 18:2W:6:ILE:HG12   | 18:2W:104:THR:HG23 | 2.03                     | 0.41              |
| 18:2W:25:ARG:NH2   | 18:2W:74:ALA:O     | 2.43                     | 0.41              |
| 20:2Y:43:ASN:ND2   | 20:2Y:65:ALA:HB3   | 2.36                     | 0.41              |
| 21:2Z:33:LEU:HD11  | 21:2Z:90:VAL:HG21  | 2.01                     | 0.41              |
| 32:2a:391:G:C6     | 32:2a:392:G:C5     | 3.09                     | 0.41              |
| 32:2a:922:G:H2'    | 32:2a:923:A:C8     | 2.56                     | 0.41              |
| 32:2a:1002:G:C2    | 32:2a:1003:G:C8    | 3.04                     | 0.41              |
| 32:2a:1036:G:H3'   | 32:2a:1037:C:C6    | 2.56                     | 0.41              |
| 32:2a:1427:U:H2'   | 32:2a:1428:A:H8    | 1.86                     | 0.41              |
| 34:2c:148:GLY:HA3  | 34:2c:172:ARG:O    | 2.21                     | 0.41              |
| 35:2d:162:LEU:HD23 | 35:2d:162:LEU:HA   | 1.91                     | 0.41              |
| 38:2g:56:GLN:HE21  | 38:2g:61:VAL:HG21  | 1.86                     | 0.41              |
| 40:2i:71:SER:HA    | 40:2i:74:ILE:HD12  | 2.03                     | 0.41              |
| 44:2m:87:TYR:N     | 50:2s:73:GLU:O     | 2.54                     | 0.41              |
| 46:2o:16:ALA:HB1   | 46:2o:21:ASP:HB3   | 2.02                     | 0.41              |
| 46:2o:43:LEU:HD13  | 46:2o:53:HIS:HD2   | 1.85                     | 0.41              |
| 47:2p:55:ARG:O     | 47:2p:58:TYR:HB3   | 2.21                     | 0.41              |
| 49:2r:66:LEU:O     | 49:2r:70:ILE:HG13  | 2.21                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:1A:562:U:O2'     | 1:1A:563:G:OP2     | 2.28                     | 0.41              |
| 1:1A:1173:G:OP2    | 1:1A:1173:G:H2'    | 2.21                     | 0.41              |
| 1:1A:1218:C:H42    | 1:1A:1231:G:H1     | 1.68                     | 0.41              |
| 1:1A:1794:U:H2'    | 1:1A:1795:C:C6     | 2.55                     | 0.41              |
| 5:1F:129:PHE:O     | 5:1F:130:ALA:C     | 2.64                     | 0.41              |
| 6:1G:109:VAL:C     | 6:1G:112:PRO:HD2   | 2.46                     | 0.41              |
| 7:1H:8:PRO:HB3     | 7:1H:51:ARG:HG2    | 2.01                     | 0.41              |
| 7:1H:54:ARG:HD3    | 7:1H:65:HIS:ND1    | 2.36                     | 0.41              |
| 13:1R:104:ARG:HG3  | 13:1R:111:LEU:HD21 | 2.03                     | 0.41              |
| 21:1Z:144:LEU:HD23 | 21:1Z:144:LEU:HA   | 1.85                     | 0.41              |
| 30:18:23:VAL:HG13  | 30:18:47:LYS:HB3   | 2.02                     | 0.41              |
| 32:1a:1029:C:N3    | 32:1a:1032:G:O6    | 2.54                     | 0.41              |
| 32:1a:1132:C:H2'   | 32:1a:1133:G:C8    | 2.56                     | 0.41              |
| 32:1a:1240:U:OP2   | 38:1g:116:ALA:N    | 2.47                     | 0.41              |
| 34:1c:43:LEU:HD23  | 34:1c:43:LEU:HA    | 1.79                     | 0.41              |
| 35:1d:160:GLN:H    | 35:1d:160:GLN:HG2  | 1.63                     | 0.41              |
| 1:2A:437:G:H2'     | 1:2A:438:G:H8      | 1.86                     | 0.41              |
| 1:2A:463:G:N1      | 1:2A:467:G:C6      | 2.89                     | 0.41              |
| 1:2A:1328:G:H2'    | 1:2A:1330:C:C5     | 2.56                     | 0.41              |
| 1:2A:2185:C:C6     | 1:2A:2185:C:C3'    | 3.04                     | 0.41              |
| 1:2A:2693:A:H2'    | 1:2A:2694:G:H8     | 1.87                     | 0.41              |
| 1:2A:2752:C:OP2    | 7:2H:4:ILE:HD11    | 2.20                     | 0.41              |
| 1:2A:2821:A:OP2    | 60:2A:3928:HOH:O   | 2.21                     | 0.41              |
| 1:2A:2823:A:OP1    | 4:2E:159:HIS:NE2   | 2.42                     | 0.41              |
| 6:2G:18:GLU:HG2    | 6:2G:175:LEU:HD21  | 2.02                     | 0.41              |
| 6:2G:43:LEU:C      | 6:2G:45:GLU:H      | 2.29                     | 0.41              |
| 8:2I:85:GLU:HB3    | 8:2I:87:LYS:N      | 2.27                     | 0.41              |
| 8:2I:88:ILE:H      | 8:2I:88:ILE:HG12   | 1.71                     | 0.41              |
| 26:24:40:HIS:C     | 26:24:44:THR:HG22  | 2.46                     | 0.41              |
| 32:2a:603:U:H2'    | 32:2a:604:G:C8     | 2.56                     | 0.41              |
| 32:2a:708:C:H2'    | 32:2a:709:G:C8     | 2.56                     | 0.41              |
| 48:2q:5:VAL:HA     | 48:2q:59:ILE:O     | 2.21                     | 0.41              |
| 1:1A:228:A:H8      | 1:1A:228:A:H3'     | 1.87                     | 0.40              |
| 1:1A:548:A:H61     | 17:1V:19:LYS:H     | 1.67                     | 0.40              |
| 1:1A:952:G:C6      | 1:1A:953:A:N7      | 2.89                     | 0.40              |
| 1:1A:1385:G:O2'    | 1:1A:1396:U:O2     | 2.31                     | 0.40              |
| 1:1A:1614:A:OP1    | 1:1A:1617:C:N4     | 2.48                     | 0.40              |
| 1:1A:1808:U:O5'    | 1:1A:1808:U:H6     | 2.04                     | 0.40              |
| 1:1A:2820:A:C8     | 4:1E:109:LYS:HE2   | 2.56                     | 0.40              |
| 60:1A:6590:HOH:O   | 3:1D:229:VAL:HG22  | 2.19                     | 0.40              |
| 2:1B:12:C:N3       | 22:10:74:ARG:NH2   | 2.66                     | 0.40              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:1B:113:G:H2'    | 2:1B:114:C:C6      | 2.56                     | 0.40              |
| 4:1E:11:MET:HE2   | 4:1E:11:MET:HB3    | 2.00                     | 0.40              |
| 4:1E:89:ASP:OD1   | 60:1E:403:HOH:O    | 2.20                     | 0.40              |
| 6:1G:50:ALA:C     | 6:1G:52:ILE:H      | 2.27                     | 0.40              |
| 8:1I:87:LYS:HE3   | 8:1I:87:LYS:HB2    | 1.60                     | 0.40              |
| 15:1T:37:GLY:HA2  | 15:1T:38:ASN:HA    | 1.70                     | 0.40              |
| 27:15:48:GLU:O    | 27:15:60:VAL:HG21  | 2.21                     | 0.40              |
| 32:1a:79:G:N1     | 32:1a:90:U:C2      | 2.89                     | 0.40              |
| 32:1a:184:G:H4'   | 32:1a:224:C:O3'    | 2.21                     | 0.40              |
| 32:1a:890:G:O2'   | 32:1a:906:G:O6     | 2.35                     | 0.40              |
| 34:1c:183:ASP:HB2 | 34:1c:204:LEU:HD11 | 2.02                     | 0.40              |
| 35:1d:111:ALA:HB2 | 35:1d:120:LEU:HD12 | 2.03                     | 0.40              |
| 37:1f:80:ARG:NH1  | 37:1f:88:VAL:O     | 2.52                     | 0.40              |
| 1:2A:13:A:N1      | 1:2A:525:U:H2'     | 2.36                     | 0.40              |
| 1:2A:309:G:N3     | 1:2A:329:G:O2'     | 2.51                     | 0.40              |
| 1:2A:729:G:C6     | 3:2D:208:LYS:HB2   | 2.56                     | 0.40              |
| 1:2A:2627:G:N2    | 1:2A:2777:G:OP2    | 2.46                     | 0.40              |
| 1:2A:2689:U:O2    | 1:2A:2689:U:H5'    | 2.21                     | 0.40              |
| 1:2A:2689:U:P     | 1:2A:2719:G:H22    | 2.44                     | 0.40              |
| 1:2A:2786:U:H2'   | 1:2A:2787:C:H6     | 1.86                     | 0.40              |
| 1:2A:2811:G:OP1   | 4:2E:60:ASN:HB2    | 2.21                     | 0.40              |
| 5:2F:155:LEU:HD11 | 5:2F:176:LEU:HD12  | 2.04                     | 0.40              |
| 6:2G:50:ALA:O     | 6:2G:53:LEU:HG     | 2.21                     | 0.40              |
| 12:2Q:35:VAL:HG12 | 12:2Q:130:LYS:O    | 2.21                     | 0.40              |
| 32:2a:381:C:OP1   | 60:2a:3231:HOH:O   | 2.22                     | 0.40              |
| 32:2a:411:A:O2'   | 32:2a:413:G:H5'    | 2.20                     | 0.40              |
| 32:2a:750:G:H21   | 46:2o:23:GLY:C     | 2.27                     | 0.40              |
| 32:2a:780:A:OP2   | 60:2a:3229:HOH:O   | 2.21                     | 0.40              |
| 32:2a:1126:U:H4'  | 32:2a:1281:U:O2'   | 2.21                     | 0.40              |
| 32:2a:1173:G:H2'  | 32:2a:1174:G:O4'   | 2.20                     | 0.40              |
| 32:2a:1469:G:H2'  | 32:2a:1470:G:H8    | 1.86                     | 0.40              |
| 32:2a:1531:A:H8   | 32:2a:1531:A:O5'   | 2.04                     | 0.40              |
| 34:2c:70:VAL:HG22 | 34:2c:72:LYS:N     | 2.26                     | 0.40              |
| 40:2i:25:LYS:HB2  | 40:2i:60:ASP:HB3   | 2.04                     | 0.40              |
| 40:2i:26:VAL:HG21 | 40:2i:47:LEU:HD21  | 2.03                     | 0.40              |
| 1:1A:1167:U:H2'   | 1:1A:1168:G:C8     | 2.56                     | 0.40              |
| 1:1A:1814:G:H4'   | 3:1D:51:VAL:HG21   | 2.03                     | 0.40              |
| 9:1N:137:LYS:HE3  | 9:1N:139:GLU:OE2   | 2.20                     | 0.40              |
| 12:1Q:42:ILE:HG13 | 12:1Q:97:VAL:HG21  | 2.03                     | 0.40              |
| 16:1U:28:ARG:HG3  | 60:1U:301:HOH:O    | 2.21                     | 0.40              |
| 23:11:73:LEU:HD23 | 23:11:73:LEU:HA    | 1.82                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 32:1a:293:G:C6    | 32:1a:294:U:C4    | 3.09                     | 0.40              |
| 32:1a:396:G:O2'   | 32:1a:398:C:OP1   | 2.34                     | 0.40              |
| 33:1b:61:LEU:HD23 | 33:1b:68:ILE:HD11 | 2.02                     | 0.40              |
| 35:1d:155:LEU:O   | 35:1d:159:ARG:HG2 | 2.21                     | 0.40              |
| 36:1e:122:GLU:O   | 36:1e:126:ARG:NH1 | 2.54                     | 0.40              |
| 42:1k:69:ALA:O    | 42:1k:73:MET:HG3  | 2.20                     | 0.40              |
| 1:2A:247:G:H4'    | 1:2A:386:G:C5     | 2.56                     | 0.40              |
| 1:2A:801:G:O6     | 5:2F:53:THR:OG1   | 2.39                     | 0.40              |
| 1:2A:1019:U:H2'   | 1:2A:1020:A:H8    | 1.87                     | 0.40              |
| 1:2A:1155:A:C5'   | 16:2U:55:ARG:HD3  | 2.50                     | 0.40              |
| 1:2A:1849:G:H2'   | 1:2A:1850:G:C8    | 2.57                     | 0.40              |
| 1:2A:1857:G:C6    | 1:2A:1858:G:C6    | 3.09                     | 0.40              |
| 1:2A:2222:G:O2'   | 3:2D:148:GLU:HG2  | 2.21                     | 0.40              |
| 1:2A:2506:U:O5'   | 60:2A:3926:HOH:O  | 2.21                     | 0.40              |
| 3:2D:2:ALA:O      | 3:2D:20:ASP:HB3   | 2.21                     | 0.40              |
| 3:2D:171:ASP:O    | 3:2D:187:GLY:N    | 2.44                     | 0.40              |
| 5:2F:137:LYS:HB3  | 5:2F:137:LYS:HE2  | 1.88                     | 0.40              |
| 7:2H:55:PRO:HB2   | 7:2H:61:HIS:CE1   | 2.55                     | 0.40              |
| 7:2H:59:ARG:HA    | 7:2H:59:ARG:HD2   | 1.98                     | 0.40              |
| 32:2a:325:A:H2'   | 32:2a:326:G:O4'   | 2.22                     | 0.40              |
| 32:2a:328:C:H4'   | 32:2a:329:A:C5'   | 2.52                     | 0.40              |
| 32:2a:407:G:H2'   | 32:2a:408:A:C8    | 2.56                     | 0.40              |
| 32:2a:953:G:H5'   | 32:2a:965:A:H61   | 1.86                     | 0.40              |
| 34:2c:13:GLY:HA3  | 45:2n:57:ARG:HH22 | 1.86                     | 0.40              |
| 39:2h:13:ILE:O    | 39:2h:17:THR:HG23 | 2.21                     | 0.40              |
| 39:2h:46:LYS:N    | 39:2h:62:TYR:O    | 2.54                     | 0.40              |
| 44:2m:3:ARG:CG    | 44:2m:9:ILE:H     | 2.34                     | 0.40              |
| 44:2m:14:ARG:HG3  | 44:2m:44:ARG:NH1  | 2.37                     | 0.40              |
| 47:2p:25:ARG:HE   | 47:2p:25:ARG:HB3  | 1.68                     | 0.40              |
| 49:2r:47:THR:O    | 49:2r:47:THR:OG1  | 2.30                     | 0.40              |
| 1:1A:271(Q):G:N7  | 60:1A:4426:HOH:O  | 2.37                     | 0.40              |
| 1:1A:303:U:O4     | 60:1A:4216:HOH:O  | 2.22                     | 0.40              |
| 1:1A:795:C:H2'    | 1:1A:796:C:C6     | 2.56                     | 0.40              |
| 1:1A:1022:G:C5    | 1:1A:1140:C:C4    | 3.09                     | 0.40              |
| 1:1A:1469:A:H2'   | 1:1A:1470:G:O4'   | 2.21                     | 0.40              |
| 1:1A:2648:C:H2'   | 1:1A:2649:U:C6    | 2.57                     | 0.40              |
| 3:1D:97:TYR:CE2   | 3:1D:103:ARG:HG3  | 2.57                     | 0.40              |
| 5:1F:178:PRO:HB2  | 5:1F:201:VAL:HG21 | 2.03                     | 0.40              |
| 10:1O:63:VAL:HG11 | 10:1O:85:VAL:HG23 | 2.03                     | 0.40              |
| 12:1Q:21:THR:HG22 | 12:1Q:98:LYS:O    | 2.22                     | 0.40              |
| 15:1T:94:ALA:HB1  | 15:1T:99:LEU:HD21 | 2.04                     | 0.40              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 32:1a:458:C:N3    | 32:1a:474:G:N1     | 2.69                     | 0.40              |
| 32:1a:578:C:O2'   | 32:1a:728:A:N3     | 2.41                     | 0.40              |
| 32:1a:667:G:O2'   | 46:1o:49:ASP:OD1   | 2.32                     | 0.40              |
| 32:1a:680:C:C2    | 32:1a:711:G:N2     | 2.90                     | 0.40              |
| 32:1a:921:U:O2    | 36:1e:19:MET:HB2   | 2.21                     | 0.40              |
| 32:1a:1201:A:H1'  | 32:1a:1202:G:OP2   | 2.21                     | 0.40              |
| 32:1a:1298:C:H2'  | 38:1g:114:ARG:HH21 | 1.85                     | 0.40              |
| 34:1c:51:GLY:O    | 34:1c:70:VAL:HG23  | 2.22                     | 0.40              |
| 34:1c:97:LYS:HE2  | 34:1c:97:LYS:HB3   | 1.97                     | 0.40              |
| 36:1e:6:PHE:HZ    | 36:1e:40:ARG:HE    | 1.69                     | 0.40              |
| 43:1l:79:GLU:HG2  | 43:1l:80:HIS:ND1   | 2.36                     | 0.40              |
| 44:1m:75:ALA:O    | 44:1m:79:LYS:N     | 2.48                     | 0.40              |
| 47:1p:75:ARG:HG3  | 47:1p:80:PHE:CD2   | 2.56                     | 0.40              |
| 1:2A:251:A:C4     | 1:2A:252:G:H1'     | 2.56                     | 0.40              |
| 1:2A:818:G:H4'    | 1:2A:838:C:O3'     | 2.21                     | 0.40              |
| 1:2A:1356:G:H2'   | 1:2A:1357:U:O4'    | 2.21                     | 0.40              |
| 1:2A:1445:A:OP1   | 60:2A:3946:HOH:O   | 2.22                     | 0.40              |
| 1:2A:1840:G:C6    | 1:2A:1841:U:C4     | 3.09                     | 0.40              |
| 1:2A:1952:A:N3    | 10:2O:22:ILE:HD12  | 2.36                     | 0.40              |
| 1:2A:2098:U:H2'   | 1:2A:2099:U:O4'    | 2.22                     | 0.40              |
| 1:2A:2159:G:H2'   | 1:2A:2160:G:C8     | 2.53                     | 0.40              |
| 3:2D:145:VAL:HB   | 3:2D:155:LEU:HB2   | 2.02                     | 0.40              |
| 5:2F:184:TYR:CE1  | 11:2P:3:LEU:HD21   | 2.56                     | 0.40              |
| 7:2H:121:ILE:HD13 | 7:2H:121:ILE:HA    | 1.86                     | 0.40              |
| 8:2I:69:LYS:HB3   | 8:2I:73:GLU:CD     | 2.46                     | 0.40              |
| 18:2W:20:VAL:HG11 | 18:2W:44:ALA:HA    | 2.02                     | 0.40              |
| 32:2a:93:G:H2'    | 32:2a:96:U:O4'     | 2.21                     | 0.40              |
| 32:2a:735:C:H2'   | 32:2a:736:C:C6     | 2.56                     | 0.40              |
| 32:2a:868:C:H2'   | 32:2a:869:G:O4'    | 2.21                     | 0.40              |
| 32:2a:974:A:P     | 45:2n:41:ARG:HH21  | 2.45                     | 0.40              |
| 32:2a:1001:A:H2'  | 32:2a:1001(A):G:C8 | 2.56                     | 0.40              |
| 39:2h:11:THR:O    | 39:2h:15:ASN:ND2   | 2.54                     | 0.40              |
| 39:2h:51:VAL:HG11 | 39:2h:60:ARG:HH11  | 1.86                     | 0.40              |
| 53:2y:13:THR:O    | 53:2y:15:ALA:N     | 2.46                     | 0.40              |
| 53:2y:88:LEU:HD23 | 53:2y:88:LEU:HA    | 1.89                     | 0.40              |
| 1:1A:328:U:H4'    | 20:1Y:68:HIS:CG    | 2.56                     | 0.40              |
| 1:1A:773:U:H2'    | 1:1A:774:A:H5'     | 2.04                     | 0.40              |
| 1:1A:863:A:H2'    | 1:1A:864:G:H8      | 1.85                     | 0.40              |
| 1:1A:1231:G:H2'   | 1:1A:1232:G:H8     | 1.86                     | 0.40              |
| 1:1A:2104:G:H2'   | 1:1A:2105:C:O4'    | 2.21                     | 0.40              |
| 1:1A:2144:U:C2'   | 1:1A:2147:G:H1     | 2.33                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:1A:2555:U:O4     | 60:1A:4153:HOH:O   | 2.15                     | 0.40              |
| 7:1H:7:LEU:HD12    | 7:1H:8:PRO:CD      | 2.51                     | 0.40              |
| 12:1Q:111:GLU:O    | 12:1Q:115:MET:HG2  | 2.21                     | 0.40              |
| 13:1R:26:LYS:HE2   | 13:1R:70:LEU:O     | 2.21                     | 0.40              |
| 18:1W:78:GLU:OE2   | 18:1W:99:ARG:HD3   | 2.21                     | 0.40              |
| 32:1a:403:C:H5''   | 35:1d:136:PRO:HD2  | 2.01                     | 0.40              |
| 32:1a:568:G:O2'    | 32:1a:574:A:N1     | 2.38                     | 0.40              |
| 32:1a:735:C:H2'    | 32:1a:736:C:H6     | 1.87                     | 0.40              |
| 32:1a:1326:C:H2'   | 32:1a:1327:C:C6    | 2.57                     | 0.40              |
| 32:1a:1333:A:H2'   | 32:1a:1334:G:O4'   | 2.21                     | 0.40              |
| 33:1b:229:VAL:HG12 | 33:1b:230:VAL:H    | 1.86                     | 0.40              |
| 35:1d:13:ARG:HB3   | 35:1d:38:TYR:O     | 2.21                     | 0.40              |
| 43:1l:111:LYS:O    | 43:1l:112:ASP:HB2  | 2.21                     | 0.40              |
| 48:1q:25:ARG:HG2   | 48:1q:38:ARG:O     | 2.21                     | 0.40              |
| 1:2A:910:A:N1      | 1:2A:2277:G:H1'    | 2.36                     | 0.40              |
| 1:2A:1198:U:H2'    | 1:2A:1199:U:C6     | 2.55                     | 0.40              |
| 1:2A:1208:C:C4     | 1:2A:1209:G:N7     | 2.89                     | 0.40              |
| 1:2A:1324:G:C2     | 1:2A:1331:A:C2     | 3.09                     | 0.40              |
| 1:2A:1877:A:C5     | 1:2A:1878:G:H1'    | 2.57                     | 0.40              |
| 1:2A:2056:G:N2     | 27:25:5:PRO:HA     | 2.36                     | 0.40              |
| 1:2A:2131:G:OP1    | 1:2A:2132:U:H5'    | 2.21                     | 0.40              |
| 1:2A:2167:U:O2     | 1:2A:2171:A:H8     | 2.03                     | 0.40              |
| 1:2A:2282:G:H4'    | 1:2A:2389:G:O2'    | 2.20                     | 0.40              |
| 7:2H:98:LEU:HD12   | 7:2H:98:LEU:HA     | 1.90                     | 0.40              |
| 21:2Z:5:LEU:O      | 21:2Z:59:LEU:HA    | 2.21                     | 0.40              |
| 21:2Z:77:ASP:OD1   | 21:2Z:80:ARG:N     | 2.46                     | 0.40              |
| 32:2a:441:A:H3'    | 32:2a:442:C:C6     | 2.56                     | 0.40              |
| 32:2a:581:G:OP1    | 46:2o:65:ARG:NH2   | 2.48                     | 0.40              |
| 32:2a:664:G:H22    | 32:2a:741:G:H1     | 1.70                     | 0.40              |
| 32:2a:973:G:OP1    | 41:2j:57:LYS:NZ    | 2.43                     | 0.40              |
| 32:2a:1516:G:H2'   | 32:2a:1518:MA6:OP2 | 2.22                     | 0.40              |
| 33:2b:42:ILE:HG21  | 33:2b:202:PRO:O    | 2.22                     | 0.40              |
| 34:2c:131:ARG:HD2  | 34:2c:131:ARG:HA   | 1.86                     | 0.40              |
| 35:2d:166:LYS:H    | 35:2d:166:LYS:HG2  | 1.77                     | 0.40              |
| 36:2e:81:GLU:HG2   | 36:2e:90:VAL:HG13  | 2.02                     | 0.40              |
| 39:2h:77:GLU:HG3   | 39:2h:78:GLN:N     | 2.36                     | 0.40              |
| 44:2m:33:ALA:HB1   | 44:2m:56:LEU:HD11  | 2.03                     | 0.40              |
| 1:1A:271(I):G:H2'  | 1:1A:271(J):C:C6   | 2.57                     | 0.40              |
| 1:1A:272(A):U:H5   | 1:1A:272(C):G:OP1  | 2.04                     | 0.40              |
| 1:1A:612:C:H2'     | 1:1A:613:G:O4'     | 2.21                     | 0.40              |
| 1:1A:890:A:H2'     | 1:1A:892:G:O4'     | 2.21                     | 0.40              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:1A:1745(A):C:H2' | 1:1A:1746:G:O4'   | 2.21                     | 0.40              |
| 1:1A:1962:5MC:OP1  | 60:1A:4221:HOH:O  | 2.22                     | 0.40              |
| 1:1A:2002:G:H1'    | 60:1A:5165:HOH:O  | 2.22                     | 0.40              |
| 2:1B:48:A:H2'      | 2:1B:49:C:C6      | 2.57                     | 0.40              |
| 2:1B:66:A:H61      | 2:1B:109:C:H5'    | 1.87                     | 0.40              |
| 7:1H:7:LEU:HG      | 7:1H:69:ARG:NH2   | 2.37                     | 0.40              |
| 17:1V:14:VAL:HB    | 17:1V:96:ILE:HG13 | 2.03                     | 0.40              |
| 32:1a:109:A:H2'    | 32:1a:326:G:N2    | 2.37                     | 0.40              |
| 32:1a:266:G:H5''   | 32:1a:267:C:C5    | 2.57                     | 0.40              |
| 32:1a:376:G:C5'    | 47:1p:5:ARG:HD3   | 2.52                     | 0.40              |
| 32:1a:439:A:C5     | 32:1a:441:A:H1'   | 2.56                     | 0.40              |
| 32:1a:645:C:H2'    | 32:1a:646:U:C6    | 2.57                     | 0.40              |
| 32:1a:701:C:O2     | 32:1a:703:G:N1    | 2.54                     | 0.40              |
| 33:1b:16:HIS:C     | 33:1b:18:GLY:N    | 2.80                     | 0.40              |
| 35:1d:112:VAL:HG22 | 35:1d:116:GLN:OE1 | 2.22                     | 0.40              |
| 35:1d:118:ARG:HG2  | 35:1d:136:PRO:HB3 | 2.04                     | 0.40              |
| 35:1d:159:ARG:HG2  | 35:1d:159:ARG:H   | 1.49                     | 0.40              |
| 39:1h:14:ARG:O     | 39:1h:18:ARG:HG2  | 2.21                     | 0.40              |
| 41:1j:55:LYS:HB2   | 41:1j:56:HIS:H    | 1.70                     | 0.40              |
| 41:1j:78:ASN:O     | 41:1j:80:LYS:N    | 2.54                     | 0.40              |
| 53:1y:60:VAL:HG23  | 53:1y:62:VAL:HG23 | 2.03                     | 0.40              |
| 1:2A:284:U:H2'     | 1:2A:285:C:C6     | 2.56                     | 0.40              |
| 1:2A:328:U:H4'     | 20:2Y:68:HIS:CE1  | 2.56                     | 0.40              |
| 1:2A:1027:A:N6     | 1:2A:1126:A:C4    | 2.89                     | 0.40              |
| 1:2A:1297:C:OP2    | 60:2A:3935:HOH:O  | 2.21                     | 0.40              |
| 1:2A:1709:U:H2'    | 1:2A:1710:C:C6    | 2.57                     | 0.40              |
| 1:2A:1879:C:H2'    | 1:2A:1880:C:O4'   | 2.21                     | 0.40              |
| 1:2A:2186:G:N1     | 1:2A:2187:G:C5    | 2.89                     | 0.40              |
| 1:2A:2199:A:N1     | 1:2A:2226:C:N4    | 2.68                     | 0.40              |
| 1:2A:2772:C:OP1    | 60:2A:3947:HOH:O  | 2.22                     | 0.40              |
| 3:2D:159:ALA:HB1   | 3:2D:198:ASN:O    | 2.21                     | 0.40              |
| 6:2G:12:TYR:HA     | 6:2G:16:ARG:CG    | 2.52                     | 0.40              |
| 6:2G:173:LEU:O     | 6:2G:178:PHE:HB2  | 2.22                     | 0.40              |
| 7:2H:3:ARG:HH21    | 7:2H:54:ARG:NH1   | 2.20                     | 0.40              |
| 9:2N:35:ARG:H      | 9:2N:35:ARG:HG2   | 1.61                     | 0.40              |
| 15:2T:41:ARG:NH2   | 32:2a:346:G:OP1   | 2.50                     | 0.40              |
| 21:2Z:30:ASN:HA    | 21:2Z:89:PHE:HE1  | 1.85                     | 0.40              |
| 21:2Z:107:THR:HA   | 21:2Z:108:PRO:HD3 | 1.96                     | 0.40              |
| 24:22:53:LEU:HA    | 24:22:53:LEU:HD23 | 1.82                     | 0.40              |
| 32:2a:11:G:C6      | 32:2a:12:U:C4     | 3.09                     | 0.40              |
| 32:2a:580:U:H2'    | 32:2a:581:G:O4'   | 2.21                     | 0.40              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 32:2a:682:G:C6    | 32:2a:709:G:C6     | 3.09                     | 0.40              |
| 32:2a:973:G:H3'   | 32:2a:974:A:H5''   | 2.03                     | 0.40              |
| 32:2a:1095:U:H2'  | 32:2a:1096:C:O4'   | 2.21                     | 0.40              |
| 32:2a:1346:A:H5'' | 40:2i:120:ARG:HH12 | 1.86                     | 0.40              |
| 33:2b:163:PHE:HA  | 33:2b:185:ILE:O    | 2.22                     | 0.40              |
| 42:2k:20:TYR:O    | 42:2k:30:VAL:HA    | 2.22                     | 0.40              |
| 43:2l:124:LYS:HA  | 43:2l:125:PRO:HD3  | 1.92                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 3   | 1D    | 273/276 (99%) | 255 (93%) | 18 (7%)  | 0        | 100         | 100 |
| 3   | 2D    | 273/276 (99%) | 255 (93%) | 18 (7%)  | 0        | 100         | 100 |
| 4   | 1E    | 202/206 (98%) | 189 (94%) | 12 (6%)  | 1 (0%)   | 24          | 42  |
| 4   | 2E    | 202/206 (98%) | 190 (94%) | 11 (5%)  | 1 (0%)   | 24          | 42  |
| 5   | 1F    | 201/210 (96%) | 193 (96%) | 7 (4%)   | 1 (0%)   | 24          | 42  |
| 5   | 2F    | 201/210 (96%) | 191 (95%) | 9 (4%)   | 1 (0%)   | 24          | 42  |
| 6   | 1G    | 179/182 (98%) | 158 (88%) | 18 (10%) | 3 (2%)   | 7           | 16  |
| 6   | 2G    | 179/182 (98%) | 155 (87%) | 19 (11%) | 5 (3%)   | 4           | 9   |
| 7   | 1H    | 172/180 (96%) | 160 (93%) | 10 (6%)  | 2 (1%)   | 10          | 22  |
| 7   | 2H    | 171/180 (95%) | 156 (91%) | 15 (9%)  | 0        | 100         | 100 |
| 8   | 1I    | 145/148 (98%) | 121 (83%) | 21 (14%) | 3 (2%)   | 5           | 13  |
| 8   | 2I    | 144/148 (97%) | 113 (78%) | 26 (18%) | 5 (4%)   | 3           | 6   |
| 9   | 1N    | 138/140 (99%) | 134 (97%) | 4 (3%)   | 0        | 100         | 100 |
| 9   | 2N    | 138/140 (99%) | 132 (96%) | 6 (4%)   | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|------------|----------|----------|-------------|-----|
| 10  | 1O    | 120/122 (98%) | 110 (92%)  | 9 (8%)   | 1 (1%)   | 16          | 31  |
| 10  | 2O    | 120/122 (98%) | 112 (93%)  | 8 (7%)   | 0        | 100         | 100 |
| 11  | 1P    | 147/150 (98%) | 139 (95%)  | 8 (5%)   | 0        | 100         | 100 |
| 11  | 2P    | 147/150 (98%) | 132 (90%)  | 12 (8%)  | 3 (2%)   | 6           | 13  |
| 12  | 1Q    | 139/141 (99%) | 131 (94%)  | 7 (5%)   | 1 (1%)   | 18          | 35  |
| 12  | 2Q    | 139/141 (99%) | 129 (93%)  | 9 (6%)   | 1 (1%)   | 18          | 35  |
| 13  | 1R    | 116/118 (98%) | 109 (94%)  | 7 (6%)   | 0        | 100         | 100 |
| 13  | 2R    | 116/118 (98%) | 110 (95%)  | 5 (4%)   | 1 (1%)   | 14          | 28  |
| 14  | 1S    | 108/112 (96%) | 100 (93%)  | 8 (7%)   | 0        | 100         | 100 |
| 14  | 2S    | 108/112 (96%) | 96 (89%)   | 11 (10%) | 1 (1%)   | 14          | 28  |
| 15  | 1T    | 129/146 (88%) | 122 (95%)  | 6 (5%)   | 1 (1%)   | 16          | 31  |
| 15  | 2T    | 129/146 (88%) | 121 (94%)  | 7 (5%)   | 1 (1%)   | 16          | 31  |
| 16  | 1U    | 114/118 (97%) | 114 (100%) | 0        | 0        | 100         | 100 |
| 16  | 2U    | 114/118 (97%) | 108 (95%)  | 5 (4%)   | 1 (1%)   | 14          | 28  |
| 17  | 1V    | 99/101 (98%)  | 95 (96%)   | 3 (3%)   | 1 (1%)   | 12          | 25  |
| 17  | 2V    | 99/101 (98%)  | 90 (91%)   | 7 (7%)   | 2 (2%)   | 6           | 13  |
| 18  | 1W    | 110/113 (97%) | 109 (99%)  | 1 (1%)   | 0        | 100         | 100 |
| 18  | 2W    | 110/113 (97%) | 106 (96%)  | 4 (4%)   | 0        | 100         | 100 |
| 19  | 1X    | 93/96 (97%)   | 92 (99%)   | 1 (1%)   | 0        | 100         | 100 |
| 19  | 2X    | 93/96 (97%)   | 86 (92%)   | 6 (6%)   | 1 (1%)   | 11          | 24  |
| 20  | 1Y    | 105/110 (96%) | 98 (93%)   | 7 (7%)   | 0        | 100         | 100 |
| 20  | 2Y    | 105/110 (96%) | 94 (90%)   | 11 (10%) | 0        | 100         | 100 |
| 21  | 1Z    | 201/206 (98%) | 184 (92%)  | 16 (8%)  | 1 (0%)   | 24          | 42  |
| 21  | 2Z    | 199/206 (97%) | 174 (87%)  | 24 (12%) | 1 (0%)   | 24          | 42  |
| 22  | 10    | 75/85 (88%)   | 74 (99%)   | 1 (1%)   | 0        | 100         | 100 |
| 22  | 20    | 75/85 (88%)   | 70 (93%)   | 5 (7%)   | 0        | 100         | 100 |
| 23  | 11    | 95/98 (97%)   | 93 (98%)   | 2 (2%)   | 0        | 100         | 100 |
| 23  | 21    | 95/98 (97%)   | 93 (98%)   | 1 (1%)   | 1 (1%)   | 11          | 24  |
| 24  | 12    | 68/72 (94%)   | 68 (100%)  | 0        | 0        | 100         | 100 |
| 24  | 22    | 68/72 (94%)   | 66 (97%)   | 2 (3%)   | 0        | 100         | 100 |
| 25  | 13    | 57/60 (95%)   | 55 (96%)   | 2 (4%)   | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 25  | 23    | 57/60 (95%)   | 51 (90%)  | 6 (10%)  | 0        | 100         | 100 |
| 26  | 14    | 67/71 (94%)   | 47 (70%)  | 15 (22%) | 5 (8%)   | 1           | 1   |
| 26  | 24    | 67/71 (94%)   | 49 (73%)  | 11 (16%) | 7 (10%)  | 0           | 0   |
| 27  | 15    | 57/60 (95%)   | 55 (96%)  | 2 (4%)   | 0        | 100         | 100 |
| 27  | 25    | 57/60 (95%)   | 53 (93%)  | 4 (7%)   | 0        | 100         | 100 |
| 28  | 16    | 51/54 (94%)   | 47 (92%)  | 4 (8%)   | 0        | 100         | 100 |
| 28  | 26    | 51/54 (94%)   | 49 (96%)  | 2 (4%)   | 0        | 100         | 100 |
| 29  | 17    | 46/49 (94%)   | 46 (100%) | 0        | 0        | 100         | 100 |
| 29  | 27    | 46/49 (94%)   | 45 (98%)  | 1 (2%)   | 0        | 100         | 100 |
| 30  | 18    | 62/65 (95%)   | 61 (98%)  | 1 (2%)   | 0        | 100         | 100 |
| 30  | 28    | 62/65 (95%)   | 58 (94%)  | 4 (6%)   | 0        | 100         | 100 |
| 31  | 19    | 35/37 (95%)   | 34 (97%)  | 1 (3%)   | 0        | 100         | 100 |
| 31  | 29    | 35/37 (95%)   | 34 (97%)  | 1 (3%)   | 0        | 100         | 100 |
| 33  | 1b    | 229/256 (90%) | 186 (81%) | 35 (15%) | 8 (4%)   | 3           | 6   |
| 33  | 2b    | 229/256 (90%) | 195 (85%) | 27 (12%) | 7 (3%)   | 3           | 7   |
| 34  | 1c    | 204/239 (85%) | 184 (90%) | 18 (9%)  | 2 (1%)   | 12          | 25  |
| 34  | 2c    | 204/239 (85%) | 183 (90%) | 15 (7%)  | 6 (3%)   | 3           | 8   |
| 35  | 1d    | 206/209 (99%) | 182 (88%) | 21 (10%) | 3 (2%)   | 8           | 18  |
| 35  | 2d    | 206/209 (99%) | 180 (87%) | 25 (12%) | 1 (0%)   | 24          | 42  |
| 36  | 1e    | 146/162 (90%) | 130 (89%) | 14 (10%) | 2 (1%)   | 9           | 19  |
| 36  | 2e    | 146/162 (90%) | 130 (89%) | 14 (10%) | 2 (1%)   | 9           | 19  |
| 37  | 1f    | 98/101 (97%)  | 91 (93%)  | 7 (7%)   | 0        | 100         | 100 |
| 37  | 2f    | 98/101 (97%)  | 91 (93%)  | 7 (7%)   | 0        | 100         | 100 |
| 38  | 1g    | 153/156 (98%) | 144 (94%) | 9 (6%)   | 0        | 100         | 100 |
| 38  | 2g    | 153/156 (98%) | 140 (92%) | 12 (8%)  | 1 (1%)   | 18          | 35  |
| 39  | 1h    | 135/138 (98%) | 124 (92%) | 11 (8%)  | 0        | 100         | 100 |
| 39  | 2h    | 135/138 (98%) | 125 (93%) | 8 (6%)   | 2 (2%)   | 8           | 18  |
| 40  | 1i    | 125/128 (98%) | 108 (86%) | 15 (12%) | 2 (2%)   | 7           | 17  |
| 40  | 2i    | 124/128 (97%) | 110 (89%) | 11 (9%)  | 3 (2%)   | 4           | 10  |
| 41  | 1j    | 95/105 (90%)  | 83 (87%)  | 9 (10%)  | 3 (3%)   | 3           | 7   |
| 41  | 2j    | 94/105 (90%)  | 78 (83%)  | 14 (15%) | 2 (2%)   | 5           | 13  |

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| Mol | Chain | Analysed          | Favoured    | Allowed  | Outliers | Percentiles |     |
|-----|-------|-------------------|-------------|----------|----------|-------------|-----|
| 42  | 1k    | 112/129 (87%)     | 100 (89%)   | 12 (11%) | 0        | 100         | 100 |
| 42  | 2k    | 112/129 (87%)     | 108 (96%)   | 4 (4%)   | 0        | 100         | 100 |
| 43  | 1l    | 119/132 (90%)     | 108 (91%)   | 11 (9%)  | 0        | 100         | 100 |
| 43  | 2l    | 119/132 (90%)     | 108 (91%)   | 10 (8%)  | 1 (1%)   | 16          | 31  |
| 44  | 1m    | 114/126 (90%)     | 104 (91%)   | 8 (7%)   | 2 (2%)   | 6           | 15  |
| 44  | 2m    | 112/126 (89%)     | 98 (88%)    | 11 (10%) | 3 (3%)   | 4           | 9   |
| 45  | 1n    | 58/61 (95%)       | 55 (95%)    | 3 (5%)   | 0        | 100         | 100 |
| 45  | 2n    | 58/61 (95%)       | 49 (84%)    | 9 (16%)  | 0        | 100         | 100 |
| 46  | 1o    | 86/89 (97%)       | 82 (95%)    | 4 (5%)   | 0        | 100         | 100 |
| 46  | 2o    | 86/89 (97%)       | 80 (93%)    | 6 (7%)   | 0        | 100         | 100 |
| 47  | 1p    | 80/88 (91%)       | 68 (85%)    | 12 (15%) | 0        | 100         | 100 |
| 47  | 2p    | 80/88 (91%)       | 69 (86%)    | 11 (14%) | 0        | 100         | 100 |
| 48  | 1q    | 97/105 (92%)      | 90 (93%)    | 6 (6%)   | 1 (1%)   | 12          | 25  |
| 48  | 2q    | 97/105 (92%)      | 91 (94%)    | 6 (6%)   | 0        | 100         | 100 |
| 49  | 1r    | 66/88 (75%)       | 58 (88%)    | 7 (11%)  | 1 (2%)   | 8           | 18  |
| 49  | 2r    | 66/88 (75%)       | 62 (94%)    | 4 (6%)   | 0        | 100         | 100 |
| 50  | 1s    | 81/93 (87%)       | 70 (86%)    | 11 (14%) | 0        | 100         | 100 |
| 50  | 2s    | 81/93 (87%)       | 70 (86%)    | 10 (12%) | 1 (1%)   | 10          | 22  |
| 51  | 1t    | 94/106 (89%)      | 85 (90%)    | 8 (8%)   | 1 (1%)   | 11          | 24  |
| 51  | 2t    | 96/106 (91%)      | 88 (92%)    | 7 (7%)   | 1 (1%)   | 12          | 25  |
| 52  | 1u    | 21/27 (78%)       | 19 (90%)    | 2 (10%)  | 0        | 100         | 100 |
| 52  | 2u    | 21/27 (78%)       | 19 (90%)    | 1 (5%)   | 1 (5%)   | 2           | 3   |
| 53  | 1y    | 95/113 (84%)      | 93 (98%)    | 2 (2%)   | 0        | 100         | 100 |
| 53  | 2y    | 94/113 (83%)      | 87 (93%)    | 5 (5%)   | 2 (2%)   | 5           | 13  |
| All | All   | 11629/12354 (94%) | 10636 (92%) | 883 (8%) | 110 (1%) | 14          | 28  |

All (110) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | 1F    | 130 | ALA  |
| 7   | 1H    | 126 | PRO  |
| 33  | 1b    | 8   | LYS  |
| 33  | 1b    | 17  | PHE  |
| 33  | 1b    | 125 | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 44  | 1m    | 67  | GLU  |
| 4   | 2E    | 51  | PHE  |
| 5   | 2F    | 130 | ALA  |
| 6   | 2G    | 43  | LEU  |
| 6   | 2G    | 81  | LYS  |
| 8   | 2I    | 10  | GLU  |
| 8   | 2I    | 85  | GLU  |
| 11  | 2P    | 36  | LYS  |
| 26  | 24    | 62  | ARG  |
| 33  | 2b    | 17  | PHE  |
| 40  | 2i    | 54  | ASP  |
| 44  | 2m    | 5   | ALA  |
| 6   | 1G    | 49  | ASP  |
| 7   | 1H    | 159 | GLU  |
| 8   | 1I    | 40  | THR  |
| 15  | 1T    | 128 | GLU  |
| 34  | 1c    | 14  | ILE  |
| 35  | 1d    | 5   | ILE  |
| 36  | 1e    | 77  | PRO  |
| 41  | 1j    | 55  | LYS  |
| 41  | 1j    | 75  | ILE  |
| 6   | 2G    | 126 | ASP  |
| 11  | 2P    | 29  | LYS  |
| 14  | 2S    | 62  | LYS  |
| 17  | 2V    | 53  | GLU  |
| 17  | 2V    | 79  | VAL  |
| 19  | 2X    | 94  | GLY  |
| 26  | 24    | 49  | PHE  |
| 26  | 24    | 54  | GLY  |
| 26  | 24    | 60  | GLN  |
| 34  | 2c    | 98  | ASN  |
| 34  | 2c    | 156 | ARG  |
| 38  | 2g    | 55  | GLY  |
| 44  | 2m    | 67  | GLU  |
| 52  | 2u    | 7   | ARG  |
| 53  | 2y    | 45  | PRO  |
| 6   | 1G    | 47  | LYS  |
| 8   | 1I    | 73  | GLU  |
| 12  | 1Q    | 59  | ARG  |
| 26  | 14    | 55  | ARG  |
| 33  | 1b    | 9   | GLU  |
| 40  | 1i    | 11  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | 2G    | 96  | ARG  |
| 23  | 21    | 3   | LYS  |
| 26  | 24    | 39  | CYS  |
| 33  | 2b    | 16  | HIS  |
| 33  | 2b    | 124 | SER  |
| 39  | 2h    | 68  | ARG  |
| 41  | 2j    | 77  | PRO  |
| 41  | 2j    | 78  | ASN  |
| 43  | 2l    | 105 | TYR  |
| 50  | 2s    | 28  | LYS  |
| 4   | 1E    | 52  | LEU  |
| 6   | 1G    | 43  | LEU  |
| 26  | 14    | 47  | GLN  |
| 26  | 14    | 49  | PHE  |
| 26  | 14    | 61  | ARG  |
| 33  | 1b    | 37  | ASN  |
| 33  | 1b    | 124 | SER  |
| 33  | 1b    | 127 | ILE  |
| 34  | 1c    | 107 | GLN  |
| 36  | 1e    | 21  | ALA  |
| 40  | 1i    | 54  | ASP  |
| 6   | 2G    | 176 | LEU  |
| 8   | 2I    | 83  | ALA  |
| 8   | 2I    | 94  | ALA  |
| 11  | 2P    | 141 | ALA  |
| 26  | 24    | 47  | GLN  |
| 26  | 24    | 55  | ARG  |
| 35  | 2d    | 37  | PRO  |
| 40  | 2i    | 11  | LYS  |
| 40  | 2i    | 44  | VAL  |
| 53  | 2y    | 9   | GLN  |
| 8   | 1I    | 103 | ARG  |
| 17  | 1V    | 79  | VAL  |
| 21  | 1Z    | 64  | GLY  |
| 33  | 1b    | 231 | GLU  |
| 35  | 1d    | 164 | ALA  |
| 35  | 1d    | 166 | LYS  |
| 41  | 1j    | 79  | ARG  |
| 48  | 1q    | 53  | LEU  |
| 49  | 1r    | 25  | THR  |
| 12  | 2Q    | 59  | ARG  |
| 33  | 2b    | 20  | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 33  | 2b    | 125 | PRO  |
| 34  | 2c    | 95  | THR  |
| 51  | 2t    | 102 | GLY  |
| 26  | 14    | 65  | ASP  |
| 44  | 1m    | 12  | ASN  |
| 33  | 2b    | 120 | ALA  |
| 44  | 2m    | 7   | VAL  |
| 10  | 1O    | 119 | PRO  |
| 34  | 2c    | 108 | ASN  |
| 36  | 2e    | 39  | GLY  |
| 8   | 2I    | 131 | LYS  |
| 13  | 2R    | 58  | GLY  |
| 16  | 2U    | 7   | GLY  |
| 36  | 2e    | 85  | GLY  |
| 33  | 2b    | 227 | GLY  |
| 34  | 2c    | 51  | GLY  |
| 34  | 2c    | 99  | VAL  |
| 51  | 1t    | 100 | ILE  |
| 15  | 2T    | 20  | PRO  |
| 21  | 2Z    | 106 | GLY  |
| 39  | 2h    | 51  | VAL  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed      | Rotameric | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|-------------|----|
| 3   | 1D    | 214/218 (98%) | 192 (90%) | 22 (10%) | 7           | 14 |
| 3   | 2D    | 215/218 (99%) | 190 (88%) | 25 (12%) | 5           | 10 |
| 4   | 1E    | 164/166 (99%) | 141 (86%) | 23 (14%) | 3           | 6  |
| 4   | 2E    | 164/166 (99%) | 146 (89%) | 18 (11%) | 6           | 12 |
| 5   | 1F    | 160/166 (96%) | 138 (86%) | 22 (14%) | 3           | 7  |
| 5   | 2F    | 159/166 (96%) | 139 (87%) | 20 (13%) | 4           | 8  |
| 6   | 1G    | 144/156 (92%) | 133 (92%) | 11 (8%)  | 12          | 26 |
| 6   | 2G    | 142/156 (91%) | 123 (87%) | 19 (13%) | 4           | 7  |

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| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 7   | 1H    | 144/148 (97%)  | 130 (90%) | 14 (10%) | 8           | 17 |
| 7   | 2H    | 143/148 (97%)  | 122 (85%) | 21 (15%) | 3           | 5  |
| 8   | 1I    | 111/124 (90%)  | 96 (86%)  | 15 (14%) | 4           | 7  |
| 8   | 2I    | 108/124 (87%)  | 80 (74%)  | 28 (26%) | 0           | 0  |
| 9   | 1N    | 119/119 (100%) | 102 (86%) | 17 (14%) | 3           | 6  |
| 9   | 2N    | 118/119 (99%)  | 100 (85%) | 18 (15%) | 3           | 5  |
| 10  | 1O    | 100/100 (100%) | 86 (86%)  | 14 (14%) | 3           | 6  |
| 10  | 2O    | 100/100 (100%) | 90 (90%)  | 10 (10%) | 7           | 16 |
| 11  | 1P    | 115/116 (99%)  | 103 (90%) | 12 (10%) | 7           | 14 |
| 11  | 2P    | 115/116 (99%)  | 102 (89%) | 13 (11%) | 5           | 11 |
| 12  | 1Q    | 111/111 (100%) | 99 (89%)  | 12 (11%) | 6           | 12 |
| 12  | 2Q    | 111/111 (100%) | 100 (90%) | 11 (10%) | 7           | 16 |
| 13  | 1R    | 101/101 (100%) | 91 (90%)  | 10 (10%) | 7           | 16 |
| 13  | 2R    | 101/101 (100%) | 86 (85%)  | 15 (15%) | 3           | 5  |
| 14  | 1S    | 87/88 (99%)    | 76 (87%)  | 11 (13%) | 4           | 8  |
| 14  | 2S    | 85/88 (97%)    | 75 (88%)  | 10 (12%) | 5           | 10 |
| 15  | 1T    | 115/127 (91%)  | 105 (91%) | 10 (9%)  | 9           | 21 |
| 15  | 2T    | 113/127 (89%)  | 104 (92%) | 9 (8%)   | 11          | 24 |
| 16  | 1U    | 93/94 (99%)    | 82 (88%)  | 11 (12%) | 5           | 10 |
| 16  | 2U    | 93/94 (99%)    | 88 (95%)  | 5 (5%)   | 20          | 42 |
| 17  | 1V    | 81/82 (99%)    | 70 (86%)  | 11 (14%) | 3           | 7  |
| 17  | 2V    | 80/82 (98%)    | 72 (90%)  | 8 (10%)  | 7           | 16 |
| 18  | 1W    | 90/92 (98%)    | 81 (90%)  | 9 (10%)  | 7           | 16 |
| 18  | 2W    | 90/92 (98%)    | 84 (93%)  | 6 (7%)   | 15          | 31 |
| 19  | 1X    | 77/78 (99%)    | 71 (92%)  | 6 (8%)   | 11          | 25 |
| 19  | 2X    | 77/78 (99%)    | 71 (92%)  | 6 (8%)   | 11          | 25 |
| 20  | 1Y    | 86/91 (94%)    | 79 (92%)  | 7 (8%)   | 11          | 23 |
| 20  | 2Y    | 86/91 (94%)    | 76 (88%)  | 10 (12%) | 5           | 10 |
| 21  | 1Z    | 169/179 (94%)  | 145 (86%) | 24 (14%) | 3           | 6  |
| 21  | 2Z    | 165/179 (92%)  | 149 (90%) | 16 (10%) | 8           | 17 |
| 22  | 10    | 61/67 (91%)    | 55 (90%)  | 6 (10%)  | 7           | 16 |

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| Mol | Chain | Analysed      | Rotameric | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|-------------|----|
| 22  | 20    | 61/67 (91%)   | 56 (92%)  | 5 (8%)   | 10          | 23 |
| 23  | 11    | 79/83 (95%)   | 71 (90%)  | 8 (10%)  | 7           | 15 |
| 23  | 21    | 81/83 (98%)   | 71 (88%)  | 10 (12%) | 4           | 8  |
| 24  | 12    | 65/67 (97%)   | 59 (91%)  | 6 (9%)   | 8           | 19 |
| 24  | 22    | 66/67 (98%)   | 56 (85%)  | 10 (15%) | 3           | 5  |
| 25  | 13    | 51/52 (98%)   | 45 (88%)  | 6 (12%)  | 5           | 10 |
| 25  | 23    | 50/52 (96%)   | 41 (82%)  | 9 (18%)  | 2           | 3  |
| 26  | 14    | 58/63 (92%)   | 53 (91%)  | 5 (9%)   | 10          | 21 |
| 26  | 24    | 54/63 (86%)   | 44 (82%)  | 10 (18%) | 1           | 2  |
| 27  | 15    | 51/52 (98%)   | 46 (90%)  | 5 (10%)  | 7           | 16 |
| 27  | 25    | 50/52 (96%)   | 43 (86%)  | 7 (14%)  | 3           | 6  |
| 28  | 16    | 51/52 (98%)   | 50 (98%)  | 1 (2%)   | 48          | 71 |
| 28  | 26    | 50/52 (96%)   | 46 (92%)  | 4 (8%)   | 11          | 24 |
| 29  | 17    | 41/42 (98%)   | 39 (95%)  | 2 (5%)   | 22          | 45 |
| 29  | 27    | 41/42 (98%)   | 37 (90%)  | 4 (10%)  | 7           | 16 |
| 30  | 18    | 54/55 (98%)   | 50 (93%)  | 4 (7%)   | 13          | 26 |
| 30  | 28    | 54/55 (98%)   | 48 (89%)  | 6 (11%)  | 6           | 12 |
| 31  | 19    | 34/34 (100%)  | 32 (94%)  | 2 (6%)   | 18          | 37 |
| 31  | 29    | 34/34 (100%)  | 32 (94%)  | 2 (6%)   | 18          | 37 |
| 33  | 1b    | 191/220 (87%) | 162 (85%) | 29 (15%) | 3           | 5  |
| 33  | 2b    | 187/220 (85%) | 163 (87%) | 24 (13%) | 4           | 7  |
| 34  | 1c    | 144/188 (77%) | 130 (90%) | 14 (10%) | 8           | 17 |
| 34  | 2c    | 140/188 (74%) | 122 (87%) | 18 (13%) | 4           | 7  |
| 35  | 1d    | 171/181 (94%) | 141 (82%) | 30 (18%) | 2           | 3  |
| 35  | 2d    | 172/181 (95%) | 154 (90%) | 18 (10%) | 6           | 13 |
| 36  | 1e    | 114/123 (93%) | 101 (89%) | 13 (11%) | 5           | 11 |
| 36  | 2e    | 114/123 (93%) | 99 (87%)  | 15 (13%) | 4           | 7  |
| 37  | 1f    | 85/90 (94%)   | 81 (95%)  | 4 (5%)   | 23          | 47 |
| 37  | 2f    | 85/90 (94%)   | 80 (94%)  | 5 (6%)   | 18          | 37 |
| 38  | 1g    | 120/127 (94%) | 115 (96%) | 5 (4%)   | 26          | 51 |
| 38  | 2g    | 119/127 (94%) | 105 (88%) | 14 (12%) | 5           | 10 |

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| Mol | Chain | Analysed         | Rotameric  | Outliers   | Percentiles |    |
|-----|-------|------------------|------------|------------|-------------|----|
| 39  | 1h    | 116/119 (98%)    | 105 (90%)  | 11 (10%)   | 8           | 17 |
| 39  | 2h    | 114/119 (96%)    | 103 (90%)  | 11 (10%)   | 8           | 17 |
| 40  | 1i    | 91/99 (92%)      | 81 (89%)   | 10 (11%)   | 6           | 12 |
| 40  | 2i    | 88/99 (89%)      | 74 (84%)   | 14 (16%)   | 2           | 4  |
| 41  | 1j    | 68/92 (74%)      | 57 (84%)   | 11 (16%)   | 2           | 4  |
| 41  | 2j    | 68/92 (74%)      | 63 (93%)   | 5 (7%)     | 13          | 26 |
| 42  | 1k    | 83/99 (84%)      | 72 (87%)   | 11 (13%)   | 4           | 7  |
| 42  | 2k    | 83/99 (84%)      | 72 (87%)   | 11 (13%)   | 4           | 7  |
| 43  | 1l    | 96/108 (89%)     | 83 (86%)   | 13 (14%)   | 4           | 7  |
| 43  | 2l    | 96/108 (89%)     | 86 (90%)   | 10 (10%)   | 7           | 14 |
| 44  | 1m    | 90/101 (89%)     | 73 (81%)   | 17 (19%)   | 1           | 2  |
| 44  | 2m    | 87/101 (86%)     | 78 (90%)   | 9 (10%)    | 7           | 14 |
| 45  | 1n    | 49/50 (98%)      | 40 (82%)   | 9 (18%)    | 1           | 2  |
| 45  | 2n    | 49/50 (98%)      | 41 (84%)   | 8 (16%)    | 2           | 4  |
| 46  | 1o    | 78/80 (98%)      | 73 (94%)   | 5 (6%)     | 16          | 33 |
| 46  | 2o    | 78/80 (98%)      | 68 (87%)   | 10 (13%)   | 4           | 7  |
| 47  | 1p    | 69/74 (93%)      | 52 (75%)   | 17 (25%)   | 1           | 0  |
| 47  | 2p    | 68/74 (92%)      | 55 (81%)   | 13 (19%)   | 1           | 2  |
| 48  | 1q    | 94/97 (97%)      | 85 (90%)   | 9 (10%)    | 8           | 17 |
| 48  | 2q    | 94/97 (97%)      | 87 (93%)   | 7 (7%)     | 13          | 26 |
| 49  | 1r    | 59/77 (77%)      | 52 (88%)   | 7 (12%)    | 5           | 10 |
| 49  | 2r    | 59/77 (77%)      | 50 (85%)   | 9 (15%)    | 3           | 5  |
| 50  | 1s    | 68/80 (85%)      | 60 (88%)   | 8 (12%)    | 5           | 10 |
| 50  | 2s    | 67/80 (84%)      | 61 (91%)   | 6 (9%)     | 9           | 19 |
| 51  | 1t    | 71/82 (87%)      | 65 (92%)   | 6 (8%)     | 10          | 22 |
| 51  | 2t    | 70/82 (85%)      | 64 (91%)   | 6 (9%)     | 10          | 21 |
| 52  | 1u    | 18/22 (82%)      | 17 (94%)   | 1 (6%)     | 19          | 40 |
| 52  | 2u    | 18/22 (82%)      | 17 (94%)   | 1 (6%)     | 19          | 40 |
| 53  | 1y    | 82/98 (84%)      | 73 (89%)   | 9 (11%)    | 6           | 12 |
| 53  | 2y    | 79/98 (81%)      | 64 (81%)   | 15 (19%)   | 1           | 2  |
| All | All   | 9524/10260 (93%) | 8415 (88%) | 1109 (12%) | 5           | 10 |

All (1109) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | 1D    | 3   | VAL  |
| 3   | 1D    | 39  | LYS  |
| 3   | 1D    | 61  | LEU  |
| 3   | 1D    | 69  | ARG  |
| 3   | 1D    | 71  | ASP  |
| 3   | 1D    | 89  | SER  |
| 3   | 1D    | 94  | LEU  |
| 3   | 1D    | 103 | ARG  |
| 3   | 1D    | 111 | LEU  |
| 3   | 1D    | 127 | VAL  |
| 3   | 1D    | 134 | ARG  |
| 3   | 1D    | 142 | VAL  |
| 3   | 1D    | 155 | LEU  |
| 3   | 1D    | 173 | VAL  |
| 3   | 1D    | 183 | ARG  |
| 3   | 1D    | 193 | VAL  |
| 3   | 1D    | 211 | ARG  |
| 3   | 1D    | 217 | ARG  |
| 3   | 1D    | 221 | VAL  |
| 3   | 1D    | 229 | VAL  |
| 3   | 1D    | 242 | ARG  |
| 3   | 1D    | 259 | THR  |
| 4   | 1E    | 1   | MET  |
| 4   | 1E    | 5   | LEU  |
| 4   | 1E    | 7   | VAL  |
| 4   | 1E    | 9   | VAL  |
| 4   | 1E    | 21  | VAL  |
| 4   | 1E    | 33  | VAL  |
| 4   | 1E    | 34  | VAL  |
| 4   | 1E    | 42  | ASP  |
| 4   | 1E    | 49  | LEU  |
| 4   | 1E    | 73  | GLU  |
| 4   | 1E    | 75  | VAL  |
| 4   | 1E    | 77  | ILE  |
| 4   | 1E    | 78  | LEU  |
| 4   | 1E    | 116 | VAL  |
| 4   | 1E    | 119 | ARG  |
| 4   | 1E    | 144 | ARG  |
| 4   | 1E    | 163 | GLU  |
| 4   | 1E    | 168 | MET  |
| 4   | 1E    | 170 | LEU  |
| 4   | 1E    | 175 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | 1E    | 178 | GLU  |
| 4   | 1E    | 181 | LEU  |
| 4   | 1E    | 195 | LEU  |
| 5   | 1F    | 12  | LEU  |
| 5   | 1F    | 15  | SER  |
| 5   | 1F    | 19  | GLU  |
| 5   | 1F    | 24  | LEU  |
| 5   | 1F    | 33  | LEU  |
| 5   | 1F    | 38  | ARG  |
| 5   | 1F    | 53  | THR  |
| 5   | 1F    | 57  | VAL  |
| 5   | 1F    | 74  | ARG  |
| 5   | 1F    | 88  | VAL  |
| 5   | 1F    | 110 | LEU  |
| 5   | 1F    | 125 | LEU  |
| 5   | 1F    | 132 | VAL  |
| 5   | 1F    | 140 | LEU  |
| 5   | 1F    | 157 | VAL  |
| 5   | 1F    | 162 | LEU  |
| 5   | 1F    | 170 | LEU  |
| 5   | 1F    | 176 | LEU  |
| 5   | 1F    | 183 | VAL  |
| 5   | 1F    | 192 | LEU  |
| 5   | 1F    | 200 | GLU  |
| 5   | 1F    | 201 | VAL  |
| 6   | 1G    | 5   | VAL  |
| 6   | 1G    | 7   | LEU  |
| 6   | 1G    | 28  | VAL  |
| 6   | 1G    | 31  | VAL  |
| 6   | 1G    | 43  | LEU  |
| 6   | 1G    | 52  | ILE  |
| 6   | 1G    | 126 | ASP  |
| 6   | 1G    | 138 | GLN  |
| 6   | 1G    | 139 | LEU  |
| 6   | 1G    | 140 | ILE  |
| 6   | 1G    | 181 | ARG  |
| 7   | 1H    | 13  | LYS  |
| 7   | 1H    | 15  | VAL  |
| 7   | 1H    | 24  | VAL  |
| 7   | 1H    | 44  | VAL  |
| 7   | 1H    | 45  | VAL  |
| 7   | 1H    | 49  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | 1H    | 71  | LEU  |
| 7   | 1H    | 84  | SER  |
| 7   | 1H    | 98  | LEU  |
| 7   | 1H    | 105 | LEU  |
| 7   | 1H    | 106 | THR  |
| 7   | 1H    | 122 | THR  |
| 7   | 1H    | 129 | THR  |
| 7   | 1H    | 153 | LYS  |
| 8   | 1I    | 3   | VAL  |
| 8   | 1I    | 5   | LEU  |
| 8   | 1I    | 20  | ASP  |
| 8   | 1I    | 57  | ARG  |
| 8   | 1I    | 75  | LEU  |
| 8   | 1I    | 78  | THR  |
| 8   | 1I    | 79  | ILE  |
| 8   | 1I    | 92  | VAL  |
| 8   | 1I    | 101 | LEU  |
| 8   | 1I    | 104 | GLN  |
| 8   | 1I    | 108 | THR  |
| 8   | 1I    | 109 | ILE  |
| 8   | 1I    | 117 | GLU  |
| 8   | 1I    | 133 | HIS  |
| 8   | 1I    | 140 | LEU  |
| 9   | 1N    | 14  | VAL  |
| 9   | 1N    | 15  | LEU  |
| 9   | 1N    | 33  | LEU  |
| 9   | 1N    | 34  | LEU  |
| 9   | 1N    | 48  | MET  |
| 9   | 1N    | 62  | VAL  |
| 9   | 1N    | 65  | LYS  |
| 9   | 1N    | 67  | LEU  |
| 9   | 1N    | 68  | GLU  |
| 9   | 1N    | 73  | THR  |
| 9   | 1N    | 87  | LEU  |
| 9   | 1N    | 89  | LYS  |
| 9   | 1N    | 97  | ARG  |
| 9   | 1N    | 99  | LEU  |
| 9   | 1N    | 121 | LYS  |
| 9   | 1N    | 133 | GLN  |
| 9   | 1N    | 138 | LEU  |
| 10  | 1O    | 1   | MET  |
| 10  | 1O    | 8   | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10  | 1O    | 10  | VAL  |
| 10  | 1O    | 20  | MET  |
| 10  | 1O    | 23  | ARG  |
| 10  | 1O    | 24  | VAL  |
| 10  | 1O    | 35  | VAL  |
| 10  | 1O    | 89  | ASN  |
| 10  | 1O    | 94  | ARG  |
| 10  | 1O    | 96  | THR  |
| 10  | 1O    | 98  | VAL  |
| 10  | 1O    | 108 | GLU  |
| 10  | 1O    | 113 | LYS  |
| 10  | 1O    | 116 | SER  |
| 11  | 1P    | 3   | LEU  |
| 11  | 1P    | 59  | LEU  |
| 11  | 1P    | 65  | ARG  |
| 11  | 1P    | 83  | VAL  |
| 11  | 1P    | 95  | VAL  |
| 11  | 1P    | 96  | THR  |
| 11  | 1P    | 99  | LEU  |
| 11  | 1P    | 112 | LEU  |
| 11  | 1P    | 114 | ILE  |
| 11  | 1P    | 125 | VAL  |
| 11  | 1P    | 147 | LEU  |
| 11  | 1P    | 149 | GLU  |
| 12  | 1Q    | 1   | MET  |
| 12  | 1Q    | 7   | MET  |
| 12  | 1Q    | 8   | LYS  |
| 12  | 1Q    | 21  | THR  |
| 12  | 1Q    | 42  | ILE  |
| 12  | 1Q    | 55  | VAL  |
| 12  | 1Q    | 60  | ARG  |
| 12  | 1Q    | 75  | THR  |
| 12  | 1Q    | 81  | VAL  |
| 12  | 1Q    | 101 | ARG  |
| 12  | 1Q    | 109 | VAL  |
| 12  | 1Q    | 130 | LYS  |
| 13  | 1R    | 6   | SER  |
| 13  | 1R    | 29  | LEU  |
| 13  | 1R    | 36  | THR  |
| 13  | 1R    | 44  | LEU  |
| 13  | 1R    | 54  | LEU  |
| 13  | 1R    | 65  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 13  | 1R    | 67  | LEU  |
| 13  | 1R    | 75  | LEU  |
| 13  | 1R    | 100 | LEU  |
| 13  | 1R    | 117 | VAL  |
| 14  | 1S    | 11  | LYS  |
| 14  | 1S    | 14  | VAL  |
| 14  | 1S    | 43  | GLU  |
| 14  | 1S    | 46  | VAL  |
| 14  | 1S    | 48  | LEU  |
| 14  | 1S    | 49  | VAL  |
| 14  | 1S    | 50  | SER  |
| 14  | 1S    | 52  | SER  |
| 14  | 1S    | 59  | LYS  |
| 14  | 1S    | 68  | GLN  |
| 14  | 1S    | 110 | LEU  |
| 15  | 1T    | 13  | ARG  |
| 15  | 1T    | 28  | VAL  |
| 15  | 1T    | 34  | VAL  |
| 15  | 1T    | 36  | GLU  |
| 15  | 1T    | 38  | ASN  |
| 15  | 1T    | 49  | VAL  |
| 15  | 1T    | 59  | THR  |
| 15  | 1T    | 85  | LYS  |
| 15  | 1T    | 96  | ARG  |
| 15  | 1T    | 111 | ARG  |
| 16  | 1U    | 8   | VAL  |
| 16  | 1U    | 20  | LEU  |
| 16  | 1U    | 31  | SER  |
| 16  | 1U    | 50  | ARG  |
| 16  | 1U    | 59  | ARG  |
| 16  | 1U    | 74  | LEU  |
| 16  | 1U    | 77  | SER  |
| 16  | 1U    | 83  | LEU  |
| 16  | 1U    | 95  | LEU  |
| 16  | 1U    | 104 | GLN  |
| 16  | 1U    | 117 | GLN  |
| 17  | 1V    | 35  | LEU  |
| 17  | 1V    | 46  | VAL  |
| 17  | 1V    | 51  | VAL  |
| 17  | 1V    | 52  | VAL  |
| 17  | 1V    | 57  | VAL  |
| 17  | 1V    | 61  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 17  | 1V    | 62  | LEU  |
| 17  | 1V    | 72  | VAL  |
| 17  | 1V    | 79  | VAL  |
| 17  | 1V    | 82  | ARG  |
| 17  | 1V    | 100 | ARG  |
| 18  | 1W    | 11  | ARG  |
| 18  | 1W    | 17  | VAL  |
| 18  | 1W    | 19  | LEU  |
| 18  | 1W    | 23  | LEU  |
| 18  | 1W    | 63  | ASP  |
| 18  | 1W    | 82  | LEU  |
| 18  | 1W    | 95  | ILE  |
| 18  | 1W    | 100 | THR  |
| 18  | 1W    | 107 | LEU  |
| 19  | 1X    | 35  | THR  |
| 19  | 1X    | 52  | VAL  |
| 19  | 1X    | 66  | LEU  |
| 19  | 1X    | 68  | ARG  |
| 19  | 1X    | 72  | LYS  |
| 19  | 1X    | 81  | VAL  |
| 20  | 1Y    | 7   | VAL  |
| 20  | 1Y    | 43  | ASN  |
| 20  | 1Y    | 44  | ILE  |
| 20  | 1Y    | 72  | VAL  |
| 20  | 1Y    | 85  | VAL  |
| 20  | 1Y    | 90  | LEU  |
| 20  | 1Y    | 99  | CYS  |
| 21  | 1Z    | 18  | LEU  |
| 21  | 1Z    | 31  | ARG  |
| 21  | 1Z    | 33  | LEU  |
| 21  | 1Z    | 41  | LEU  |
| 21  | 1Z    | 61  | LEU  |
| 21  | 1Z    | 71  | VAL  |
| 21  | 1Z    | 74  | VAL  |
| 21  | 1Z    | 76  | LEU  |
| 21  | 1Z    | 86  | VAL  |
| 21  | 1Z    | 87  | ASP  |
| 21  | 1Z    | 93  | ASP  |
| 21  | 1Z    | 126 | VAL  |
| 21  | 1Z    | 135 | GLU  |
| 21  | 1Z    | 150 | LEU  |
| 21  | 1Z    | 154 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 21  | 1Z    | 155 | LEU  |
| 21  | 1Z    | 161 | VAL  |
| 21  | 1Z    | 163 | LEU  |
| 21  | 1Z    | 165 | VAL  |
| 21  | 1Z    | 170 | THR  |
| 21  | 1Z    | 180 | VAL  |
| 21  | 1Z    | 191 | VAL  |
| 21  | 1Z    | 193 | GLU  |
| 21  | 1Z    | 203 | GLU  |
| 22  | 10    | 11  | ARG  |
| 22  | 10    | 29  | GLN  |
| 22  | 10    | 37  | LEU  |
| 22  | 10    | 39  | ARG  |
| 22  | 10    | 53  | MET  |
| 22  | 10    | 64  | ASP  |
| 23  | 11    | 11  | ARG  |
| 23  | 11    | 21  | ARG  |
| 23  | 11    | 51  | VAL  |
| 23  | 11    | 56  | GLN  |
| 23  | 11    | 59  | THR  |
| 23  | 11    | 80  | LEU  |
| 23  | 11    | 95  | LEU  |
| 23  | 11    | 98  | LEU  |
| 24  | 12    | 1   | MET  |
| 24  | 12    | 32  | LEU  |
| 24  | 12    | 53  | LEU  |
| 24  | 12    | 54  | LYS  |
| 24  | 12    | 64  | LEU  |
| 24  | 12    | 68  | ARG  |
| 25  | 13    | 8   | LEU  |
| 25  | 13    | 23  | LEU  |
| 25  | 13    | 40  | THR  |
| 25  | 13    | 54  | VAL  |
| 25  | 13    | 56  | VAL  |
| 25  | 13    | 58  | VAL  |
| 26  | 14    | 1   | MET  |
| 26  | 14    | 14  | ILE  |
| 26  | 14    | 49  | PHE  |
| 26  | 14    | 60  | GLN  |
| 26  | 14    | 61  | ARG  |
| 27  | 15    | 6   | VAL  |
| 27  | 15    | 16  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 27  | 15    | 29  | THR  |
| 27  | 15    | 35  | GLU  |
| 27  | 15    | 58  | LEU  |
| 28  | 16    | 48  | VAL  |
| 29  | 17    | 24  | THR  |
| 29  | 17    | 43  | THR  |
| 30  | 18    | 14  | VAL  |
| 30  | 18    | 30  | ARG  |
| 30  | 18    | 32  | LEU  |
| 30  | 18    | 37  | SER  |
| 31  | 19    | 17  | ILE  |
| 31  | 19    | 35  | ARG  |
| 33  | 1b    | 7   | VAL  |
| 33  | 1b    | 8   | LYS  |
| 33  | 1b    | 15  | VAL  |
| 33  | 1b    | 23  | ARG  |
| 33  | 1b    | 27  | LYS  |
| 33  | 1b    | 43  | ASP  |
| 33  | 1b    | 47  | THR  |
| 33  | 1b    | 67  | THR  |
| 33  | 1b    | 71  | VAL  |
| 33  | 1b    | 95  | GLN  |
| 33  | 1b    | 96  | ARG  |
| 33  | 1b    | 112 | VAL  |
| 33  | 1b    | 118 | LEU  |
| 33  | 1b    | 134 | GLU  |
| 33  | 1b    | 142 | LEU  |
| 33  | 1b    | 144 | ARG  |
| 33  | 1b    | 160 | ASP  |
| 33  | 1b    | 164 | VAL  |
| 33  | 1b    | 168 | THR  |
| 33  | 1b    | 178 | ARG  |
| 33  | 1b    | 184 | VAL  |
| 33  | 1b    | 185 | ILE  |
| 33  | 1b    | 197 | VAL  |
| 33  | 1b    | 200 | ILE  |
| 33  | 1b    | 208 | ILE  |
| 33  | 1b    | 211 | ILE  |
| 33  | 1b    | 221 | LEU  |
| 33  | 1b    | 226 | ARG  |
| 33  | 1b    | 229 | VAL  |
| 34  | 1c    | 3   | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 34  | 1c    | 17  | ASP  |
| 34  | 1c    | 26  | LYS  |
| 34  | 1c    | 28  | GLN  |
| 34  | 1c    | 32  | LEU  |
| 34  | 1c    | 36  | ASP  |
| 34  | 1c    | 47  | LEU  |
| 34  | 1c    | 64  | VAL  |
| 34  | 1c    | 89  | GLU  |
| 34  | 1c    | 103 | VAL  |
| 34  | 1c    | 112 | SER  |
| 34  | 1c    | 115 | LEU  |
| 34  | 1c    | 116 | VAL  |
| 34  | 1c    | 192 | THR  |
| 35  | 1d    | 3   | ARG  |
| 35  | 1d    | 5   | ILE  |
| 35  | 1d    | 28  | SER  |
| 35  | 1d    | 49  | ARG  |
| 35  | 1d    | 58  | LEU  |
| 35  | 1d    | 59  | ARG  |
| 35  | 1d    | 76  | ARG  |
| 35  | 1d    | 85  | LYS  |
| 35  | 1d    | 89  | THR  |
| 35  | 1d    | 97  | LEU  |
| 35  | 1d    | 104 | VAL  |
| 35  | 1d    | 105 | VAL  |
| 35  | 1d    | 108 | LEU  |
| 35  | 1d    | 126 | ILE  |
| 35  | 1d    | 127 | THR  |
| 35  | 1d    | 135 | LEU  |
| 35  | 1d    | 148 | VAL  |
| 35  | 1d    | 155 | LEU  |
| 35  | 1d    | 157 | LEU  |
| 35  | 1d    | 158 | ILE  |
| 35  | 1d    | 159 | ARG  |
| 35  | 1d    | 173 | TRP  |
| 35  | 1d    | 178 | VAL  |
| 35  | 1d    | 182 | LYS  |
| 35  | 1d    | 184 | LYS  |
| 35  | 1d    | 188 | LEU  |
| 35  | 1d    | 190 | ASP  |
| 35  | 1d    | 194 | LEU  |
| 35  | 1d    | 196 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 35  | 1d    | 201 | GLN  |
| 36  | 1e    | 12  | LEU  |
| 36  | 1e    | 16  | THR  |
| 36  | 1e    | 24  | ARG  |
| 36  | 1e    | 31  | LEU  |
| 36  | 1e    | 34  | VAL  |
| 36  | 1e    | 41  | VAL  |
| 36  | 1e    | 47  | LYS  |
| 36  | 1e    | 51  | VAL  |
| 36  | 1e    | 78  | HIS  |
| 36  | 1e    | 79  | GLU  |
| 36  | 1e    | 91  | LEU  |
| 36  | 1e    | 100 | VAL  |
| 36  | 1e    | 107 | ARG  |
| 37  | 1f    | 25  | ILE  |
| 37  | 1f    | 64  | GLN  |
| 37  | 1f    | 69  | GLU  |
| 37  | 1f    | 72  | VAL  |
| 38  | 1g    | 21  | VAL  |
| 38  | 1g    | 30  | ILE  |
| 38  | 1g    | 41  | ARG  |
| 38  | 1g    | 135 | VAL  |
| 38  | 1g    | 144 | MET  |
| 39  | 1h    | 19  | VAL  |
| 39  | 1h    | 24  | THR  |
| 39  | 1h    | 26  | VAL  |
| 39  | 1h    | 39  | LEU  |
| 39  | 1h    | 41  | ARG  |
| 39  | 1h    | 51  | VAL  |
| 39  | 1h    | 52  | ASP  |
| 39  | 1h    | 60  | ARG  |
| 39  | 1h    | 99  | GLU  |
| 39  | 1h    | 127 | LEU  |
| 39  | 1h    | 137 | VAL  |
| 40  | 1i    | 7   | THR  |
| 40  | 1i    | 27  | THR  |
| 40  | 1i    | 53  | VAL  |
| 40  | 1i    | 56  | LEU  |
| 40  | 1i    | 66  | ARG  |
| 40  | 1i    | 81  | ILE  |
| 40  | 1i    | 96  | LEU  |
| 40  | 1i    | 103 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 40  | 1i    | 125 | TYR  |
| 40  | 1i    | 127 | LYS  |
| 41  | 1j    | 19  | SER  |
| 41  | 1j    | 30  | SER  |
| 41  | 1j    | 34  | VAL  |
| 41  | 1j    | 38  | ILE  |
| 41  | 1j    | 43  | ARG  |
| 41  | 1j    | 49  | VAL  |
| 41  | 1j    | 55  | LYS  |
| 41  | 1j    | 72  | VAL  |
| 41  | 1j    | 84  | GLN  |
| 41  | 1j    | 96  | ILE  |
| 41  | 1j    | 100 | THR  |
| 42  | 1k    | 28  | THR  |
| 42  | 1k    | 31  | THR  |
| 42  | 1k    | 48  | ILE  |
| 42  | 1k    | 81  | ASP  |
| 42  | 1k    | 87  | THR  |
| 42  | 1k    | 91  | ARG  |
| 42  | 1k    | 95  | ILE  |
| 42  | 1k    | 109 | VAL  |
| 42  | 1k    | 112 | THR  |
| 42  | 1k    | 114 | VAL  |
| 42  | 1k    | 117 | ASN  |
| 43  | 1l    | 6   | THR  |
| 43  | 1l    | 18  | VAL  |
| 43  | 1l    | 22  | SER  |
| 43  | 1l    | 33  | ARG  |
| 43  | 1l    | 39  | VAL  |
| 43  | 1l    | 42  | THR  |
| 43  | 1l    | 44  | THR  |
| 43  | 1l    | 52  | LEU  |
| 43  | 1l    | 58  | VAL  |
| 43  | 1l    | 60  | LEU  |
| 43  | 1l    | 67  | THR  |
| 43  | 1l    | 83  | VAL  |
| 43  | 1l    | 118 | SER  |
| 44  | 1m    | 4   | ILE  |
| 44  | 1m    | 12  | ASN  |
| 44  | 1m    | 17  | VAL  |
| 44  | 1m    | 19  | LEU  |
| 44  | 1m    | 25  | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 44  | 1m    | 27  | LYS  |
| 44  | 1m    | 43  | THR  |
| 44  | 1m    | 47  | ASP  |
| 44  | 1m    | 56  | LEU  |
| 44  | 1m    | 66  | LEU  |
| 44  | 1m    | 70  | LEU  |
| 44  | 1m    | 81  | LEU  |
| 44  | 1m    | 86  | CYS  |
| 44  | 1m    | 102 | ARG  |
| 44  | 1m    | 105 | THR  |
| 44  | 1m    | 109 | THR  |
| 44  | 1m    | 111 | LYS  |
| 45  | 1n    | 3   | ARG  |
| 45  | 1n    | 7   | ILE  |
| 45  | 1n    | 13  | THR  |
| 45  | 1n    | 18  | VAL  |
| 45  | 1n    | 22  | THR  |
| 45  | 1n    | 33  | VAL  |
| 45  | 1n    | 41  | ARG  |
| 45  | 1n    | 46  | GLU  |
| 45  | 1n    | 60  | SER  |
| 46  | 1o    | 3   | ILE  |
| 46  | 1o    | 39  | LEU  |
| 46  | 1o    | 64  | ARG  |
| 46  | 1o    | 76  | GLU  |
| 46  | 1o    | 88  | ARG  |
| 47  | 1p    | 1   | MET  |
| 47  | 1p    | 2   | VAL  |
| 47  | 1p    | 5   | ARG  |
| 47  | 1p    | 6   | LEU  |
| 47  | 1p    | 8   | ARG  |
| 47  | 1p    | 11  | SER  |
| 47  | 1p    | 19  | ILE  |
| 47  | 1p    | 20  | VAL  |
| 47  | 1p    | 29  | ASP  |
| 47  | 1p    | 33  | ILE  |
| 47  | 1p    | 45  | THR  |
| 47  | 1p    | 49  | LEU  |
| 47  | 1p    | 51  | VAL  |
| 47  | 1p    | 60  | LEU  |
| 47  | 1p    | 62  | VAL  |
| 47  | 1p    | 67  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 47  | 1p    | 74  | LEU  |
| 48  | 1q    | 9   | VAL  |
| 48  | 1q    | 35  | VAL  |
| 48  | 1q    | 39  | SER  |
| 48  | 1q    | 50  | LYS  |
| 48  | 1q    | 60  | ILE  |
| 48  | 1q    | 72  | ARG  |
| 48  | 1q    | 75  | ARG  |
| 48  | 1q    | 81  | ARG  |
| 48  | 1q    | 87  | LYS  |
| 49  | 1r    | 31  | LEU  |
| 49  | 1r    | 37  | VAL  |
| 49  | 1r    | 42  | ARG  |
| 49  | 1r    | 70  | ILE  |
| 49  | 1r    | 76  | LEU  |
| 49  | 1r    | 78  | LEU  |
| 49  | 1r    | 86  | VAL  |
| 50  | 1s    | 4   | SER  |
| 50  | 1s    | 28  | LYS  |
| 50  | 1s    | 37  | ARG  |
| 50  | 1s    | 40  | ILE  |
| 50  | 1s    | 41  | VAL  |
| 50  | 1s    | 63  | THR  |
| 50  | 1s    | 79  | THR  |
| 50  | 1s    | 83  | HIS  |
| 51  | 1t    | 10  | LEU  |
| 51  | 1t    | 18  | GLN  |
| 51  | 1t    | 54  | LYS  |
| 51  | 1t    | 62  | LEU  |
| 51  | 1t    | 64  | ASP  |
| 51  | 1t    | 100 | ILE  |
| 52  | 1u    | 15  | ARG  |
| 53  | 1y    | 3   | MET  |
| 53  | 1y    | 5   | ILE  |
| 53  | 1y    | 23  | ARG  |
| 53  | 1y    | 40  | ILE  |
| 53  | 1y    | 41  | LEU  |
| 53  | 1y    | 60  | VAL  |
| 53  | 1y    | 74  | ILE  |
| 53  | 1y    | 87  | LYS  |
| 53  | 1y    | 96  | ARG  |
| 3   | 2D    | 3   | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | 2D    | 4   | LYS  |
| 3   | 2D    | 32  | SER  |
| 3   | 2D    | 46  | GLN  |
| 3   | 2D    | 61  | LEU  |
| 3   | 2D    | 64  | ILE  |
| 3   | 2D    | 94  | LEU  |
| 3   | 2D    | 103 | ARG  |
| 3   | 2D    | 105 | ILE  |
| 3   | 2D    | 106 | ILE  |
| 3   | 2D    | 111 | LEU  |
| 3   | 2D    | 113 | VAL  |
| 3   | 2D    | 127 | VAL  |
| 3   | 2D    | 138 | VAL  |
| 3   | 2D    | 141 | VAL  |
| 3   | 2D    | 142 | VAL  |
| 3   | 2D    | 155 | LEU  |
| 3   | 2D    | 171 | ASP  |
| 3   | 2D    | 173 | VAL  |
| 3   | 2D    | 183 | ARG  |
| 3   | 2D    | 193 | VAL  |
| 3   | 2D    | 211 | ARG  |
| 3   | 2D    | 221 | VAL  |
| 3   | 2D    | 229 | VAL  |
| 3   | 2D    | 242 | ARG  |
| 4   | 2E    | 9   | VAL  |
| 4   | 2E    | 12  | THR  |
| 4   | 2E    | 21  | VAL  |
| 4   | 2E    | 33  | VAL  |
| 4   | 2E    | 34  | VAL  |
| 4   | 2E    | 38  | THR  |
| 4   | 2E    | 52  | LEU  |
| 4   | 2E    | 75  | VAL  |
| 4   | 2E    | 77  | ILE  |
| 4   | 2E    | 78  | LEU  |
| 4   | 2E    | 116 | VAL  |
| 4   | 2E    | 144 | ARG  |
| 4   | 2E    | 170 | LEU  |
| 4   | 2E    | 175 | VAL  |
| 4   | 2E    | 181 | LEU  |
| 4   | 2E    | 184 | VAL  |
| 4   | 2E    | 197 | ILE  |
| 4   | 2E    | 202 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | 2F    | 20  | LEU  |
| 5   | 2F    | 27  | GLU  |
| 5   | 2F    | 33  | LEU  |
| 5   | 2F    | 53  | THR  |
| 5   | 2F    | 57  | VAL  |
| 5   | 2F    | 74  | ARG  |
| 5   | 2F    | 88  | VAL  |
| 5   | 2F    | 132 | VAL  |
| 5   | 2F    | 135 | LYS  |
| 5   | 2F    | 153 | SER  |
| 5   | 2F    | 157 | VAL  |
| 5   | 2F    | 158 | THR  |
| 5   | 2F    | 165 | ARG  |
| 5   | 2F    | 170 | LEU  |
| 5   | 2F    | 183 | VAL  |
| 5   | 2F    | 192 | LEU  |
| 5   | 2F    | 195 | ASP  |
| 5   | 2F    | 197 | ASP  |
| 5   | 2F    | 200 | GLU  |
| 5   | 2F    | 201 | VAL  |
| 6   | 2G    | 5   | VAL  |
| 6   | 2G    | 27  | ASN  |
| 6   | 2G    | 28  | VAL  |
| 6   | 2G    | 31  | VAL  |
| 6   | 2G    | 40  | ASN  |
| 6   | 2G    | 47  | LYS  |
| 6   | 2G    | 86  | MET  |
| 6   | 2G    | 88  | ILE  |
| 6   | 2G    | 103 | LEU  |
| 6   | 2G    | 106 | LEU  |
| 6   | 2G    | 113 | ARG  |
| 6   | 2G    | 126 | ASP  |
| 6   | 2G    | 138 | GLN  |
| 6   | 2G    | 139 | LEU  |
| 6   | 2G    | 145 | THR  |
| 6   | 2G    | 152 | LEU  |
| 6   | 2G    | 159 | VAL  |
| 6   | 2G    | 167 | GLU  |
| 6   | 2G    | 172 | LEU  |
| 7   | 2H    | 7   | LEU  |
| 7   | 2H    | 16  | SER  |
| 7   | 2H    | 23  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | 2H    | 47  | GLU  |
| 7   | 2H    | 49  | VAL  |
| 7   | 2H    | 68  | THR  |
| 7   | 2H    | 71  | LEU  |
| 7   | 2H    | 81  | GLU  |
| 7   | 2H    | 86  | GLU  |
| 7   | 2H    | 88  | LEU  |
| 7   | 2H    | 95  | ARG  |
| 7   | 2H    | 98  | LEU  |
| 7   | 2H    | 105 | LEU  |
| 7   | 2H    | 113 | VAL  |
| 7   | 2H    | 114 | VAL  |
| 7   | 2H    | 121 | ILE  |
| 7   | 2H    | 134 | SER  |
| 7   | 2H    | 136 | ILE  |
| 7   | 2H    | 139 | GLN  |
| 7   | 2H    | 148 | ILE  |
| 7   | 2H    | 175 | LYS  |
| 8   | 2I    | 15  | VAL  |
| 8   | 2I    | 37  | VAL  |
| 8   | 2I    | 38  | LEU  |
| 8   | 2I    | 42  | SER  |
| 8   | 2I    | 44  | LEU  |
| 8   | 2I    | 48  | GLU  |
| 8   | 2I    | 52  | ARG  |
| 8   | 2I    | 54  | GLN  |
| 8   | 2I    | 57  | ARG  |
| 8   | 2I    | 58  | LEU  |
| 8   | 2I    | 77  | LEU  |
| 8   | 2I    | 81  | VAL  |
| 8   | 2I    | 87  | LYS  |
| 8   | 2I    | 88  | ILE  |
| 8   | 2I    | 92  | VAL  |
| 8   | 2I    | 93  | THR  |
| 8   | 2I    | 96  | ASP  |
| 8   | 2I    | 101 | LEU  |
| 8   | 2I    | 108 | THR  |
| 8   | 2I    | 117 | GLU  |
| 8   | 2I    | 122 | GLU  |
| 8   | 2I    | 123 | LEU  |
| 8   | 2I    | 126 | TYR  |
| 8   | 2I    | 129 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8   | 2I    | 133 | HIS  |
| 8   | 2I    | 143 | SER  |
| 8   | 2I    | 144 | VAL  |
| 8   | 2I    | 145 | VAL  |
| 9   | 2N    | 5   | VAL  |
| 9   | 2N    | 15  | LEU  |
| 9   | 2N    | 28  | THR  |
| 9   | 2N    | 33  | LEU  |
| 9   | 2N    | 34  | LEU  |
| 9   | 2N    | 35  | ARG  |
| 9   | 2N    | 43  | THR  |
| 9   | 2N    | 46  | VAL  |
| 9   | 2N    | 62  | VAL  |
| 9   | 2N    | 65  | LYS  |
| 9   | 2N    | 68  | GLU  |
| 9   | 2N    | 73  | THR  |
| 9   | 2N    | 87  | LEU  |
| 9   | 2N    | 89  | LYS  |
| 9   | 2N    | 99  | LEU  |
| 9   | 2N    | 122 | VAL  |
| 9   | 2N    | 133 | GLN  |
| 9   | 2N    | 140 | VAL  |
| 10  | 2O    | 10  | VAL  |
| 10  | 2O    | 23  | ARG  |
| 10  | 2O    | 24  | VAL  |
| 10  | 2O    | 32  | TYR  |
| 10  | 2O    | 35  | VAL  |
| 10  | 2O    | 52  | VAL  |
| 10  | 2O    | 53  | LYS  |
| 10  | 2O    | 78  | ARG  |
| 10  | 2O    | 96  | THR  |
| 10  | 2O    | 98  | VAL  |
| 11  | 2P    | 45  | LEU  |
| 11  | 2P    | 59  | LEU  |
| 11  | 2P    | 65  | ARG  |
| 11  | 2P    | 83  | VAL  |
| 11  | 2P    | 86  | LYS  |
| 11  | 2P    | 95  | VAL  |
| 11  | 2P    | 96  | THR  |
| 11  | 2P    | 100 | LEU  |
| 11  | 2P    | 125 | VAL  |
| 11  | 2P    | 133 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11  | 2P    | 135 | LEU  |
| 11  | 2P    | 144 | GLU  |
| 11  | 2P    | 148 | LEU  |
| 12  | 2Q    | 21  | THR  |
| 12  | 2Q    | 42  | ILE  |
| 12  | 2Q    | 54  | MET  |
| 12  | 2Q    | 55  | VAL  |
| 12  | 2Q    | 56  | ARG  |
| 12  | 2Q    | 106 | VAL  |
| 12  | 2Q    | 109 | VAL  |
| 12  | 2Q    | 110 | THR  |
| 12  | 2Q    | 131 | ILE  |
| 12  | 2Q    | 135 | ASP  |
| 12  | 2Q    | 139 | GLU  |
| 13  | 2R    | 18  | LEU  |
| 13  | 2R    | 24  | GLN  |
| 13  | 2R    | 27  | SER  |
| 13  | 2R    | 29  | LEU  |
| 13  | 2R    | 36  | THR  |
| 13  | 2R    | 44  | LEU  |
| 13  | 2R    | 65  | LEU  |
| 13  | 2R    | 75  | LEU  |
| 13  | 2R    | 79  | LEU  |
| 13  | 2R    | 86  | ARG  |
| 13  | 2R    | 96  | ARG  |
| 13  | 2R    | 100 | LEU  |
| 13  | 2R    | 102 | GLU  |
| 13  | 2R    | 111 | LEU  |
| 13  | 2R    | 114 | VAL  |
| 14  | 2S    | 8   | GLU  |
| 14  | 2S    | 23  | ARG  |
| 14  | 2S    | 27  | SER  |
| 14  | 2S    | 36  | TYR  |
| 14  | 2S    | 46  | VAL  |
| 14  | 2S    | 52  | SER  |
| 14  | 2S    | 64  | GLU  |
| 14  | 2S    | 68  | GLN  |
| 14  | 2S    | 85  | VAL  |
| 14  | 2S    | 110 | LEU  |
| 15  | 2T    | 23  | ARG  |
| 15  | 2T    | 27  | THR  |
| 15  | 2T    | 51  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 15  | 2T    | 67  | SER  |
| 15  | 2T    | 89  | VAL  |
| 15  | 2T    | 93  | ARG  |
| 15  | 2T    | 107 | ASP  |
| 15  | 2T    | 118 | ARG  |
| 15  | 2T    | 123 | GLN  |
| 16  | 2U    | 8   | VAL  |
| 16  | 2U    | 36  | ARG  |
| 16  | 2U    | 74  | LEU  |
| 16  | 2U    | 83  | LEU  |
| 16  | 2U    | 100 | VAL  |
| 17  | 2V    | 21  | ARG  |
| 17  | 2V    | 25  | LEU  |
| 17  | 2V    | 35  | LEU  |
| 17  | 2V    | 46  | VAL  |
| 17  | 2V    | 51  | VAL  |
| 17  | 2V    | 62  | LEU  |
| 17  | 2V    | 72  | VAL  |
| 17  | 2V    | 82  | ARG  |
| 18  | 2W    | 11  | ARG  |
| 18  | 2W    | 17  | VAL  |
| 18  | 2W    | 23  | LEU  |
| 18  | 2W    | 100 | THR  |
| 18  | 2W    | 103 | ILE  |
| 18  | 2W    | 107 | LEU  |
| 19  | 2X    | 38  | GLU  |
| 19  | 2X    | 49  | VAL  |
| 19  | 2X    | 57  | LEU  |
| 19  | 2X    | 70  | LEU  |
| 19  | 2X    | 81  | VAL  |
| 19  | 2X    | 82  | GLN  |
| 20  | 2Y    | 3   | VAL  |
| 20  | 2Y    | 37  | VAL  |
| 20  | 2Y    | 50  | ARG  |
| 20  | 2Y    | 61  | ILE  |
| 20  | 2Y    | 70  | SER  |
| 20  | 2Y    | 72  | VAL  |
| 20  | 2Y    | 85  | VAL  |
| 20  | 2Y    | 90  | LEU  |
| 20  | 2Y    | 98  | VAL  |
| 20  | 2Y    | 99  | CYS  |
| 21  | 2Z    | 5   | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 21  | 2Z    | 18  | LEU  |
| 21  | 2Z    | 27  | VAL  |
| 21  | 2Z    | 39  | VAL  |
| 21  | 2Z    | 41  | LEU  |
| 21  | 2Z    | 42  | VAL  |
| 21  | 2Z    | 86  | VAL  |
| 21  | 2Z    | 94  | GLU  |
| 21  | 2Z    | 124 | ILE  |
| 21  | 2Z    | 126 | VAL  |
| 21  | 2Z    | 142 | SER  |
| 21  | 2Z    | 150 | LEU  |
| 21  | 2Z    | 155 | LEU  |
| 21  | 2Z    | 185 | GLU  |
| 21  | 2Z    | 186 | GLU  |
| 21  | 2Z    | 196 | VAL  |
| 22  | 20    | 29  | GLN  |
| 22  | 20    | 30  | VAL  |
| 22  | 20    | 39  | ARG  |
| 22  | 20    | 46  | LYS  |
| 22  | 20    | 63  | VAL  |
| 23  | 21    | 4   | VAL  |
| 23  | 21    | 11  | ARG  |
| 23  | 21    | 30  | VAL  |
| 23  | 21    | 35  | THR  |
| 23  | 21    | 37  | ILE  |
| 23  | 21    | 40  | ARG  |
| 23  | 21    | 51  | VAL  |
| 23  | 21    | 80  | LEU  |
| 23  | 21    | 85  | LEU  |
| 23  | 21    | 97  | LEU  |
| 24  | 22    | 15  | LYS  |
| 24  | 22    | 16  | LEU  |
| 24  | 22    | 32  | LEU  |
| 24  | 22    | 33  | MET  |
| 24  | 22    | 38  | GLN  |
| 24  | 22    | 40  | SER  |
| 24  | 22    | 44  | LEU  |
| 24  | 22    | 50  | ILE  |
| 24  | 22    | 53  | LEU  |
| 24  | 22    | 57  | ILE  |
| 25  | 23    | 3   | ARG  |
| 25  | 23    | 6   | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 25  | 23    | 18  | ASP  |
| 25  | 23    | 23  | LEU  |
| 25  | 23    | 31  | LEU  |
| 25  | 23    | 40  | THR  |
| 25  | 23    | 54  | VAL  |
| 25  | 23    | 56  | VAL  |
| 25  | 23    | 59  | VAL  |
| 26  | 24    | 1   | MET  |
| 26  | 24    | 3   | GLU  |
| 26  | 24    | 21  | VAL  |
| 26  | 24    | 31  | ILE  |
| 26  | 24    | 33  | VAL  |
| 26  | 24    | 50  | VAL  |
| 26  | 24    | 53  | GLU  |
| 26  | 24    | 58  | ARG  |
| 26  | 24    | 61  | ARG  |
| 26  | 24    | 63  | TYR  |
| 27  | 25    | 6   | VAL  |
| 27  | 25    | 29  | THR  |
| 27  | 25    | 33  | CYS  |
| 27  | 25    | 55  | ARG  |
| 27  | 25    | 57  | VAL  |
| 27  | 25    | 58  | LEU  |
| 27  | 25    | 59  | GLU  |
| 28  | 26    | 5   | VAL  |
| 28  | 26    | 6   | ARG  |
| 28  | 26    | 14  | THR  |
| 28  | 26    | 28  | ARG  |
| 29  | 27    | 1   | MET  |
| 29  | 27    | 4   | THR  |
| 29  | 27    | 23  | ARG  |
| 29  | 27    | 43  | THR  |
| 30  | 28    | 14  | VAL  |
| 30  | 28    | 23  | VAL  |
| 30  | 28    | 27  | THR  |
| 30  | 28    | 34  | TRP  |
| 30  | 28    | 46  | ARG  |
| 30  | 28    | 59  | LYS  |
| 31  | 29    | 3   | VAL  |
| 31  | 29    | 12  | ASP  |
| 33  | 2b    | 8   | LYS  |
| 33  | 2b    | 17  | PHE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 33  | 2b    | 27  | LYS  |
| 33  | 2b    | 44  | LEU  |
| 33  | 2b    | 45  | GLN  |
| 33  | 2b    | 48  | MET  |
| 33  | 2b    | 67  | THR  |
| 33  | 2b    | 68  | ILE  |
| 33  | 2b    | 80  | ILE  |
| 33  | 2b    | 94  | ASN  |
| 33  | 2b    | 96  | ARG  |
| 33  | 2b    | 97  | TRP  |
| 33  | 2b    | 109 | SER  |
| 33  | 2b    | 111 | ARG  |
| 33  | 2b    | 117 | GLU  |
| 33  | 2b    | 136 | VAL  |
| 33  | 2b    | 158 | LEU  |
| 33  | 2b    | 160 | ASP  |
| 33  | 2b    | 189 | ASP  |
| 33  | 2b    | 196 | LEU  |
| 33  | 2b    | 197 | VAL  |
| 33  | 2b    | 200 | ILE  |
| 33  | 2b    | 208 | ILE  |
| 33  | 2b    | 230 | VAL  |
| 34  | 2c    | 15  | THR  |
| 34  | 2c    | 32  | LEU  |
| 34  | 2c    | 35  | GLU  |
| 34  | 2c    | 52  | LEU  |
| 34  | 2c    | 56  | ASP  |
| 34  | 2c    | 77  | ILE  |
| 34  | 2c    | 85  | ARG  |
| 34  | 2c    | 101 | LEU  |
| 34  | 2c    | 102 | ASN  |
| 34  | 2c    | 115 | LEU  |
| 34  | 2c    | 128 | PHE  |
| 34  | 2c    | 152 | ILE  |
| 34  | 2c    | 154 | SER  |
| 34  | 2c    | 166 | GLU  |
| 34  | 2c    | 192 | THR  |
| 34  | 2c    | 195 | VAL  |
| 34  | 2c    | 206 | GLU  |
| 34  | 2c    | 207 | VAL  |
| 35  | 2d    | 8   | VAL  |
| 35  | 2d    | 12  | CYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 35  | 2d    | 26  | CYS  |
| 35  | 2d    | 38  | TYR  |
| 35  | 2d    | 58  | LEU  |
| 35  | 2d    | 83  | SER  |
| 35  | 2d    | 105 | VAL  |
| 35  | 2d    | 108 | LEU  |
| 35  | 2d    | 115 | ARG  |
| 35  | 2d    | 127 | THR  |
| 35  | 2d    | 135 | LEU  |
| 35  | 2d    | 150 | GLU  |
| 35  | 2d    | 152 | SER  |
| 35  | 2d    | 155 | LEU  |
| 35  | 2d    | 170 | VAL  |
| 35  | 2d    | 194 | LEU  |
| 35  | 2d    | 200 | GLU  |
| 35  | 2d    | 201 | GLN  |
| 36  | 2e    | 10  | MET  |
| 36  | 2e    | 11  | ILE  |
| 36  | 2e    | 31  | LEU  |
| 36  | 2e    | 40  | ARG  |
| 36  | 2e    | 41  | VAL  |
| 36  | 2e    | 47  | LYS  |
| 36  | 2e    | 55  | VAL  |
| 36  | 2e    | 56  | GLN  |
| 36  | 2e    | 69  | VAL  |
| 36  | 2e    | 72  | GLN  |
| 36  | 2e    | 91  | LEU  |
| 36  | 2e    | 112 | LEU  |
| 36  | 2e    | 120 | THR  |
| 36  | 2e    | 126 | ARG  |
| 36  | 2e    | 135 | THR  |
| 37  | 2f    | 17  | SER  |
| 37  | 2f    | 22  | GLU  |
| 37  | 2f    | 46  | ARG  |
| 37  | 2f    | 72  | VAL  |
| 37  | 2f    | 74  | ASP  |
| 38  | 2g    | 9   | VAL  |
| 38  | 2g    | 13  | GLN  |
| 38  | 2g    | 16  | LEU  |
| 38  | 2g    | 22  | LEU  |
| 38  | 2g    | 24  | THR  |
| 38  | 2g    | 64  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 38  | 2g    | 75  | VAL  |
| 38  | 2g    | 80  | VAL  |
| 38  | 2g    | 97  | GLN  |
| 38  | 2g    | 104 | LEU  |
| 38  | 2g    | 113 | GLU  |
| 38  | 2g    | 115 | ARG  |
| 38  | 2g    | 118 | VAL  |
| 38  | 2g    | 148 | ASN  |
| 39  | 2h    | 8   | ASP  |
| 39  | 2h    | 25  | ASP  |
| 39  | 2h    | 52  | ASP  |
| 39  | 2h    | 63  | LEU  |
| 39  | 2h    | 97  | VAL  |
| 39  | 2h    | 104 | ARG  |
| 39  | 2h    | 112 | LEU  |
| 39  | 2h    | 127 | LEU  |
| 39  | 2h    | 129 | VAL  |
| 39  | 2h    | 133 | LEU  |
| 39  | 2h    | 137 | VAL  |
| 40  | 2i    | 17  | VAL  |
| 40  | 2i    | 20  | ARG  |
| 40  | 2i    | 29  | ASN  |
| 40  | 2i    | 53  | VAL  |
| 40  | 2i    | 54  | ASP  |
| 40  | 2i    | 60  | ASP  |
| 40  | 2i    | 64  | THR  |
| 40  | 2i    | 65  | VAL  |
| 40  | 2i    | 71  | SER  |
| 40  | 2i    | 81  | ILE  |
| 40  | 2i    | 86  | VAL  |
| 40  | 2i    | 92  | TYR  |
| 40  | 2i    | 102 | LEU  |
| 40  | 2i    | 108 | VAL  |
| 41  | 2j    | 6   | ILE  |
| 41  | 2j    | 38  | ILE  |
| 41  | 2j    | 69  | ASN  |
| 41  | 2j    | 81  | THR  |
| 41  | 2j    | 92  | THR  |
| 42  | 2k    | 14  | VAL  |
| 42  | 2k    | 18  | ARG  |
| 42  | 2k    | 28  | THR  |
| 42  | 2k    | 33  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 42  | 2k    | 48  | ILE  |
| 42  | 2k    | 87  | THR  |
| 42  | 2k    | 103 | LEU  |
| 42  | 2k    | 114 | VAL  |
| 42  | 2k    | 116 | HIS  |
| 42  | 2k    | 117 | ASN  |
| 42  | 2k    | 119 | CYS  |
| 43  | 2l    | 6   | THR  |
| 43  | 2l    | 27  | LEU  |
| 43  | 2l    | 33  | ARG  |
| 43  | 2l    | 36  | VAL  |
| 43  | 2l    | 82  | VAL  |
| 43  | 2l    | 83  | VAL  |
| 43  | 2l    | 97  | ARG  |
| 43  | 2l    | 104 | VAL  |
| 43  | 2l    | 113 | ARG  |
| 43  | 2l    | 124 | LYS  |
| 44  | 2m    | 4   | ILE  |
| 44  | 2m    | 19  | LEU  |
| 44  | 2m    | 35  | GLU  |
| 44  | 2m    | 47  | ASP  |
| 44  | 2m    | 57  | ARG  |
| 44  | 2m    | 61  | GLU  |
| 44  | 2m    | 70  | LEU  |
| 44  | 2m    | 115 | LYS  |
| 44  | 2m    | 116 | THR  |
| 45  | 2n    | 9   | LYS  |
| 45  | 2n    | 11  | LYS  |
| 45  | 2n    | 18  | VAL  |
| 45  | 2n    | 33  | VAL  |
| 45  | 2n    | 35  | ARG  |
| 45  | 2n    | 44  | LEU  |
| 45  | 2n    | 46  | GLU  |
| 45  | 2n    | 53  | LEU  |
| 46  | 2o    | 3   | ILE  |
| 46  | 2o    | 4   | THR  |
| 46  | 2o    | 26  | GLU  |
| 46  | 2o    | 27  | VAL  |
| 46  | 2o    | 32  | LEU  |
| 46  | 2o    | 39  | LEU  |
| 46  | 2o    | 64  | ARG  |
| 46  | 2o    | 83  | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 46  | 2o    | 84  | LYS  |
| 46  | 2o    | 87  | ILE  |
| 47  | 2p    | 1   | MET  |
| 47  | 2p    | 2   | VAL  |
| 47  | 2p    | 6   | LEU  |
| 47  | 2p    | 11  | SER  |
| 47  | 2p    | 20  | VAL  |
| 47  | 2p    | 21  | VAL  |
| 47  | 2p    | 25  | ARG  |
| 47  | 2p    | 42  | ARG  |
| 47  | 2p    | 54  | GLU  |
| 47  | 2p    | 60  | LEU  |
| 47  | 2p    | 62  | VAL  |
| 47  | 2p    | 67  | THR  |
| 47  | 2p    | 69  | THR  |
| 48  | 2q    | 6   | LEU  |
| 48  | 2q    | 9   | VAL  |
| 48  | 2q    | 19  | VAL  |
| 48  | 2q    | 60  | ILE  |
| 48  | 2q    | 74  | LEU  |
| 48  | 2q    | 96  | GLU  |
| 48  | 2q    | 97  | SER  |
| 49  | 2r    | 25  | THR  |
| 49  | 2r    | 37  | VAL  |
| 49  | 2r    | 47  | THR  |
| 49  | 2r    | 54  | ARG  |
| 49  | 2r    | 74  | ARG  |
| 49  | 2r    | 75  | ILE  |
| 49  | 2r    | 76  | LEU  |
| 49  | 2r    | 85  | LEU  |
| 49  | 2r    | 86  | VAL  |
| 50  | 2s    | 9   | VAL  |
| 50  | 2s    | 27  | GLU  |
| 50  | 2s    | 40  | ILE  |
| 50  | 2s    | 48  | THR  |
| 50  | 2s    | 71  | LEU  |
| 50  | 2s    | 79  | THR  |
| 51  | 2t    | 24  | LEU  |
| 51  | 2t    | 33  | ILE  |
| 51  | 2t    | 45  | GLN  |
| 51  | 2t    | 56  | MET  |
| 51  | 2t    | 71  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 51  | 2t    | 100 | ILE  |
| 52  | 2u    | 8   | THR  |
| 53  | 2y    | 8   | LYS  |
| 53  | 2y    | 9   | GLN  |
| 53  | 2y    | 11  | GLU  |
| 53  | 2y    | 16  | ILE  |
| 53  | 2y    | 23  | ARG  |
| 53  | 2y    | 24  | LEU  |
| 53  | 2y    | 27  | LEU  |
| 53  | 2y    | 29  | LYS  |
| 53  | 2y    | 39  | ILE  |
| 53  | 2y    | 41  | LEU  |
| 53  | 2y    | 54  | ILE  |
| 53  | 2y    | 60  | VAL  |
| 53  | 2y    | 62  | VAL  |
| 53  | 2y    | 77  | LEU  |
| 53  | 2y    | 96  | ARG  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (138) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | 1D    | 166 | GLN  |
| 3   | 1D    | 253 | GLN  |
| 4   | 1E    | 48  | GLN  |
| 5   | 1F    | 69  | HIS  |
| 5   | 1F    | 203 | GLN  |
| 5   | 1F    | 204 | ASN  |
| 6   | 1G    | 26  | GLN  |
| 6   | 1G    | 108 | ASN  |
| 6   | 1G    | 132 | ASN  |
| 8   | 1I    | 43  | ASN  |
| 8   | 1I    | 74  | ASN  |
| 8   | 1I    | 104 | GLN  |
| 8   | 1I    | 133 | HIS  |
| 9   | 1N    | 133 | GLN  |
| 10  | 1O    | 89  | ASN  |
| 13  | 1R    | 50  | HIS  |
| 13  | 1R    | 71  | GLN  |
| 15  | 1T    | 58  | ASN  |
| 15  | 1T    | 84  | GLN  |
| 16  | 1U    | 94  | ASN  |
| 19  | 1X    | 31  | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 19  | 1X    | 82  | GLN  |
| 20  | 1Y    | 6   | HIS  |
| 20  | 1Y    | 92  | ASN  |
| 21  | 1Z    | 73  | GLN  |
| 22  | 10    | 29  | GLN  |
| 23  | 11    | 16  | ASN  |
| 23  | 11    | 56  | GLN  |
| 25  | 13    | 32  | GLN  |
| 33  | 1b    | 16  | HIS  |
| 33  | 1b    | 40  | HIS  |
| 34  | 1c    | 3   | ASN  |
| 34  | 1c    | 6   | HIS  |
| 34  | 1c    | 98  | ASN  |
| 34  | 1c    | 176 | HIS  |
| 35  | 1d    | 77  | ASN  |
| 35  | 1d    | 201 | GLN  |
| 36  | 1e    | 78  | HIS  |
| 37  | 1f    | 7   | ASN  |
| 37  | 1f    | 13  | ASN  |
| 37  | 1f    | 57  | GLN  |
| 37  | 1f    | 100 | ASN  |
| 38  | 1g    | 28  | ASN  |
| 38  | 1g    | 51  | GLN  |
| 38  | 1g    | 56  | GLN  |
| 38  | 1g    | 64  | GLN  |
| 38  | 1g    | 122 | HIS  |
| 38  | 1g    | 148 | ASN  |
| 38  | 1g    | 153 | HIS  |
| 40  | 1i    | 3   | GLN  |
| 41  | 1j    | 56  | HIS  |
| 41  | 1j    | 84  | GLN  |
| 42  | 1k    | 38  | ASN  |
| 42  | 1k    | 62  | GLN  |
| 43  | 1l    | 99  | HIS  |
| 44  | 1m    | 12  | ASN  |
| 46  | 1o    | 28  | GLN  |
| 46  | 1o    | 62  | GLN  |
| 48  | 1q    | 16  | GLN  |
| 48  | 1q    | 94  | ASN  |
| 50  | 1s    | 69  | HIS  |
| 53  | 1y    | 4   | ASN  |
| 53  | 1y    | 38  | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 53  | 1y    | 89  | GLN  |
| 3   | 2D    | 126 | GLN  |
| 3   | 2D    | 253 | GLN  |
| 4   | 2E    | 48  | GLN  |
| 4   | 2E    | 85  | ASN  |
| 4   | 2E    | 143 | ASN  |
| 5   | 2F    | 69  | HIS  |
| 6   | 2G    | 27  | ASN  |
| 6   | 2G    | 40  | ASN  |
| 6   | 2G    | 66  | GLN  |
| 6   | 2G    | 108 | ASN  |
| 6   | 2G    | 132 | ASN  |
| 8   | 2I    | 43  | ASN  |
| 8   | 2I    | 139 | GLN  |
| 9   | 2N    | 94  | HIS  |
| 9   | 2N    | 133 | GLN  |
| 10  | 2O    | 3   | GLN  |
| 10  | 2O    | 5   | GLN  |
| 10  | 2O    | 89  | ASN  |
| 11  | 2P    | 81  | GLN  |
| 12  | 2Q    | 123 | HIS  |
| 13  | 2R    | 13  | HIS  |
| 13  | 2R    | 50  | HIS  |
| 15  | 2T    | 79  | HIS  |
| 15  | 2T    | 123 | GLN  |
| 16  | 2U    | 72  | HIS  |
| 16  | 2U    | 94  | ASN  |
| 16  | 2U    | 104 | GLN  |
| 17  | 2V    | 64  | HIS  |
| 18  | 2W    | 60  | ASN  |
| 19  | 2X    | 82  | GLN  |
| 20  | 2Y    | 57  | GLN  |
| 21  | 2Z    | 73  | GLN  |
| 21  | 2Z    | 132 | ASN  |
| 22  | 20    | 70  | GLN  |
| 24  | 22    | 38  | GLN  |
| 25  | 23    | 32  | GLN  |
| 26  | 24    | 46  | GLN  |
| 31  | 29    | 29  | ASN  |
| 33  | 2b    | 135 | GLN  |
| 33  | 2b    | 212 | GLN  |
| 34  | 2c    | 123 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 34  | 2c    | 181 | ASN  |
| 35  | 2d    | 77  | ASN  |
| 35  | 2d    | 116 | GLN  |
| 35  | 2d    | 119 | GLN  |
| 35  | 2d    | 160 | GLN  |
| 35  | 2d    | 161 | ASN  |
| 35  | 2d    | 201 | GLN  |
| 36  | 2e    | 56  | GLN  |
| 37  | 2f    | 13  | ASN  |
| 38  | 2g    | 13  | GLN  |
| 38  | 2g    | 28  | ASN  |
| 38  | 2g    | 68  | ASN  |
| 38  | 2g    | 86  | GLN  |
| 38  | 2g    | 109 | ASN  |
| 40  | 2i    | 3   | GLN  |
| 40  | 2i    | 31  | GLN  |
| 41  | 2j    | 21  | GLN  |
| 41  | 2j    | 68  | HIS  |
| 42  | 2k    | 26  | ASN  |
| 42  | 2k    | 99  | GLN  |
| 42  | 2k    | 104 | GLN  |
| 42  | 2k    | 117 | ASN  |
| 44  | 2m    | 62  | ASN  |
| 44  | 2m    | 77  | ASN  |
| 46  | 2o    | 28  | GLN  |
| 46  | 2o    | 62  | GLN  |
| 47  | 2p    | 13  | HIS  |
| 48  | 2q    | 16  | GLN  |
| 50  | 2s    | 23  | ASN  |
| 50  | 2s    | 83  | HIS  |
| 53  | 2y    | 4   | ASN  |
| 53  | 2y    | 84  | GLN  |
| 53  | 2y    | 89  | GLN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1   | 1A    | 2865/2915 (98%) | 446 (15%)         | 31 (1%)         |
| 1   | 2A    | 2858/2915 (98%) | 509 (17%)         | 31 (1%)         |
| 2   | 1B    | 119/121 (98%)   | 11 (9%)           | 0               |
| 2   | 2B    | 119/121 (98%)   | 20 (16%)          | 0               |

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| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 32  | 1a    | 1497/1521 (98%) | 288 (19%)         | 0               |
| 32  | 2a    | 1501/1521 (98%) | 284 (18%)         | 0               |
| All | All   | 8959/9114 (98%) | 1558 (17%)        | 62 (0%)         |

All (1558) RNA backbone outliers are listed below:

| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | 1A    | 11     | G    |
| 1   | 1A    | 12     | U    |
| 1   | 1A    | 13     | A    |
| 1   | 1A    | 34     | C    |
| 1   | 1A    | 45     | C    |
| 1   | 1A    | 59     | U    |
| 1   | 1A    | 71     | A    |
| 1   | 1A    | 72     | U    |
| 1   | 1A    | 74     | A    |
| 1   | 1A    | 75     | G    |
| 1   | 1A    | 92     | A    |
| 1   | 1A    | 94     | C    |
| 1   | 1A    | 95     | G    |
| 1   | 1A    | 118    | A    |
| 1   | 1A    | 119    | A    |
| 1   | 1A    | 120    | U    |
| 1   | 1A    | 140    | G    |
| 1   | 1A    | 172    | C    |
| 1   | 1A    | 173    | G    |
| 1   | 1A    | 181    | A    |
| 1   | 1A    | 182    | A    |
| 1   | 1A    | 196    | A    |
| 1   | 1A    | 199    | A    |
| 1   | 1A    | 205    | G    |
| 1   | 1A    | 215    | G    |
| 1   | 1A    | 216    | A    |
| 1   | 1A    | 221    | A    |
| 1   | 1A    | 222    | A    |
| 1   | 1A    | 229    | A    |
| 1   | 1A    | 233    | A    |
| 1   | 1A    | 248    | G    |
| 1   | 1A    | 271(I) | G    |
| 1   | 1A    | 271(K) | U    |
| 1   | 1A    | 271(L) | U    |
| 1   | 1A    | 271(M) | G    |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | 1A    | 271(N) | U    |
| 1   | 1A    | 271(O) | C    |
| 1   | 1A    | 272(A) | U    |
| 1   | 1A    | 272(B) | G    |
| 1   | 1A    | 275    | G    |
| 1   | 1A    | 279    | C    |
| 1   | 1A    | 283    | A    |
| 1   | 1A    | 311    | A    |
| 1   | 1A    | 317    | G    |
| 1   | 1A    | 324    | A    |
| 1   | 1A    | 327    | G    |
| 1   | 1A    | 330    | A    |
| 1   | 1A    | 352    | G    |
| 1   | 1A    | 363    | G    |
| 1   | 1A    | 386    | G    |
| 1   | 1A    | 396    | G    |
| 1   | 1A    | 404    | C    |
| 1   | 1A    | 405    | U    |
| 1   | 1A    | 407    | G    |
| 1   | 1A    | 411    | G    |
| 1   | 1A    | 412    | A    |
| 1   | 1A    | 421    | U    |
| 1   | 1A    | 428    | A    |
| 1   | 1A    | 448    | U    |
| 1   | 1A    | 455    | C    |
| 1   | 1A    | 456    | C    |
| 1   | 1A    | 457    | A    |
| 1   | 1A    | 479    | A    |
| 1   | 1A    | 481    | G    |
| 1   | 1A    | 504    | U    |
| 1   | 1A    | 505    | A    |
| 1   | 1A    | 508    | G    |
| 1   | 1A    | 509    | C    |
| 1   | 1A    | 518    | G    |
| 1   | 1A    | 530    | G    |
| 1   | 1A    | 531    | C    |
| 1   | 1A    | 532    | A    |
| 1   | 1A    | 533    | G    |
| 1   | 1A    | 545    | G    |
| 1   | 1A    | 549    | G    |
| 1   | 1A    | 551    | G    |
| 1   | 1A    | 563    | G    |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | 1A    | 573    | G    |
| 1   | 1A    | 575    | A    |
| 1   | 1A    | 586    | A    |
| 1   | 1A    | 603    | A    |
| 1   | 1A    | 604    | G    |
| 1   | 1A    | 607    | U    |
| 1   | 1A    | 614(B) | G    |
| 1   | 1A    | 615    | G    |
| 1   | 1A    | 616    | G    |
| 1   | 1A    | 627    | A    |
| 1   | 1A    | 637    | A    |
| 1   | 1A    | 645    | C    |
| 1   | 1A    | 646    | A    |
| 1   | 1A    | 652(E) | G    |
| 1   | 1A    | 652(T) | C    |
| 1   | 1A    | 652(U) | G    |
| 1   | 1A    | 669    | G    |
| 1   | 1A    | 686    | G    |
| 1   | 1A    | 717    | G    |
| 1   | 1A    | 730    | C    |
| 1   | 1A    | 775    | G    |
| 1   | 1A    | 776    | G    |
| 1   | 1A    | 778    | G    |
| 1   | 1A    | 782    | A    |
| 1   | 1A    | 784    | A    |
| 1   | 1A    | 785    | G    |
| 1   | 1A    | 790    | C    |
| 1   | 1A    | 792    | G    |
| 1   | 1A    | 805    | G    |
| 1   | 1A    | 812    | C    |
| 1   | 1A    | 827    | U    |
| 1   | 1A    | 828    | U    |
| 1   | 1A    | 859    | G    |
| 1   | 1A    | 878    | A    |
| 1   | 1A    | 879    | G    |
| 1   | 1A    | 881    | G    |
| 1   | 1A    | 882    | G    |
| 1   | 1A    | 886    | C    |
| 1   | 1A    | 888    | C    |
| 1   | 1A    | 889    | C    |
| 1   | 1A    | 890    | A    |
| 1   | 1A    | 896    | A    |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 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    | 959    | A    |
| 1   | 1A    | 961    | C    |
| 1   | 1A    | 967    | C    |
| 1   | 1A    | 974    | G    |
| 1   | 1A    | 975    | C    |
| 1   | 1A    | 975(A) | G    |
| 1   | 1A    | 983    | A    |
| 1   | 1A    | 990    | A    |
| 1   | 1A    | 996    | A    |
| 1   | 1A    | 1012   | U    |
| 1   | 1A    | 1013   | C    |
| 1   | 1A    | 1022   | G    |
| 1   | 1A    | 1026   | U    |
| 1   | 1A    | 1027   | A    |
| 1   | 1A    | 1033   | U    |
| 1   | 1A    | 1039   | G    |
| 1   | 1A    | 1042   | G    |
| 1   | 1A    | 1046   | A    |
| 1   | 1A    | 1047   | G    |
| 1   | 1A    | 1050   | A    |
| 1   | 1A    | 1054   | A    |
| 1   | 1A    | 1055   | G    |
| 1   | 1A    | 1060   | U    |
| 1   | 1A    | 1061   | U    |
| 1   | 1A    | 1062   | G    |
| 1   | 1A    | 1063   | G    |
| 1   | 1A    | 1064   | C    |
| 1   | 1A    | 1065   | U    |
| 1   | 1A    | 1070   | A    |
| 1   | 1A    | 1071   | G    |
| 1   | 1A    | 1073   | A    |
| 1   | 1A    | 1075   | C    |
| 1   | 1A    | 1076   | C    |
| 1   | 1A    | 1077   | A    |
| 1   | 1A    | 1080   | C    |
| 1   | 1A    | 1087   | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 1A    | 1088 | A    |
| 1   | 1A    | 1090 | U    |
| 1   | 1A    | 1096 | A    |
| 1   | 1A    | 1097 | U    |
| 1   | 1A    | 1106 | G    |
| 1   | 1A    | 1109 | C    |
| 1   | 1A    | 1112 | G    |
| 1   | 1A    | 1115 | G    |
| 1   | 1A    | 1116 | C    |
| 1   | 1A    | 1128 | A    |
| 1   | 1A    | 1129 | A    |
| 1   | 1A    | 1130 | U    |
| 1   | 1A    | 1135 | C    |
| 1   | 1A    | 1136 | G    |
| 1   | 1A    | 1139 | G    |
| 1   | 1A    | 1141 | U    |
| 1   | 1A    | 1170 | G    |
| 1   | 1A    | 1171 | G    |
| 1   | 1A    | 1173 | G    |
| 1   | 1A    | 1174 | A    |
| 1   | 1A    | 1175 | U    |
| 1   | 1A    | 1176 | G    |
| 1   | 1A    | 1177 | A    |
| 1   | 1A    | 1178 | C    |
| 1   | 1A    | 1211 | U    |
| 1   | 1A    | 1218 | C    |
| 1   | 1A    | 1236 | G    |
| 1   | 1A    | 1241 | A    |
| 1   | 1A    | 1250 | G    |
| 1   | 1A    | 1253 | A    |
| 1   | 1A    | 1256 | G    |
| 1   | 1A    | 1271 | G    |
| 1   | 1A    | 1272 | A    |
| 1   | 1A    | 1273 | U    |
| 1   | 1A    | 1276 | A    |
| 1   | 1A    | 1300 | U    |
| 1   | 1A    | 1301 | A    |
| 1   | 1A    | 1303 | G    |
| 1   | 1A    | 1342 | A    |
| 1   | 1A    | 1349 | A    |
| 1   | 1A    | 1352 | U    |
| 1   | 1A    | 1359 | A    |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 1   | 1A    | 1360    | A    |
| 1   | 1A    | 1365    | A    |
| 1   | 1A    | 1370    | C    |
| 1   | 1A    | 1380    | G    |
| 1   | 1A    | 1384    | A    |
| 1   | 1A    | 1385    | G    |
| 1   | 1A    | 1386    | C    |
| 1   | 1A    | 1395    | A    |
| 1   | 1A    | 1416    | G    |
| 1   | 1A    | 1417    | C    |
| 1   | 1A    | 1420    | U    |
| 1   | 1A    | 1421    | G    |
| 1   | 1A    | 1428    | C    |
| 1   | 1A    | 1437    | C    |
| 1   | 1A    | 1445    | A    |
| 1   | 1A    | 1450    | G    |
| 1   | 1A    | 1452    | A    |
| 1   | 1A    | 1453    | U    |
| 1   | 1A    | 1455    | G    |
| 1   | 1A    | 1460    | A    |
| 1   | 1A    | 1467    | C    |
| 1   | 1A    | 1471    | A    |
| 1   | 1A    | 1479    | G    |
| 1   | 1A    | 1482    | G    |
| 1   | 1A    | 1493    | C    |
| 1   | 1A    | 1509    | C    |
| 1   | 1A    | 1509(A) | A    |
| 1   | 1A    | 1539    | G    |
| 1   | 1A    | 1542    | A    |
| 1   | 1A    | 1543    | C    |
| 1   | 1A    | 1558    | A    |
| 1   | 1A    | 1569    | A    |
| 1   | 1A    | 1578    | U    |
| 1   | 1A    | 1579    | A    |
| 1   | 1A    | 1580    | A    |
| 1   | 1A    | 1581    | G    |
| 1   | 1A    | 1584    | C    |
| 1   | 1A    | 1586    | A    |
| 1   | 1A    | 1607    | C    |
| 1   | 1A    | 1608    | A    |
| 1   | 1A    | 1609    | A    |
| 1   | 1A    | 1610    | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 1A    | 1648 | C    |
| 1   | 1A    | 1654 | A    |
| 1   | 1A    | 1674 | G    |
| 1   | 1A    | 1696 | G    |
| 1   | 1A    | 1700 | A    |
| 1   | 1A    | 1701 | A    |
| 1   | 1A    | 1722 | A    |
| 1   | 1A    | 1739 | U    |
| 1   | 1A    | 1740 | G    |
| 1   | 1A    | 1756 | G    |
| 1   | 1A    | 1757 | U    |
| 1   | 1A    | 1763 | G    |
| 1   | 1A    | 1764 | G    |
| 1   | 1A    | 1773 | A    |
| 1   | 1A    | 1780 | A    |
| 1   | 1A    | 1782 | C    |
| 1   | 1A    | 1786 | A    |
| 1   | 1A    | 1791 | A    |
| 1   | 1A    | 1800 | C    |
| 1   | 1A    | 1801 | G    |
| 1   | 1A    | 1811 | G    |
| 1   | 1A    | 1812 | A    |
| 1   | 1A    | 1816 | G    |
| 1   | 1A    | 1847 | A    |
| 1   | 1A    | 1877 | A    |
| 1   | 1A    | 1878 | G    |
| 1   | 1A    | 1889 | A    |
| 1   | 1A    | 1896 | G    |
| 1   | 1A    | 1900 | A    |
| 1   | 1A    | 1906 | G    |
| 1   | 1A    | 1910 | G    |
| 1   | 1A    | 1913 | A    |
| 1   | 1A    | 1915 | 5MU  |
| 1   | 1A    | 1929 | G    |
| 1   | 1A    | 1930 | G    |
| 1   | 1A    | 1931 | U    |
| 1   | 1A    | 1938 | A    |
| 1   | 1A    | 1955 | U    |
| 1   | 1A    | 1963 | U    |
| 1   | 1A    | 1965 | C    |
| 1   | 1A    | 1967 | C    |
| 1   | 1A    | 1970 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 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    | 2062 | A    |
| 1   | 1A    | 2069 | G    |
| 1   | 1A    | 2070 | G    |
| 1   | 1A    | 2102 | U    |
| 1   | 1A    | 2103 | C    |
| 1   | 1A    | 2104 | G    |
| 1   | 1A    | 2106 | G    |
| 1   | 1A    | 2107 | C    |
| 1   | 1A    | 2108 | C    |
| 1   | 1A    | 2109 | U    |
| 1   | 1A    | 2116 | G    |
| 1   | 1A    | 2117 | A    |
| 1   | 1A    | 2121 | G    |
| 1   | 1A    | 2123 | G    |
| 1   | 1A    | 2126 | A    |
| 1   | 1A    | 2127 | G    |
| 1   | 1A    | 2130 | U    |
| 1   | 1A    | 2132 | U    |
| 1   | 1A    | 2133 | G    |
| 1   | 1A    | 2135 | A    |
| 1   | 1A    | 2136 | C    |
| 1   | 1A    | 2138 | C    |
| 1   | 1A    | 2142 | C    |
| 1   | 1A    | 2144 | U    |
| 1   | 1A    | 2146 | C    |
| 1   | 1A    | 2147 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 1A    | 2153 | 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    | 2170 | A    |
| 1   | 1A    | 2173 | A    |
| 1   | 1A    | 2180 | U    |
| 1   | 1A    | 2181 | G    |
| 1   | 1A    | 2183 | C    |
| 1   | 1A    | 2184 | G    |
| 1   | 1A    | 2186 | G    |
| 1   | 1A    | 2187 | G    |
| 1   | 1A    | 2188 | C    |
| 1   | 1A    | 2190 | G    |
| 1   | 1A    | 2191 | G    |
| 1   | 1A    | 2192 | G    |
| 1   | 1A    | 2198 | A    |
| 1   | 1A    | 2206 | G    |
| 1   | 1A    | 2207 | G    |
| 1   | 1A    | 2208 | A    |
| 1   | 1A    | 2218 | U    |
| 1   | 1A    | 2219 | G    |
| 1   | 1A    | 2225 | A    |
| 1   | 1A    | 2238 | G    |
| 1   | 1A    | 2239 | G    |
| 1   | 1A    | 2268 | A    |
| 1   | 1A    | 2278 | A    |
| 1   | 1A    | 2283 | C    |
| 1   | 1A    | 2286 | A    |
| 1   | 1A    | 2287 | A    |
| 1   | 1A    | 2289 | G    |
| 1   | 1A    | 2305 | A    |
| 1   | 1A    | 2308 | G    |
| 1   | 1A    | 2320 | A    |
| 1   | 1A    | 2325 | G    |
| 1   | 1A    | 2334 | G    |
| 1   | 1A    | 2336 | A    |
| 1   | 1A    | 2347 | C    |
| 1   | 1A    | 2350 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 1A    | 2354 | G    |
| 1   | 1A    | 2361 | A    |
| 1   | 1A    | 2383 | G    |
| 1   | 1A    | 2385 | C    |
| 1   | 1A    | 2406 | U    |
| 1   | 1A    | 2410 | G    |
| 1   | 1A    | 2414 | G    |
| 1   | 1A    | 2422 | A    |
| 1   | 1A    | 2423 | U    |
| 1   | 1A    | 2424 | C    |
| 1   | 1A    | 2425 | A    |
| 1   | 1A    | 2429 | G    |
| 1   | 1A    | 2430 | A    |
| 1   | 1A    | 2435 | A    |
| 1   | 1A    | 2439 | A    |
| 1   | 1A    | 2441 | C    |
| 1   | 1A    | 2445 | G    |
| 1   | 1A    | 2448 | A    |
| 1   | 1A    | 2468 | G    |
| 1   | 1A    | 2469 | A    |
| 1   | 1A    | 2475 | C    |
| 1   | 1A    | 2476 | A    |
| 1   | 1A    | 2490 | G    |
| 1   | 1A    | 2502 | G    |
| 1   | 1A    | 2505 | G    |
| 1   | 1A    | 2506 | U    |
| 1   | 1A    | 2507 | C    |
| 1   | 1A    | 2518 | A    |
| 1   | 1A    | 2529 | G    |
| 1   | 1A    | 2535 | G    |
| 1   | 1A    | 2554 | U    |
| 1   | 1A    | 2566 | A    |
| 1   | 1A    | 2567 | G    |
| 1   | 1A    | 2573 | C    |
| 1   | 1A    | 2582 | G    |
| 1   | 1A    | 2585 | U    |
| 1   | 1A    | 2602 | A    |
| 1   | 1A    | 2603 | G    |
| 1   | 1A    | 2609 | U    |
| 1   | 1A    | 2611 | U    |
| 1   | 1A    | 2612 | C    |
| 1   | 1A    | 2629 | A    |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 1   | 1A    | 2630    | G    |
| 1   | 1A    | 2632    | A    |
| 1   | 1A    | 2654    | A    |
| 1   | 1A    | 2663    | G    |
| 1   | 1A    | 2689    | U    |
| 1   | 1A    | 2690    | C    |
| 1   | 1A    | 2702    | U    |
| 1   | 1A    | 2703    | C    |
| 1   | 1A    | 2712(A) | A    |
| 1   | 1A    | 2713    | A    |
| 1   | 1A    | 2714    | G    |
| 1   | 1A    | 2726    | U    |
| 1   | 1A    | 2733    | A    |
| 1   | 1A    | 2758    | A    |
| 1   | 1A    | 2764    | A    |
| 1   | 1A    | 2765    | A    |
| 1   | 1A    | 2766    | G    |
| 1   | 1A    | 2769    | C    |
| 1   | 1A    | 2778    | A    |
| 1   | 1A    | 2789    | C    |
| 1   | 1A    | 2790    | A    |
| 1   | 1A    | 2791    | C    |
| 1   | 1A    | 2802    | G    |
| 1   | 1A    | 2805    | G    |
| 1   | 1A    | 2820    | A    |
| 1   | 1A    | 2821    | A    |
| 1   | 1A    | 2833    | G    |
| 1   | 1A    | 2835    | A    |
| 1   | 1A    | 2872    | G    |
| 1   | 1A    | 2873    | A    |
| 1   | 1A    | 2880    | C    |
| 1   | 1A    | 2892    | A    |
| 1   | 1A    | 2894    | G    |
| 2   | 1B    | 13      | A    |
| 2   | 1B    | 45      | A    |
| 2   | 1B    | 50      | G    |
| 2   | 1B    | 52      | A    |
| 2   | 1B    | 53      | A    |
| 2   | 1B    | 56      | G    |
| 2   | 1B    | 66      | A    |
| 2   | 1B    | 73      | A    |
| 2   | 1B    | 85      | G    |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 2   | 1B    | 106    | G    |
| 2   | 1B    | 110    | G    |
| 32  | 1a    | 7      | G    |
| 32  | 1a    | 9      | G    |
| 32  | 1a    | 32     | A    |
| 32  | 1a    | 33     | A    |
| 32  | 1a    | 39     | G    |
| 32  | 1a    | 47     | C    |
| 32  | 1a    | 48     | C    |
| 32  | 1a    | 50     | A    |
| 32  | 1a    | 51     | A    |
| 32  | 1a    | 61     | G    |
| 32  | 1a    | 70     | G    |
| 32  | 1a    | 71     | C    |
| 32  | 1a    | 72     | C    |
| 32  | 1a    | 73     | G    |
| 32  | 1a    | 79     | G    |
| 32  | 1a    | 92     | C    |
| 32  | 1a    | 96     | U    |
| 32  | 1a    | 97     | G    |
| 32  | 1a    | 100    | C    |
| 32  | 1a    | 101    | A    |
| 32  | 1a    | 115    | G    |
| 32  | 1a    | 116    | A    |
| 32  | 1a    | 121    | C    |
| 32  | 1a    | 131    | C    |
| 32  | 1a    | 137    | C    |
| 32  | 1a    | 143    | A    |
| 32  | 1a    | 150    | C    |
| 32  | 1a    | 151    | A    |
| 32  | 1a    | 153    | C    |
| 32  | 1a    | 156    | G    |
| 32  | 1a    | 157    | G    |
| 32  | 1a    | 163    | C    |
| 32  | 1a    | 166    | G    |
| 32  | 1a    | 174    | C    |
| 32  | 1a    | 182    | U    |
| 32  | 1a    | 189(E) | U    |
| 32  | 1a    | 189(F) | U    |
| 32  | 1a    | 189(G) | G    |
| 32  | 1a    | 195    | A    |
| 32  | 1a    | 197    | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 32  | 1a    | 202 | U    |
| 32  | 1a    | 204 | U    |
| 32  | 1a    | 216 | G    |
| 32  | 1a    | 222 | U    |
| 32  | 1a    | 231 | G    |
| 32  | 1a    | 247 | G    |
| 32  | 1a    | 251 | G    |
| 32  | 1a    | 266 | G    |
| 32  | 1a    | 267 | C    |
| 32  | 1a    | 289 | G    |
| 32  | 1a    | 305 | G    |
| 32  | 1a    | 321 | A    |
| 32  | 1a    | 328 | C    |
| 32  | 1a    | 329 | A    |
| 32  | 1a    | 330 | C    |
| 32  | 1a    | 332 | G    |
| 32  | 1a    | 348 | G    |
| 32  | 1a    | 351 | G    |
| 32  | 1a    | 352 | C    |
| 32  | 1a    | 353 | A    |
| 32  | 1a    | 354 | G    |
| 32  | 1a    | 362 | G    |
| 32  | 1a    | 363 | A    |
| 32  | 1a    | 367 | U    |
| 32  | 1a    | 371 | G    |
| 32  | 1a    | 372 | C    |
| 32  | 1a    | 373 | A    |
| 32  | 1a    | 382 | A    |
| 32  | 1a    | 384 | G    |
| 32  | 1a    | 388 | G    |
| 32  | 1a    | 390 | C    |
| 32  | 1a    | 398 | C    |
| 32  | 1a    | 406 | G    |
| 32  | 1a    | 412 | A    |
| 32  | 1a    | 413 | G    |
| 32  | 1a    | 424 | G    |
| 32  | 1a    | 429 | U    |
| 32  | 1a    | 439 | A    |
| 32  | 1a    | 442 | C    |
| 32  | 1a    | 452 | A    |
| 32  | 1a    | 461 | A    |
| 32  | 1a    | 470 | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 32  | 1a    | 471 | G    |
| 32  | 1a    | 477 | A    |
| 32  | 1a    | 479 | C    |
| 32  | 1a    | 483 | C    |
| 32  | 1a    | 485 | G    |
| 32  | 1a    | 496 | A    |
| 32  | 1a    | 498 | U    |
| 32  | 1a    | 505 | G    |
| 32  | 1a    | 509 | A    |
| 32  | 1a    | 510 | A    |
| 32  | 1a    | 511 | C    |
| 32  | 1a    | 513 | C    |
| 32  | 1a    | 518 | C    |
| 32  | 1a    | 531 | U    |
| 32  | 1a    | 532 | A    |
| 32  | 1a    | 533 | A    |
| 32  | 1a    | 536 | C    |
| 32  | 1a    | 547 | A    |
| 32  | 1a    | 550 | G    |
| 32  | 1a    | 559 | A    |
| 32  | 1a    | 561 | U    |
| 32  | 1a    | 572 | A    |
| 32  | 1a    | 573 | A    |
| 32  | 1a    | 576 | G    |
| 32  | 1a    | 577 | G    |
| 32  | 1a    | 592 | G    |
| 32  | 1a    | 596 | C    |
| 32  | 1a    | 618 | C    |
| 32  | 1a    | 619 | U    |
| 32  | 1a    | 630 | G    |
| 32  | 1a    | 632 | A    |
| 32  | 1a    | 633 | G    |
| 32  | 1a    | 653 | A    |
| 32  | 1a    | 661 | G    |
| 32  | 1a    | 665 | A    |
| 32  | 1a    | 673 | G    |
| 32  | 1a    | 687 | A    |
| 32  | 1a    | 688 | G    |
| 32  | 1a    | 702 | A    |
| 32  | 1a    | 703 | G    |
| 32  | 1a    | 723 | U    |
| 32  | 1a    | 731 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 32  | 1a    | 742 | G    |
| 32  | 1a    | 755 | G    |
| 32  | 1a    | 759 | A    |
| 32  | 1a    | 760 | G    |
| 32  | 1a    | 777 | A    |
| 32  | 1a    | 792 | A    |
| 32  | 1a    | 793 | U    |
| 32  | 1a    | 794 | A    |
| 32  | 1a    | 802 | A    |
| 32  | 1a    | 810 | C    |
| 32  | 1a    | 815 | A    |
| 32  | 1a    | 816 | A    |
| 32  | 1a    | 817 | C    |
| 32  | 1a    | 818 | G    |
| 32  | 1a    | 828 | A    |
| 32  | 1a    | 829 | G    |
| 32  | 1a    | 839 | U    |
| 32  | 1a    | 840 | C    |
| 32  | 1a    | 841 | U    |
| 32  | 1a    | 848 | C    |
| 32  | 1a    | 851 | G    |
| 32  | 1a    | 874 | G    |
| 32  | 1a    | 902 | G    |
| 32  | 1a    | 914 | A    |
| 32  | 1a    | 916 | G    |
| 32  | 1a    | 922 | G    |
| 32  | 1a    | 926 | G    |
| 32  | 1a    | 927 | G    |
| 32  | 1a    | 931 | C    |
| 32  | 1a    | 934 | C    |
| 32  | 1a    | 942 | G    |
| 32  | 1a    | 960 | U    |
| 32  | 1a    | 961 | U    |
| 32  | 1a    | 968 | A    |
| 32  | 1a    | 969 | A    |
| 32  | 1a    | 971 | G    |
| 32  | 1a    | 974 | A    |
| 32  | 1a    | 975 | A    |
| 32  | 1a    | 976 | G    |
| 32  | 1a    | 977 | A    |
| 32  | 1a    | 978 | A    |
| 32  | 1a    | 981 | U    |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 32  | 1a    | 991     | U    |
| 32  | 1a    | 992     | U    |
| 32  | 1a    | 993     | G    |
| 32  | 1a    | 994     | A    |
| 32  | 1a    | 998     | G    |
| 32  | 1a    | 1003    | G    |
| 32  | 1a    | 1004    | A    |
| 32  | 1a    | 1006    | C    |
| 32  | 1a    | 1022    | G    |
| 32  | 1a    | 1023    | G    |
| 32  | 1a    | 1024    | G    |
| 32  | 1a    | 1025    | U    |
| 32  | 1a    | 1026    | G    |
| 32  | 1a    | 1027    | C    |
| 32  | 1a    | 1028    | C    |
| 32  | 1a    | 1029    | C    |
| 32  | 1a    | 1030(A) | G    |
| 32  | 1a    | 1030(B) | C    |
| 32  | 1a    | 1030(D) | A    |
| 32  | 1a    | 1031    | G    |
| 32  | 1a    | 1032    | G    |
| 32  | 1a    | 1033    | G    |
| 32  | 1a    | 1034    | G    |
| 32  | 1a    | 1037    | C    |
| 32  | 1a    | 1044    | A    |
| 32  | 1a    | 1053    | G    |
| 32  | 1a    | 1056    | U    |
| 32  | 1a    | 1062    | U    |
| 32  | 1a    | 1065    | U    |
| 32  | 1a    | 1066    | C    |
| 32  | 1a    | 1068    | G    |
| 32  | 1a    | 1081    | G    |
| 32  | 1a    | 1086    | U    |
| 32  | 1a    | 1089    | G    |
| 32  | 1a    | 1094    | G    |
| 32  | 1a    | 1095    | U    |
| 32  | 1a    | 1101    | A    |
| 32  | 1a    | 1120    | G    |
| 32  | 1a    | 1123    | A    |
| 32  | 1a    | 1124    | G    |
| 32  | 1a    | 1125    | U    |
| 32  | 1a    | 1130    | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 32  | 1a    | 1132 | C    |
| 32  | 1a    | 1134 | G    |
| 32  | 1a    | 1136 | U    |
| 32  | 1a    | 1138 | G    |
| 32  | 1a    | 1139 | G    |
| 32  | 1a    | 1140 | C    |
| 32  | 1a    | 1150 | U    |
| 32  | 1a    | 1152 | A    |
| 32  | 1a    | 1154 | G    |
| 32  | 1a    | 1159 | U    |
| 32  | 1a    | 1160 | G    |
| 32  | 1a    | 1165 | C    |
| 32  | 1a    | 1166 | G    |
| 32  | 1a    | 1168 | A    |
| 32  | 1a    | 1182 | G    |
| 32  | 1a    | 1183 | A    |
| 32  | 1a    | 1184 | G    |
| 32  | 1a    | 1193 | G    |
| 32  | 1a    | 1196 | U    |
| 32  | 1a    | 1197 | G    |
| 32  | 1a    | 1200 | C    |
| 32  | 1a    | 1202 | G    |
| 32  | 1a    | 1206 | G    |
| 32  | 1a    | 1208 | C    |
| 32  | 1a    | 1212 | U    |
| 32  | 1a    | 1213 | A    |
| 32  | 1a    | 1220 | G    |
| 32  | 1a    | 1224 | G    |
| 32  | 1a    | 1227 | A    |
| 32  | 1a    | 1238 | A    |
| 32  | 1a    | 1250 | A    |
| 32  | 1a    | 1253 | G    |
| 32  | 1a    | 1256 | A    |
| 32  | 1a    | 1257 | U    |
| 32  | 1a    | 1258 | G    |
| 32  | 1a    | 1270 | C    |
| 32  | 1a    | 1273 | G    |
| 32  | 1a    | 1278 | U    |
| 32  | 1a    | 1279 | A    |
| 32  | 1a    | 1280 | A    |
| 32  | 1a    | 1286 | A    |
| 32  | 1a    | 1287 | A    |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 32  | 1a    | 1297    | C    |
| 32  | 1a    | 1299    | A    |
| 32  | 1a    | 1300    | G    |
| 32  | 1a    | 1302    | U    |
| 32  | 1a    | 1338    | G    |
| 32  | 1a    | 1340    | A    |
| 32  | 1a    | 1346    | A    |
| 32  | 1a    | 1347    | G    |
| 32  | 1a    | 1353    | G    |
| 32  | 1a    | 1361    | G    |
| 32  | 1a    | 1363    | C    |
| 32  | 1a    | 1368    | G    |
| 32  | 1a    | 1370    | G    |
| 32  | 1a    | 1377    | A    |
| 32  | 1a    | 1378    | C    |
| 32  | 1a    | 1397    | C    |
| 32  | 1a    | 1398    | A    |
| 32  | 1a    | 1402    | 4OC  |
| 32  | 1a    | 1409    | C    |
| 32  | 1a    | 1419    | G    |
| 32  | 1a    | 1442    | G    |
| 32  | 1a    | 1442(A) | G    |
| 32  | 1a    | 1452    | C    |
| 32  | 1a    | 1456    | G    |
| 32  | 1a    | 1487    | G    |
| 32  | 1a    | 1491    | G    |
| 32  | 1a    | 1492    | A    |
| 32  | 1a    | 1493    | A    |
| 32  | 1a    | 1497    | G    |
| 32  | 1a    | 1499    | A    |
| 32  | 1a    | 1503    | A    |
| 32  | 1a    | 1504    | G    |
| 32  | 1a    | 1506    | U    |
| 32  | 1a    | 1507    | A    |
| 32  | 1a    | 1517    | G    |
| 32  | 1a    | 1520    | G    |
| 32  | 1a    | 1529    | G    |
| 32  | 1a    | 1530    | G    |
| 1   | 2A    | 10      | G    |
| 1   | 2A    | 15      | G    |
| 1   | 2A    | 34      | C    |
| 1   | 2A    | 45      | C    |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | 2A    | 55     | G    |
| 1   | 2A    | 61     | G    |
| 1   | 2A    | 71     | A    |
| 1   | 2A    | 74     | A    |
| 1   | 2A    | 75     | G    |
| 1   | 2A    | 84     | A    |
| 1   | 2A    | 90     | U    |
| 1   | 2A    | 94     | C    |
| 1   | 2A    | 95     | G    |
| 1   | 2A    | 102    | G    |
| 1   | 2A    | 118    | A    |
| 1   | 2A    | 119    | A    |
| 1   | 2A    | 120    | U    |
| 1   | 2A    | 141    | A    |
| 1   | 2A    | 153    | C    |
| 1   | 2A    | 157    | U    |
| 1   | 2A    | 173    | G    |
| 1   | 2A    | 181    | A    |
| 1   | 2A    | 182    | A    |
| 1   | 2A    | 196    | A    |
| 1   | 2A    | 199    | A    |
| 1   | 2A    | 205    | G    |
| 1   | 2A    | 215    | G    |
| 1   | 2A    | 216    | A    |
| 1   | 2A    | 221    | A    |
| 1   | 2A    | 222    | A    |
| 1   | 2A    | 228    | A    |
| 1   | 2A    | 229    | A    |
| 1   | 2A    | 230    | U    |
| 1   | 2A    | 232    | G    |
| 1   | 2A    | 248    | G    |
| 1   | 2A    | 250    | 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(A) | U    |
| 1   | 2A    | 272(B) | G    |
| 1   | 2A    | 277    | C    |
| 1   | 2A    | 278    | A    |
| 1   | 2A    | 302    | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 2A    | 311 | A    |
| 1   | 2A    | 324 | A    |
| 1   | 2A    | 327 | G    |
| 1   | 2A    | 329 | G    |
| 1   | 2A    | 330 | A    |
| 1   | 2A    | 346 | A    |
| 1   | 2A    | 352 | G    |
| 1   | 2A    | 355 | G    |
| 1   | 2A    | 362 | U    |
| 1   | 2A    | 363 | G    |
| 1   | 2A    | 370 | G    |
| 1   | 2A    | 386 | G    |
| 1   | 2A    | 399 | G    |
| 1   | 2A    | 407 | G    |
| 1   | 2A    | 411 | G    |
| 1   | 2A    | 428 | A    |
| 1   | 2A    | 434 | U    |
| 1   | 2A    | 435 | C    |
| 1   | 2A    | 444 | C    |
| 1   | 2A    | 451 | C    |
| 1   | 2A    | 455 | C    |
| 1   | 2A    | 456 | C    |
| 1   | 2A    | 457 | A    |
| 1   | 2A    | 470 | A    |
| 1   | 2A    | 481 | G    |
| 1   | 2A    | 504 | U    |
| 1   | 2A    | 505 | A    |
| 1   | 2A    | 509 | C    |
| 1   | 2A    | 518 | G    |
| 1   | 2A    | 530 | G    |
| 1   | 2A    | 531 | C    |
| 1   | 2A    | 532 | A    |
| 1   | 2A    | 533 | G    |
| 1   | 2A    | 545 | G    |
| 1   | 2A    | 556 | G    |
| 1   | 2A    | 563 | G    |
| 1   | 2A    | 568 | U    |
| 1   | 2A    | 573 | G    |
| 1   | 2A    | 575 | A    |
| 1   | 2A    | 593 | G    |
| 1   | 2A    | 595 | C    |
| 1   | 2A    | 603 | A    |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | 2A    | 604    | G    |
| 1   | 2A    | 607    | U    |
| 1   | 2A    | 614(B) | G    |
| 1   | 2A    | 614(C) | A    |
| 1   | 2A    | 615    | G    |
| 1   | 2A    | 627    | A    |
| 1   | 2A    | 634    | C    |
| 1   | 2A    | 637    | A    |
| 1   | 2A    | 645    | C    |
| 1   | 2A    | 646    | A    |
| 1   | 2A    | 652(A) | A    |
| 1   | 2A    | 652(B) | A    |
| 1   | 2A    | 652(C) | G    |
| 1   | 2A    | 652(U) | G    |
| 1   | 2A    | 653    | A    |
| 1   | 2A    | 668    | G    |
| 1   | 2A    | 669    | G    |
| 1   | 2A    | 686    | G    |
| 1   | 2A    | 717    | G    |
| 1   | 2A    | 730    | C    |
| 1   | 2A    | 738    | G    |
| 1   | 2A    | 740    | U    |
| 1   | 2A    | 753    | C    |
| 1   | 2A    | 775    | G    |
| 1   | 2A    | 776    | G    |
| 1   | 2A    | 782    | A    |
| 1   | 2A    | 784    | A    |
| 1   | 2A    | 785    | G    |
| 1   | 2A    | 790    | C    |
| 1   | 2A    | 792    | G    |
| 1   | 2A    | 805    | G    |
| 1   | 2A    | 812    | C    |
| 1   | 2A    | 827    | U    |
| 1   | 2A    | 828    | U    |
| 1   | 2A    | 829    | A    |
| 1   | 2A    | 832    | G    |
| 1   | 2A    | 848    | G    |
| 1   | 2A    | 859    | G    |
| 1   | 2A    | 866    | A    |
| 1   | 2A    | 880    | G    |
| 1   | 2A    | 881    | G    |
| 1   | 2A    | 886    | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 2A    | 887  | A    |
| 1   | 2A    | 888  | C    |
| 1   | 2A    | 889  | C    |
| 1   | 2A    | 890  | A    |
| 1   | 2A    | 893  | C    |
| 1   | 2A    | 896  | A    |
| 1   | 2A    | 900  | A    |
| 1   | 2A    | 910  | A    |
| 1   | 2A    | 914  | C    |
| 1   | 2A    | 917  | A    |
| 1   | 2A    | 932  | G    |
| 1   | 2A    | 938  | G    |
| 1   | 2A    | 941  | A    |
| 1   | 2A    | 945  | A    |
| 1   | 2A    | 946  | G    |
| 1   | 2A    | 959  | A    |
| 1   | 2A    | 961  | C    |
| 1   | 2A    | 968  | G    |
| 1   | 2A    | 974  | G    |
| 1   | 2A    | 975  | C    |
| 1   | 2A    | 980  | A    |
| 1   | 2A    | 983  | A    |
| 1   | 2A    | 996  | A    |
| 1   | 2A    | 1012 | U    |
| 1   | 2A    | 1013 | C    |
| 1   | 2A    | 1020 | A    |
| 1   | 2A    | 1025 | G    |
| 1   | 2A    | 1026 | U    |
| 1   | 2A    | 1033 | U    |
| 1   | 2A    | 1038 | C    |
| 1   | 2A    | 1041 | C    |
| 1   | 2A    | 1044 | G    |
| 1   | 2A    | 1045 | A    |
| 1   | 2A    | 1046 | A    |
| 1   | 2A    | 1047 | G    |
| 1   | 2A    | 1052 | C    |
| 1   | 2A    | 1053 | C    |
| 1   | 2A    | 1054 | A    |
| 1   | 2A    | 1058 | G    |
| 1   | 2A    | 1060 | U    |
| 1   | 2A    | 1063 | G    |
| 1   | 2A    | 1064 | C    |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 1   | 2A    | 1065    | U    |
| 1   | 2A    | 1066    | U    |
| 1   | 2A    | 1067    | A    |
| 1   | 2A    | 1068    | G    |
| 1   | 2A    | 1069    | A    |
| 1   | 2A    | 1070    | A    |
| 1   | 2A    | 1071    | G    |
| 1   | 2A    | 1072    | C    |
| 1   | 2A    | 1073    | A    |
| 1   | 2A    | 1074    | G    |
| 1   | 2A    | 1076    | C    |
| 1   | 2A    | 1077    | A    |
| 1   | 2A    | 1078    | U    |
| 1   | 2A    | 1079    | C    |
| 1   | 2A    | 1082    | U    |
| 1   | 2A    | 1083    | U    |
| 1   | 2A    | 1084    | A    |
| 1   | 2A    | 1085    | A    |
| 1   | 2A    | 1086    | A    |
| 1   | 2A    | 1088    | A    |
| 1   | 2A    | 1089    | G    |
| 1   | 2A    | 1090    | U    |
| 1   | 2A    | 1091    | G    |
| 1   | 2A    | 1092    | C    |
| 1   | 2A    | 1093    | G    |
| 1   | 2A    | 1094    | U    |
| 1   | 2A    | 1096    | A    |
| 1   | 2A    | 1107    | G    |
| 1   | 2A    | 1108    | U    |
| 1   | 2A    | 1109    | C    |
| 1   | 2A    | 1112    | G    |
| 1   | 2A    | 1115    | G    |
| 1   | 2A    | 1116    | C    |
| 1   | 2A    | 1117    | G    |
| 1   | 2A    | 1130    | U    |
| 1   | 2A    | 1135    | C    |
| 1   | 2A    | 1136    | G    |
| 1   | 2A    | 1142    | U    |
| 1   | 2A    | 1142(A) | A    |
| 1   | 2A    | 1156    | A    |
| 1   | 2A    | 1170    | G    |
| 1   | 2A    | 1171    | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 2A    | 1211 | U    |
| 1   | 2A    | 1220 | A    |
| 1   | 2A    | 1229 | G    |
| 1   | 2A    | 1236 | G    |
| 1   | 2A    | 1244 | G    |
| 1   | 2A    | 1250 | G    |
| 1   | 2A    | 1253 | A    |
| 1   | 2A    | 1256 | G    |
| 1   | 2A    | 1265 | A    |
| 1   | 2A    | 1271 | G    |
| 1   | 2A    | 1272 | A    |
| 1   | 2A    | 1273 | U    |
| 1   | 2A    | 1282 | U    |
| 1   | 2A    | 1284 | A    |
| 1   | 2A    | 1296 | G    |
| 1   | 2A    | 1300 | U    |
| 1   | 2A    | 1301 | A    |
| 1   | 2A    | 1312 | U    |
| 1   | 2A    | 1313 | U    |
| 1   | 2A    | 1314 | C    |
| 1   | 2A    | 1329 | U    |
| 1   | 2A    | 1342 | A    |
| 1   | 2A    | 1345 | C    |
| 1   | 2A    | 1352 | U    |
| 1   | 2A    | 1359 | A    |
| 1   | 2A    | 1360 | A    |
| 1   | 2A    | 1365 | A    |
| 1   | 2A    | 1368 | G    |
| 1   | 2A    | 1380 | G    |
| 1   | 2A    | 1384 | A    |
| 1   | 2A    | 1385 | G    |
| 1   | 2A    | 1386 | C    |
| 1   | 2A    | 1405 | U    |
| 1   | 2A    | 1416 | G    |
| 1   | 2A    | 1417 | C    |
| 1   | 2A    | 1419 | A    |
| 1   | 2A    | 1420 | U    |
| 1   | 2A    | 1421 | G    |
| 1   | 2A    | 1427 | A    |
| 1   | 2A    | 1428 | C    |
| 1   | 2A    | 1445 | A    |
| 1   | 2A    | 1450 | G    |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 1   | 2A    | 1459    | 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    | 1497    | U    |
| 1   | 2A    | 1508    | A    |
| 1   | 2A    | 1509    | C    |
| 1   | 2A    | 1509(A) | A    |
| 1   | 2A    | 1525    | G    |
| 1   | 2A    | 1531    | C    |
| 1   | 2A    | 1537    | G    |
| 1   | 2A    | 1539    | G    |
| 1   | 2A    | 1542    | A    |
| 1   | 2A    | 1543    | C    |
| 1   | 2A    | 1558    | A    |
| 1   | 2A    | 1566    | A    |
| 1   | 2A    | 1569    | A    |
| 1   | 2A    | 1578    | U    |
| 1   | 2A    | 1580    | A    |
| 1   | 2A    | 1584    | C    |
| 1   | 2A    | 1586    | A    |
| 1   | 2A    | 1608    | A    |
| 1   | 2A    | 1609    | A    |
| 1   | 2A    | 1610    | A    |
| 1   | 2A    | 1640    | C    |
| 1   | 2A    | 1648    | C    |
| 1   | 2A    | 1654    | A    |
| 1   | 2A    | 1674    | G    |
| 1   | 2A    | 1696    | G    |
| 1   | 2A    | 1700    | A    |
| 1   | 2A    | 1701    | A    |
| 1   | 2A    | 1703    | G    |
| 1   | 2A    | 1721    | G    |
| 1   | 2A    | 1722    | A    |
| 1   | 2A    | 1756    | G    |
| 1   | 2A    | 1758    | G    |
| 1   | 2A    | 1762    | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 2A    | 1763 | G    |
| 1   | 2A    | 1764 | G    |
| 1   | 2A    | 1773 | A    |
| 1   | 2A    | 1780 | A    |
| 1   | 2A    | 1782 | C    |
| 1   | 2A    | 1786 | A    |
| 1   | 2A    | 1791 | A    |
| 1   | 2A    | 1800 | C    |
| 1   | 2A    | 1801 | G    |
| 1   | 2A    | 1816 | G    |
| 1   | 2A    | 1829 | A    |
| 1   | 2A    | 1835 | G    |
| 1   | 2A    | 1839 | G    |
| 1   | 2A    | 1847 | A    |
| 1   | 2A    | 1848 | A    |
| 1   | 2A    | 1861 | G    |
| 1   | 2A    | 1877 | A    |
| 1   | 2A    | 1878 | G    |
| 1   | 2A    | 1900 | A    |
| 1   | 2A    | 1906 | G    |
| 1   | 2A    | 1914 | C    |
| 1   | 2A    | 1929 | G    |
| 1   | 2A    | 1930 | G    |
| 1   | 2A    | 1938 | A    |
| 1   | 2A    | 1955 | U    |
| 1   | 2A    | 1963 | U    |
| 1   | 2A    | 1967 | C    |
| 1   | 2A    | 1970 | A    |
| 1   | 2A    | 1971 | A    |
| 1   | 2A    | 1972 | A    |
| 1   | 2A    | 1984 | G    |
| 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    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 2A    | 2060 | A    |
| 1   | 2A    | 2061 | G    |
| 1   | 2A    | 2062 | A    |
| 1   | 2A    | 2063 | C    |
| 1   | 2A    | 2069 | G    |
| 1   | 2A    | 2097 | C    |
| 1   | 2A    | 2099 | U    |
| 1   | 2A    | 2103 | C    |
| 1   | 2A    | 2104 | G    |
| 1   | 2A    | 2105 | C    |
| 1   | 2A    | 2107 | C    |
| 1   | 2A    | 2108 | C    |
| 1   | 2A    | 2110 | G    |
| 1   | 2A    | 2111 | C    |
| 1   | 2A    | 2112 | G    |
| 1   | 2A    | 2116 | G    |
| 1   | 2A    | 2117 | A    |
| 1   | 2A    | 2118 | U    |
| 1   | 2A    | 2119 | A    |
| 1   | 2A    | 2123 | G    |
| 1   | 2A    | 2124 | G    |
| 1   | 2A    | 2126 | A    |
| 1   | 2A    | 2127 | G    |
| 1   | 2A    | 2129 | C    |
| 1   | 2A    | 2130 | U    |
| 1   | 2A    | 2132 | U    |
| 1   | 2A    | 2133 | G    |
| 1   | 2A    | 2134 | A    |
| 1   | 2A    | 2136 | C    |
| 1   | 2A    | 2137 | C    |
| 1   | 2A    | 2138 | C    |
| 1   | 2A    | 2141 | G    |
| 1   | 2A    | 2142 | C    |
| 1   | 2A    | 2145 | C    |
| 1   | 2A    | 2146 | C    |
| 1   | 2A    | 2147 | G    |
| 1   | 2A    | 2148 | G    |
| 1   | 2A    | 2151 | G    |
| 1   | 2A    | 2154 | G    |
| 1   | 2A    | 2158 | A    |
| 1   | 2A    | 2159 | G    |
| 1   | 2A    | 2161 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 2A    | 2162 | G    |
| 1   | 2A    | 2163 | C    |
| 1   | 2A    | 2164 | C    |
| 1   | 2A    | 2165 | G    |
| 1   | 2A    | 2166 | G    |
| 1   | 2A    | 2168 | G    |
| 1   | 2A    | 2172 | U    |
| 1   | 2A    | 2173 | A    |
| 1   | 2A    | 2174 | C    |
| 1   | 2A    | 2178 | C    |
| 1   | 2A    | 2180 | U    |
| 1   | 2A    | 2182 | G    |
| 1   | 2A    | 2185 | C    |
| 1   | 2A    | 2186 | 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    | 2218 | U    |
| 1   | 2A    | 2225 | A    |
| 1   | 2A    | 2235 | G    |
| 1   | 2A    | 2239 | G    |
| 1   | 2A    | 2268 | A    |
| 1   | 2A    | 2269 | A    |
| 1   | 2A    | 2273 | A    |
| 1   | 2A    | 2275 | C    |
| 1   | 2A    | 2278 | A    |
| 1   | 2A    | 2281 | C    |
| 1   | 2A    | 2283 | C    |
| 1   | 2A    | 2287 | A    |
| 1   | 2A    | 2288 | A    |
| 1   | 2A    | 2289 | G    |
| 1   | 2A    | 2305 | A    |
| 1   | 2A    | 2308 | G    |
| 1   | 2A    | 2309 | A    |
| 1   | 2A    | 2311 | A    |
| 1   | 2A    | 2312 | U    |
| 1   | 2A    | 2318 | G    |
| 1   | 2A    | 2319 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 2A    | 2321 | G    |
| 1   | 2A    | 2322 | A    |
| 1   | 2A    | 2325 | G    |
| 1   | 2A    | 2335 | A    |
| 1   | 2A    | 2336 | A    |
| 1   | 2A    | 2343 | C    |
| 1   | 2A    | 2347 | C    |
| 1   | 2A    | 2350 | C    |
| 1   | 2A    | 2366 | A    |
| 1   | 2A    | 2379 | G    |
| 1   | 2A    | 2383 | G    |
| 1   | 2A    | 2385 | C    |
| 1   | 2A    | 2388 | A    |
| 1   | 2A    | 2406 | U    |
| 1   | 2A    | 2410 | G    |
| 1   | 2A    | 2414 | G    |
| 1   | 2A    | 2422 | A    |
| 1   | 2A    | 2423 | U    |
| 1   | 2A    | 2425 | A    |
| 1   | 2A    | 2429 | G    |
| 1   | 2A    | 2430 | A    |
| 1   | 2A    | 2435 | A    |
| 1   | 2A    | 2439 | A    |
| 1   | 2A    | 2441 | C    |
| 1   | 2A    | 2445 | G    |
| 1   | 2A    | 2448 | A    |
| 1   | 2A    | 2476 | A    |
| 1   | 2A    | 2490 | G    |
| 1   | 2A    | 2491 | U    |
| 1   | 2A    | 2502 | G    |
| 1   | 2A    | 2505 | G    |
| 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    |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 1   | 2A    | 2582    | G    |
| 1   | 2A    | 2602    | A    |
| 1   | 2A    | 2603    | G    |
| 1   | 2A    | 2611    | U    |
| 1   | 2A    | 2612    | C    |
| 1   | 2A    | 2615    | U    |
| 1   | 2A    | 2629    | A    |
| 1   | 2A    | 2630    | G    |
| 1   | 2A    | 2632    | A    |
| 1   | 2A    | 2654    | A    |
| 1   | 2A    | 2663    | G    |
| 1   | 2A    | 2682    | U    |
| 1   | 2A    | 2689    | U    |
| 1   | 2A    | 2690    | C    |
| 1   | 2A    | 2691    | C    |
| 1   | 2A    | 2702    | U    |
| 1   | 2A    | 2703    | C    |
| 1   | 2A    | 2712(A) | A    |
| 1   | 2A    | 2713    | A    |
| 1   | 2A    | 2714    | G    |
| 1   | 2A    | 2726    | U    |
| 1   | 2A    | 2732    | G    |
| 1   | 2A    | 2733    | A    |
| 1   | 2A    | 2748    | A    |
| 1   | 2A    | 2750    | A    |
| 1   | 2A    | 2751    | G    |
| 1   | 2A    | 2757    | A    |
| 1   | 2A    | 2765    | A    |
| 1   | 2A    | 2766    | G    |
| 1   | 2A    | 2778    | A    |
| 1   | 2A    | 2793    | G    |
| 1   | 2A    | 2818    | G    |
| 1   | 2A    | 2820    | A    |
| 1   | 2A    | 2821    | A    |
| 1   | 2A    | 2839    | G    |
| 1   | 2A    | 2872    | G    |
| 1   | 2A    | 2873    | A    |
| 1   | 2A    | 2875    | C    |
| 1   | 2A    | 2880    | C    |
| 1   | 2A    | 2887    | U    |
| 1   | 2A    | 2891    | G    |
| 1   | 2A    | 2894    | G    |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | 2A    | 2897   | U    |
| 2   | 2B    | 2      | C    |
| 2   | 2B    | 7      | G    |
| 2   | 2B    | 8      | U    |
| 2   | 2B    | 9      | G    |
| 2   | 2B    | 12     | C    |
| 2   | 2B    | 13     | A    |
| 2   | 2B    | 18     | G    |
| 2   | 2B    | 30     | C    |
| 2   | 2B    | 52     | A    |
| 2   | 2B    | 56     | G    |
| 2   | 2B    | 73     | A    |
| 2   | 2B    | 75     | G    |
| 2   | 2B    | 84     | C    |
| 2   | 2B    | 85     | G    |
| 2   | 2B    | 91     | C    |
| 2   | 2B    | 94     | C    |
| 2   | 2B    | 106    | G    |
| 2   | 2B    | 110    | G    |
| 2   | 2B    | 116    | G    |
| 2   | 2B    | 120    | A    |
| 32  | 2a    | 5      | U    |
| 32  | 2a    | 7      | G    |
| 32  | 2a    | 9      | G    |
| 32  | 2a    | 22     | G    |
| 32  | 2a    | 32     | A    |
| 32  | 2a    | 39     | G    |
| 32  | 2a    | 47     | C    |
| 32  | 2a    | 48     | C    |
| 32  | 2a    | 51     | A    |
| 32  | 2a    | 65     | U    |
| 32  | 2a    | 66     | G    |
| 32  | 2a    | 80     | G    |
| 32  | 2a    | 88     | A    |
| 32  | 2a    | 89     | C    |
| 32  | 2a    | 98     | G    |
| 32  | 2a    | 101    | A    |
| 32  | 2a    | 105    | G    |
| 32  | 2a    | 116    | A    |
| 32  | 2a    | 120    | A    |
| 32  | 2a    | 121    | C    |
| 32  | 2a    | 129(A) | G    |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 32  | 2a    | 131    | C    |
| 32  | 2a    | 151    | A    |
| 32  | 2a    | 156    | G    |
| 32  | 2a    | 163    | C    |
| 32  | 2a    | 174    | C    |
| 32  | 2a    | 181    | G    |
| 32  | 2a    | 182    | U    |
| 32  | 2a    | 189(F) | U    |
| 32  | 2a    | 189(H) | G    |
| 32  | 2a    | 195    | A    |
| 32  | 2a    | 197    | A    |
| 32  | 2a    | 202    | U    |
| 32  | 2a    | 203    | U    |
| 32  | 2a    | 204    | U    |
| 32  | 2a    | 216    | G    |
| 32  | 2a    | 220    | 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    | 298    | A    |
| 32  | 2a    | 321    | A    |
| 32  | 2a    | 328    | C    |
| 32  | 2a    | 332    | G    |
| 32  | 2a    | 350    | G    |
| 32  | 2a    | 351    | G    |
| 32  | 2a    | 352    | C    |
| 32  | 2a    | 353    | A    |
| 32  | 2a    | 354    | G    |
| 32  | 2a    | 367    | U    |
| 32  | 2a    | 372    | C    |
| 32  | 2a    | 373    | A    |
| 32  | 2a    | 375    | U    |
| 32  | 2a    | 384    | G    |
| 32  | 2a    | 397    | A    |
| 32  | 2a    | 398    | C    |
| 32  | 2a    | 406    | G    |
| 32  | 2a    | 412    | A    |
| 32  | 2a    | 423    | G    |
| 32  | 2a    | 424    | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 32  | 2a    | 429 | U    |
| 32  | 2a    | 430 | A    |
| 32  | 2a    | 434 | U    |
| 32  | 2a    | 438 | G    |
| 32  | 2a    | 439 | A    |
| 32  | 2a    | 442 | C    |
| 32  | 2a    | 452 | A    |
| 32  | 2a    | 461 | A    |
| 32  | 2a    | 470 | C    |
| 32  | 2a    | 471 | G    |
| 32  | 2a    | 482 | A    |
| 32  | 2a    | 485 | G    |
| 32  | 2a    | 496 | A    |
| 32  | 2a    | 498 | U    |
| 32  | 2a    | 500 | G    |
| 32  | 2a    | 501 | C    |
| 32  | 2a    | 505 | G    |
| 32  | 2a    | 506 | G    |
| 32  | 2a    | 509 | A    |
| 32  | 2a    | 510 | A    |
| 32  | 2a    | 511 | C    |
| 32  | 2a    | 518 | C    |
| 32  | 2a    | 528 | C    |
| 32  | 2a    | 530 | G    |
| 32  | 2a    | 531 | U    |
| 32  | 2a    | 532 | A    |
| 32  | 2a    | 533 | A    |
| 32  | 2a    | 536 | C    |
| 32  | 2a    | 545 | C    |
| 32  | 2a    | 547 | A    |
| 32  | 2a    | 559 | A    |
| 32  | 2a    | 560 | U    |
| 32  | 2a    | 561 | U    |
| 32  | 2a    | 564 | C    |
| 32  | 2a    | 572 | A    |
| 32  | 2a    | 573 | A    |
| 32  | 2a    | 574 | A    |
| 32  | 2a    | 576 | G    |
| 32  | 2a    | 577 | G    |
| 32  | 2a    | 587 | G    |
| 32  | 2a    | 607 | A    |
| 32  | 2a    | 618 | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 32  | 2a    | 630 | G    |
| 32  | 2a    | 632 | A    |
| 32  | 2a    | 639 | G    |
| 32  | 2a    | 653 | A    |
| 32  | 2a    | 657 | G    |
| 32  | 2a    | 665 | A    |
| 32  | 2a    | 687 | A    |
| 32  | 2a    | 688 | G    |
| 32  | 2a    | 695 | A    |
| 32  | 2a    | 723 | U    |
| 32  | 2a    | 724 | G    |
| 32  | 2a    | 731 | G    |
| 32  | 2a    | 749 | C    |
| 32  | 2a    | 753 | A    |
| 32  | 2a    | 755 | G    |
| 32  | 2a    | 760 | G    |
| 32  | 2a    | 773 | G    |
| 32  | 2a    | 774 | G    |
| 32  | 2a    | 777 | A    |
| 32  | 2a    | 785 | G    |
| 32  | 2a    | 793 | U    |
| 32  | 2a    | 794 | A    |
| 32  | 2a    | 799 | G    |
| 32  | 2a    | 810 | C    |
| 32  | 2a    | 815 | A    |
| 32  | 2a    | 816 | A    |
| 32  | 2a    | 817 | C    |
| 32  | 2a    | 821 | G    |
| 32  | 2a    | 827 | U    |
| 32  | 2a    | 828 | A    |
| 32  | 2a    | 829 | G    |
| 32  | 2a    | 840 | C    |
| 32  | 2a    | 841 | U    |
| 32  | 2a    | 848 | C    |
| 32  | 2a    | 851 | G    |
| 32  | 2a    | 859 | A    |
| 32  | 2a    | 870 | U    |
| 32  | 2a    | 871 | U    |
| 32  | 2a    | 902 | G    |
| 32  | 2a    | 914 | A    |
| 32  | 2a    | 916 | G    |
| 32  | 2a    | 926 | G    |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 32  | 2a    | 927     | G    |
| 32  | 2a    | 934     | C    |
| 32  | 2a    | 960     | U    |
| 32  | 2a    | 961     | U    |
| 32  | 2a    | 966     | M2G  |
| 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    | 992     | U    |
| 32  | 2a    | 993     | G    |
| 32  | 2a    | 994     | A    |
| 32  | 2a    | 1001    | A    |
| 32  | 2a    | 1004    | A    |
| 32  | 2a    | 1006    | C    |
| 32  | 2a    | 1017    | G    |
| 32  | 2a    | 1020    | U    |
| 32  | 2a    | 1023    | G    |
| 32  | 2a    | 1025    | U    |
| 32  | 2a    | 1026    | G    |
| 32  | 2a    | 1027    | C    |
| 32  | 2a    | 1028    | C    |
| 32  | 2a    | 1030    | C    |
| 32  | 2a    | 1030(A) | G    |
| 32  | 2a    | 1030(B) | C    |
| 32  | 2a    | 1030(C) | G    |
| 32  | 2a    | 1030(D) | A    |
| 32  | 2a    | 1031    | G    |
| 32  | 2a    | 1032    | G    |
| 32  | 2a    | 1033    | G    |
| 32  | 2a    | 1041    | A    |
| 32  | 2a    | 1053    | G    |
| 32  | 2a    | 1054    | C    |
| 32  | 2a    | 1055    | A    |
| 32  | 2a    | 1065    | U    |
| 32  | 2a    | 1066    | C    |
| 32  | 2a    | 1068    | G    |
| 32  | 2a    | 1081    | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 32  | 2a    | 1088 | G    |
| 32  | 2a    | 1094 | G    |
| 32  | 2a    | 1095 | U    |
| 32  | 2a    | 1101 | A    |
| 32  | 2a    | 1117 | G    |
| 32  | 2a    | 1123 | A    |
| 32  | 2a    | 1125 | U    |
| 32  | 2a    | 1128 | C    |
| 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    | 1147 | C    |
| 32  | 2a    | 1152 | A    |
| 32  | 2a    | 1157 | A    |
| 32  | 2a    | 1159 | U    |
| 32  | 2a    | 1162 | C    |
| 32  | 2a    | 1166 | G    |
| 32  | 2a    | 1183 | A    |
| 32  | 2a    | 1184 | G    |
| 32  | 2a    | 1187 | G    |
| 32  | 2a    | 1193 | G    |
| 32  | 2a    | 1196 | U    |
| 32  | 2a    | 1197 | G    |
| 32  | 2a    | 1211 | U    |
| 32  | 2a    | 1212 | U    |
| 32  | 2a    | 1213 | A    |
| 32  | 2a    | 1214 | C    |
| 32  | 2a    | 1224 | G    |
| 32  | 2a    | 1226 | C    |
| 32  | 2a    | 1227 | A    |
| 32  | 2a    | 1229 | A    |
| 32  | 2a    | 1236 | A    |
| 32  | 2a    | 1238 | A    |
| 32  | 2a    | 1240 | U    |
| 32  | 2a    | 1241 | G    |
| 32  | 2a    | 1250 | A    |
| 32  | 2a    | 1256 | A    |
| 32  | 2a    | 1257 | U    |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 32  | 2a    | 1258    | G    |
| 32  | 2a    | 1260    | C    |
| 32  | 2a    | 1261    | A    |
| 32  | 2a    | 1270    | C    |
| 32  | 2a    | 1278    | U    |
| 32  | 2a    | 1279    | A    |
| 32  | 2a    | 1280    | A    |
| 32  | 2a    | 1281    | U    |
| 32  | 2a    | 1282    | C    |
| 32  | 2a    | 1286    | A    |
| 32  | 2a    | 1287    | A    |
| 32  | 2a    | 1293    | G    |
| 32  | 2a    | 1294    | G    |
| 32  | 2a    | 1300    | G    |
| 32  | 2a    | 1303    | C    |
| 32  | 2a    | 1305    | G    |
| 32  | 2a    | 1312    | G    |
| 32  | 2a    | 1317    | C    |
| 32  | 2a    | 1320    | C    |
| 32  | 2a    | 1322    | C    |
| 32  | 2a    | 1323    | G    |
| 32  | 2a    | 1340    | A    |
| 32  | 2a    | 1347    | G    |
| 32  | 2a    | 1353    | G    |
| 32  | 2a    | 1358    | U    |
| 32  | 2a    | 1363    | C    |
| 32  | 2a    | 1364    | U    |
| 32  | 2a    | 1365    | G    |
| 32  | 2a    | 1368    | G    |
| 32  | 2a    | 1370    | G    |
| 32  | 2a    | 1399    | C    |
| 32  | 2a    | 1402    | 4OC  |
| 32  | 2a    | 1406    | U    |
| 32  | 2a    | 1413    | 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    | 1487    | G    |
| 32  | 2a    | 1492    | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 32  | 2a    | 1499 | A    |
| 32  | 2a    | 1503 | A    |
| 32  | 2a    | 1504 | G    |
| 32  | 2a    | 1505 | G    |
| 32  | 2a    | 1506 | U    |
| 32  | 2a    | 1507 | A    |
| 32  | 2a    | 1517 | G    |
| 32  | 2a    | 1520 | G    |
| 32  | 2a    | 1529 | G    |
| 32  | 2a    | 1530 | G    |
| 32  | 2a    | 1532 | U    |

All (62) RNA pucker outliers are listed below:

| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | 1A    | 196    | A    |
| 1   | 1A    | 266    | G    |
| 1   | 1A    | 271(K) | U    |
| 1   | 1A    | 278    | A    |
| 1   | 1A    | 573    | G    |
| 1   | 1A    | 764    | A    |
| 1   | 1A    | 774    | A    |
| 1   | 1A    | 827    | U    |
| 1   | 1A    | 839    | U    |
| 1   | 1A    | 840    | C    |
| 1   | 1A    | 887    | A    |
| 1   | 1A    | 888    | C    |
| 1   | 1A    | 895    | U    |
| 1   | 1A    | 974    | G    |
| 1   | 1A    | 1065   | U    |
| 1   | 1A    | 1067   | A    |
| 1   | 1A    | 1089   | G    |
| 1   | 1A    | 1176   | G    |
| 1   | 1A    | 1210   | A    |
| 1   | 1A    | 1275   | A    |
| 1   | 1A    | 1420   | U    |
| 1   | 1A    | 1442   | G    |
| 1   | 1A    | 1608   | A    |
| 1   | 1A    | 1653   | G    |
| 1   | 1A    | 2019   | A    |
| 1   | 1A    | 2126   | A    |
| 1   | 1A    | 2172   | U    |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | 1A    | 2406   | U    |
| 1   | 1A    | 2602   | A    |
| 1   | 1A    | 2689   | U    |
| 1   | 1A    | 2893   | G    |
| 1   | 2A    | 9      | U    |
| 1   | 2A    | 195    | A    |
| 1   | 2A    | 266    | G    |
| 1   | 2A    | 271(M) | G    |
| 1   | 2A    | 277    | C    |
| 1   | 2A    | 752    | A    |
| 1   | 2A    | 764    | A    |
| 1   | 2A    | 827    | U    |
| 1   | 2A    | 840    | C    |
| 1   | 2A    | 1053   | C    |
| 1   | 2A    | 1057   | A    |
| 1   | 2A    | 1063   | G    |
| 1   | 2A    | 1065   | U    |
| 1   | 2A    | 1067   | A    |
| 1   | 2A    | 1073   | A    |
| 1   | 2A    | 1210   | A    |
| 1   | 2A    | 1379   | A    |
| 1   | 2A    | 1420   | U    |
| 1   | 2A    | 1442   | G    |
| 1   | 2A    | 1491   | G    |
| 1   | 2A    | 1992   | G    |
| 1   | 2A    | 2126   | A    |
| 1   | 2A    | 2171   | A    |
| 1   | 2A    | 2172   | U    |
| 1   | 2A    | 2318   | G    |
| 1   | 2A    | 2321   | G    |
| 1   | 2A    | 2406   | U    |
| 1   | 2A    | 2602   | A    |
| 1   | 2A    | 2689   | U    |
| 1   | 2A    | 2750   | A    |
| 1   | 2A    | 2756   | U    |

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The



Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res  | Link  | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|-------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 32  | 5MC  | 1a    | 1400 | 32    | 19,22,23     | 1.64 | 3 (15%)  | 26,32,35    | 1.24 | 3 (11%)  |
| 1   | OMU  | 2A    | 2552 | 1,54  | 19,22,23     | 1.16 | 3 (15%)  | 25,31,34    | 1.88 | 5 (20%)  |
| 32  | UR3  | 2a    | 1498 | 32    | 19,22,23     | 0.96 | 1 (5%)   | 26,32,35    | 1.73 | 2 (7%)   |
| 32  | MA6  | 1a    | 1518 | 32    | 23,26,27     | 0.43 | 0        | 33,38,41    | 2.03 | 9 (27%)  |
| 32  | G7M  | 1a    | 527  | 32    | 23,26,27     | 1.59 | 3 (13%)  | 34,39,42    | 1.68 | 4 (11%)  |
| 32  | 4OC  | 1a    | 1402 | 32    | 20,23,24     | 0.78 | 0        | 25,32,35    | 0.94 | 1 (4%)   |
| 32  | 5MC  | 1a    | 1407 | 32    | 19,22,23     | 1.68 | 2 (10%)  | 26,32,35    | 1.10 | 3 (11%)  |
| 1   | OMG  | 2A    | 2251 | 1     | 23,26,27     | 1.22 | 3 (13%)  | 32,38,41    | 2.06 | 6 (18%)  |
| 1   | PSU  | 2A    | 2605 | 1     | 18,21,22     | 1.30 | 2 (11%)  | 21,30,33    | 1.95 | 4 (19%)  |
| 1   | 5MU  | 1A    | 1939 | 1,54  | 19,22,23     | 1.40 | 5 (26%)  | 27,32,35    | 2.18 | 6 (22%)  |
| 1   | OMU  | 1A    | 2552 | 1,54  | 19,22,23     | 1.30 | 3 (15%)  | 25,31,34    | 1.83 | 6 (24%)  |
| 32  | PSU  | 2a    | 516  | 54,32 | 18,21,22     | 1.37 | 3 (16%)  | 21,30,33    | 2.19 | 5 (23%)  |
| 32  | 5MC  | 1a    | 1404 | 32    | 19,22,23     | 1.80 | 3 (15%)  | 26,32,35    | 1.19 | 3 (11%)  |
| 32  | MA6  | 2a    | 1519 | 32    | 23,26,27     | 0.74 | 1 (4%)   | 33,38,41    | 2.27 | 10 (30%) |
| 1   | OMC  | 1A    | 1920 | 1     | 19,22,23     | 0.80 | 0        | 25,31,34    | 1.02 | 1 (4%)   |
| 1   | 5MC  | 2A    | 1942 | 1,54  | 19,22,23     | 1.78 | 3 (15%)  | 26,32,35    | 1.14 | 3 (11%)  |
| 43  | 0TD  | 1l    | 92   | 43    | 8,9,10       | 4.52 | 1 (12%)  | 6,11,13     | 7.23 | 1 (16%)  |
| 1   | 2MA  | 2A    | 2503 | 1,54  | 22,25,26     | 1.52 | 4 (18%)  | 32,37,40    | 2.42 | 8 (25%)  |
| 1   | 5MU  | 2A    | 1915 | 1     | 19,22,23     | 1.46 | 4 (21%)  | 27,32,35    | 2.16 | 8 (29%)  |
| 32  | 2MG  | 2a    | 1207 | 32    | 23,26,27     | 1.27 | 4 (17%)  | 33,38,41    | 2.00 | 7 (21%)  |
| 1   | PSU  | 1A    | 2605 | 1,54  | 18,21,22     | 1.37 | 2 (11%)  | 21,30,33    | 2.06 | 4 (19%)  |
| 32  | 5MC  | 2a    | 1400 | 32    | 19,22,23     | 1.68 | 3 (15%)  | 26,32,35    | 1.21 | 4 (15%)  |
| 1   | PSU  | 2A    | 1911 | 1     | 18,21,22     | 1.37 | 2 (11%)  | 21,30,33    | 1.99 | 4 (19%)  |
| 32  | 5MC  | 2a    | 1407 | 32    | 19,22,23     | 1.66 | 3 (15%)  | 26,32,35    | 1.16 | 3 (11%)  |
| 1   | 2MA  | 1A    | 2503 | 1,54  | 22,25,26     | 1.47 | 4 (18%)  | 32,37,40    | 2.38 | 7 (21%)  |
| 32  | 5MC  | 2a    | 967  | 32    | 19,22,23     | 1.79 | 3 (15%)  | 26,32,35    | 1.13 | 2 (7%)   |
| 1   | OMC  | 2A    | 1920 | 1     | 19,22,23     | 0.79 | 0        | 25,31,34    | 0.98 | 1 (4%)   |
| 1   | PSU  | 2A    | 1917 | 1     | 18,21,22     | 1.39 | 2 (11%)  | 21,30,33    | 1.97 | 4 (19%)  |
| 32  | M2G  | 2a    | 966  | 32    | 24,27,28     | 1.29 | 3 (12%)  | 33,40,43    | 1.89 | 5 (15%)  |
| 43  | 0TD  | 2l    | 92   | 43    | 8,9,10       | 4.47 | 1 (12%)  | 6,11,13     | 2.76 | 3 (50%)  |
| 1   | OMG  | 1A    | 2251 | 1,54  | 23,26,27     | 1.25 | 2 (8%)   | 32,38,41    | 2.02 | 7 (21%)  |

| Mol | Type | Chain | Res  | Link  | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|-------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 32  | PSU  | 1a    | 516  | 54,32 | 18,21,22     | 1.36 | 2 (11%)  | 21,30,33    | 1.94 | 5 (23%)  |
| 1   | 5MU  | 1A    | 1915 | 1     | 19,22,23     | 1.49 | 5 (26%)  | 27,32,35    | 2.36 | 10 (37%) |
| 32  | 5MC  | 2a    | 1404 | 32    | 19,22,23     | 1.80 | 3 (15%)  | 26,32,35    | 1.20 | 3 (11%)  |
| 32  | MA6  | 1a    | 1519 | 32    | 23,26,27     | 0.44 | 0        | 33,38,41    | 2.02 | 9 (27%)  |
| 1   | PSU  | 1A    | 1911 | 1     | 18,21,22     | 1.38 | 2 (11%)  | 21,30,33    | 2.01 | 5 (23%)  |
| 1   | PSU  | 1A    | 1917 | 1     | 18,21,22     | 1.42 | 3 (16%)  | 21,30,33    | 2.03 | 4 (19%)  |
| 32  | 5MC  | 1a    | 967  | 32    | 19,22,23     | 1.67 | 3 (15%)  | 26,32,35    | 1.09 | 2 (7%)   |
| 32  | 4OC  | 2a    | 1402 | 32    | 20,23,24     | 0.77 | 0        | 25,32,35    | 0.98 | 1 (4%)   |
| 32  | UR3  | 1a    | 1498 | 32    | 19,22,23     | 1.03 | 2 (10%)  | 26,32,35    | 1.68 | 4 (15%)  |
| 1   | 5MC  | 2A    | 1962 | 1     | 19,22,23     | 1.60 | 3 (15%)  | 26,32,35    | 1.11 | 2 (7%)   |
| 1   | 5MC  | 1A    | 1942 | 1     | 19,22,23     | 1.39 | 3 (15%)  | 26,32,35    | 1.23 | 2 (7%)   |
| 32  | M2G  | 1a    | 966  | 32    | 24,27,28     | 1.31 | 4 (16%)  | 33,40,43    | 1.81 | 6 (18%)  |
| 32  | 2MG  | 1a    | 1207 | 54,32 | 23,26,27     | 1.25 | 3 (13%)  | 33,38,41    | 2.33 | 9 (27%)  |
| 32  | MA6  | 2a    | 1518 | 32    | 23,26,27     | 0.41 | 0        | 33,38,41    | 1.97 | 9 (27%)  |
| 32  | G7M  | 2a    | 527  | 54,32 | 23,26,27     | 1.43 | 4 (17%)  | 34,39,42    | 1.66 | 5 (14%)  |
| 1   | 5MU  | 2A    | 1939 | 1,54  | 19,22,23     | 1.36 | 5 (26%)  | 27,32,35    | 2.11 | 6 (22%)  |
| 1   | 5MC  | 1A    | 1962 | 1,54  | 19,22,23     | 1.51 | 3 (15%)  | 26,32,35    | 1.22 | 3 (11%)  |

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

| Mol | Type | Chain | Res  | Link  | Chirals | Torsions   | Rings   |
|-----|------|-------|------|-------|---------|------------|---------|
| 32  | 5MC  | 1a    | 1400 | 32    | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | OMU  | 2A    | 2552 | 1,54  | -       | 0/9/27/28  | 0/2/2/2 |
| 32  | UR3  | 2a    | 1498 | 32    | -       | 0/7/25/26  | 0/2/2/2 |
| 32  | MA6  | 1a    | 1518 | 32    | -       | 0/11/29/30 | 0/3/3/3 |
| 32  | G7M  | 1a    | 527  | 32    | -       | 2/7/25/26  | 0/3/3/3 |
| 32  | 4OC  | 1a    | 1402 | 32    | -       | 2/9/29/30  | 0/2/2/2 |
| 32  | 5MC  | 1a    | 1407 | 32    | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | OMG  | 2A    | 2251 | 1     | -       | 0/9/27/28  | 0/3/3/3 |
| 1   | PSU  | 2A    | 2605 | 1     | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | 5MU  | 1A    | 1939 | 1,54  | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | OMU  | 1A    | 2552 | 1,54  | -       | 0/9/27/28  | 0/2/2/2 |
| 32  | PSU  | 2a    | 516  | 54,32 | -       | 1/7/25/26  | 0/2/2/2 |
| 32  | 5MC  | 1a    | 1404 | 32    | -       | 0/7/25/26  | 0/2/2/2 |
| 32  | MA6  | 2a    | 1519 | 32    | -       | 2/11/29/30 | 0/3/3/3 |

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| Mol | Type | Chain | Res  | Link  | Chirals | Torsions   | Rings   |
|-----|------|-------|------|-------|---------|------------|---------|
| 1   | OMC  | 1A    | 1920 | 1     | -       | 1/9/27/28  | 0/2/2/2 |
| 1   | 5MC  | 2A    | 1942 | 1,54  | -       | 0/7/25/26  | 0/2/2/2 |
| 43  | 0TD  | 1l    | 92   | 43    | -       | 3/7/12/14  | -       |
| 1   | 2MA  | 2A    | 2503 | 1,54  | -       | 2/7/25/26  | 0/3/3/3 |
| 1   | 5MU  | 2A    | 1915 | 1     | -       | 2/7/25/26  | 0/2/2/2 |
| 32  | 2MG  | 2a    | 1207 | 32    | -       | 0/9/27/28  | 0/3/3/3 |
| 1   | PSU  | 1A    | 2605 | 1,54  | -       | 0/7/25/26  | 0/2/2/2 |
| 32  | 5MC  | 2a    | 1400 | 32    | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | PSU  | 2A    | 1911 | 1     | -       | 0/7/25/26  | 0/2/2/2 |
| 32  | 5MC  | 2a    | 1407 | 32    | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | 2MA  | 1A    | 2503 | 1,54  | -       | 2/7/25/26  | 0/3/3/3 |
| 32  | 5MC  | 2a    | 967  | 32    | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | OMC  | 2A    | 1920 | 1     | -       | 1/9/27/28  | 0/2/2/2 |
| 1   | PSU  | 2A    | 1917 | 1     | -       | 0/7/25/26  | 0/2/2/2 |
| 32  | M2G  | 2a    | 966  | 32    | -       | 0/11/29/30 | 0/3/3/3 |
| 43  | 0TD  | 2l    | 92   | 43    | -       | 2/7/12/14  | -       |
| 1   | OMG  | 1A    | 2251 | 1,54  | -       | 1/9/27/28  | 0/3/3/3 |
| 32  | PSU  | 1a    | 516  | 54,32 | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | 5MU  | 1A    | 1915 | 1     | -       | 4/7/25/26  | 0/2/2/2 |
| 32  | 5MC  | 2a    | 1404 | 32    | -       | 0/7/25/26  | 0/2/2/2 |
| 32  | MA6  | 1a    | 1519 | 32    | -       | 2/11/29/30 | 0/3/3/3 |
| 1   | PSU  | 1A    | 1911 | 1     | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | PSU  | 1A    | 1917 | 1     | -       | 2/7/25/26  | 0/2/2/2 |
| 32  | 5MC  | 1a    | 967  | 32    | -       | 0/7/25/26  | 0/2/2/2 |
| 32  | 4OC  | 2a    | 1402 | 32    | -       | 3/9/29/30  | 0/2/2/2 |
| 32  | UR3  | 1a    | 1498 | 32    | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | 5MC  | 2A    | 1962 | 1     | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | 5MC  | 1A    | 1942 | 1     | -       | 0/7/25/26  | 0/2/2/2 |
| 32  | M2G  | 1a    | 966  | 32    | -       | 0/11/29/30 | 0/3/3/3 |
| 32  | 2MG  | 1a    | 1207 | 54,32 | -       | 3/9/27/28  | 0/3/3/3 |
| 32  | MA6  | 2a    | 1518 | 32    | -       | 0/11/29/30 | 0/3/3/3 |
| 32  | G7M  | 2a    | 527  | 54,32 | -       | 1/7/25/26  | 0/3/3/3 |
| 1   | 5MU  | 2A    | 1939 | 1,54  | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | 5MC  | 1A    | 1962 | 1,54  | -       | 0/7/25/26  | 0/2/2/2 |

All (118) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 43  | 1l    | 92  | 0TD  | CB-SB | -12.36 | 1.69        | 1.82     |
| 43  | 2l    | 92  | 0TD  | CB-SB | -12.34 | 1.69        | 1.82     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 32  | 1a    | 1404 | 5MC  | C5-C4 | 6.77  | 1.49        | 1.44     |
| 32  | 2a    | 1404 | 5MC  | C5-C4 | 6.76  | 1.49        | 1.44     |
| 32  | 2a    | 967  | 5MC  | C5-C4 | 6.72  | 1.49        | 1.44     |
| 1   | 2A    | 1942 | 5MC  | C5-C4 | 6.56  | 1.49        | 1.44     |
| 32  | 2a    | 1400 | 5MC  | C5-C4 | 6.23  | 1.48        | 1.44     |
| 32  | 1a    | 1407 | 5MC  | C5-C4 | 6.14  | 1.48        | 1.44     |
| 32  | 1a    | 967  | 5MC  | C5-C4 | 6.05  | 1.48        | 1.44     |
| 32  | 2a    | 1407 | 5MC  | C5-C4 | 6.00  | 1.48        | 1.44     |
| 32  | 1a    | 1400 | 5MC  | C5-C4 | 5.83  | 1.48        | 1.44     |
| 1   | 2A    | 1962 | 5MC  | C5-C4 | 5.68  | 1.48        | 1.44     |
| 1   | 1A    | 1962 | 5MC  | C5-C4 | 5.16  | 1.48        | 1.44     |
| 32  | 1a    | 527  | G7M  | C5-N7 | -5.05 | 1.33        | 1.39     |
| 1   | 1A    | 1942 | 5MC  | C5-C4 | 4.64  | 1.47        | 1.44     |
| 1   | 2A    | 2503 | 2MA  | C5-C4 | 4.49  | 1.47        | 1.39     |
| 1   | 1A    | 2503 | 2MA  | C5-C4 | 4.27  | 1.46        | 1.39     |
| 32  | 2a    | 527  | G7M  | C5-N7 | -4.04 | 1.34        | 1.39     |
| 1   | 1A    | 1911 | PSU  | C6-C5 | 3.69  | 1.39        | 1.35     |
| 32  | 1a    | 516  | PSU  | C6-C5 | 3.63  | 1.39        | 1.35     |
| 1   | 2A    | 1911 | PSU  | C6-C5 | 3.61  | 1.39        | 1.35     |
| 1   | 2A    | 1917 | PSU  | C6-C5 | 3.52  | 1.39        | 1.35     |
| 1   | 1A    | 1917 | PSU  | C6-C5 | 3.48  | 1.39        | 1.35     |
| 32  | 1a    | 527  | G7M  | C5-C4 | 3.35  | 1.46        | 1.38     |
| 32  | 2a    | 1207 | 2MG  | C5-C4 | 3.33  | 1.47        | 1.38     |
| 32  | 2a    | 516  | PSU  | C6-C5 | 3.30  | 1.38        | 1.35     |
| 32  | 1a    | 966  | M2G  | C5-C4 | 3.29  | 1.47        | 1.38     |
| 1   | 1A    | 1915 | 5MU  | C2-N1 | 3.20  | 1.43        | 1.38     |
| 32  | 2a    | 966  | M2G  | C5-C4 | 3.19  | 1.47        | 1.38     |
| 1   | 2A    | 2605 | PSU  | C6-C5 | 3.19  | 1.38        | 1.35     |
| 32  | 1a    | 1207 | 2MG  | C5-C4 | 3.18  | 1.47        | 1.38     |
| 32  | 2a    | 527  | G7M  | C5-C4 | 3.17  | 1.46        | 1.38     |
| 1   | 2A    | 1915 | 5MU  | C2-N1 | 3.12  | 1.43        | 1.38     |
| 1   | 2A    | 2251 | OMG  | C5-C4 | 3.07  | 1.47        | 1.38     |
| 1   | 1A    | 2251 | OMG  | C6-N1 | -3.04 | 1.33        | 1.38     |
| 1   | 1A    | 2251 | OMG  | C5-C4 | 3.01  | 1.47        | 1.38     |
| 1   | 1A    | 2552 | OMU  | C4-N3 | -2.96 | 1.33        | 1.38     |
| 1   | 1A    | 2552 | OMU  | C2-N3 | -2.93 | 1.32        | 1.38     |
| 1   | 1A    | 2503 | 2MA  | C5-N7 | -2.90 | 1.33        | 1.39     |
| 1   | 1A    | 1939 | 5MU  | C4-N3 | -2.86 | 1.33        | 1.38     |
| 1   | 2A    | 1915 | 5MU  | C6-C5 | 2.86  | 1.39        | 1.34     |
| 1   | 1A    | 2605 | PSU  | C4-N3 | -2.85 | 1.33        | 1.38     |
| 32  | 2a    | 1407 | 5MC  | C6-C5 | 2.84  | 1.39        | 1.34     |
| 1   | 1A    | 1915 | 5MU  | C4-N3 | -2.83 | 1.33        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 32  | 1a    | 967  | 5MC  | C6-C5 | 2.82  | 1.39        | 1.34     |
| 32  | 1a    | 966  | M2G  | C2-N2 | 2.82  | 1.40        | 1.35     |
| 32  | 2a    | 966  | M2G  | C2-N2 | 2.79  | 1.40        | 1.35     |
| 32  | 2a    | 967  | 5MC  | C6-C5 | 2.79  | 1.39        | 1.34     |
| 1   | 2A    | 1942 | 5MC  | C6-C5 | 2.78  | 1.39        | 1.34     |
| 1   | 1A    | 1962 | 5MC  | C6-C5 | 2.77  | 1.39        | 1.34     |
| 1   | 1A    | 1939 | 5MU  | C6-C5 | 2.76  | 1.39        | 1.34     |
| 1   | 2A    | 2251 | OMG  | C6-N1 | -2.74 | 1.33        | 1.38     |
| 32  | 1a    | 1407 | 5MC  | C6-C5 | 2.73  | 1.39        | 1.34     |
| 1   | 2A    | 2552 | OMU  | C4-N3 | -2.72 | 1.34        | 1.38     |
| 1   | 1A    | 1942 | 5MC  | C6-C5 | 2.71  | 1.39        | 1.34     |
| 32  | 1a    | 1400 | 5MC  | C6-C5 | 2.71  | 1.39        | 1.34     |
| 1   | 2A    | 1939 | 5MU  | C6-C5 | 2.71  | 1.39        | 1.34     |
| 1   | 1A    | 1917 | PSU  | C4-N3 | -2.70 | 1.33        | 1.38     |
| 1   | 2A    | 1911 | PSU  | C4-N3 | -2.67 | 1.33        | 1.38     |
| 1   | 2A    | 1962 | 5MC  | C6-C5 | 2.66  | 1.38        | 1.34     |
| 1   | 2A    | 1939 | 5MU  | C4-N3 | -2.66 | 1.33        | 1.38     |
| 1   | 2A    | 2503 | 2MA  | C5-C6 | 2.65  | 1.48        | 1.41     |
| 1   | 1A    | 1911 | PSU  | C4-N3 | -2.62 | 1.33        | 1.38     |
| 32  | 2a    | 516  | PSU  | C4-N3 | -2.61 | 1.34        | 1.38     |
| 32  | 2a    | 1404 | 5MC  | C6-C5 | 2.61  | 1.38        | 1.34     |
| 1   | 1A    | 1915 | 5MU  | C6-C5 | 2.60  | 1.38        | 1.34     |
| 1   | 2A    | 1917 | PSU  | C4-N3 | -2.58 | 1.34        | 1.38     |
| 32  | 1a    | 527  | G7M  | C6-N1 | -2.56 | 1.34        | 1.38     |
| 1   | 1A    | 1939 | 5MU  | C2-N3 | -2.54 | 1.33        | 1.38     |
| 32  | 1a    | 1404 | 5MC  | C6-C5 | 2.53  | 1.38        | 1.34     |
| 1   | 2A    | 2605 | PSU  | C4-N3 | -2.53 | 1.34        | 1.38     |
| 32  | 1a    | 966  | M2G  | C6-N1 | -2.53 | 1.34        | 1.38     |
| 32  | 2a    | 966  | M2G  | C6-N1 | -2.53 | 1.34        | 1.38     |
| 1   | 2A    | 2503 | 2MA  | C5-N7 | -2.52 | 1.34        | 1.39     |
| 32  | 2a    | 1400 | 5MC  | C6-C5 | 2.49  | 1.38        | 1.34     |
| 32  | 1a    | 1400 | 5MC  | C6-N1 | -2.49 | 1.33        | 1.38     |
| 32  | 1a    | 1404 | 5MC  | C6-N1 | -2.49 | 1.33        | 1.38     |
| 1   | 2A    | 1915 | 5MU  | C4-C5 | 2.47  | 1.48        | 1.44     |
| 1   | 2A    | 1915 | 5MU  | C4-N3 | -2.47 | 1.34        | 1.38     |
| 32  | 1a    | 1498 | UR3  | C2-N1 | 2.44  | 1.41        | 1.38     |
| 32  | 1a    | 1207 | 2MG  | C6-N1 | -2.41 | 1.34        | 1.38     |
| 1   | 1A    | 2605 | PSU  | C6-C5 | 2.41  | 1.38        | 1.35     |
| 1   | 2A    | 1939 | 5MU  | C2-N3 | -2.41 | 1.33        | 1.38     |
| 32  | 2a    | 1207 | 2MG  | C6-N1 | -2.39 | 1.34        | 1.38     |
| 32  | 1a    | 516  | PSU  | C4-N3 | -2.38 | 1.34        | 1.38     |
| 1   | 1A    | 1939 | 5MU  | C6-N1 | -2.38 | 1.34        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 32  | 2a    | 1404 | 5MC  | C6-N1   | -2.37 | 1.34        | 1.38     |
| 1   | 1A    | 1915 | 5MU  | C4-C5   | 2.36  | 1.48        | 1.44     |
| 1   | 1A    | 1962 | 5MC  | C6-N1   | -2.35 | 1.34        | 1.38     |
| 1   | 2A    | 1962 | 5MC  | C6-N1   | -2.35 | 1.34        | 1.38     |
| 32  | 2a    | 527  | G7M  | C6-N1   | -2.33 | 1.34        | 1.38     |
| 1   | 2A    | 2503 | 2MA  | C8-N7   | 2.30  | 1.36        | 1.31     |
| 1   | 2A    | 1942 | 5MC  | C6-N1   | -2.28 | 1.34        | 1.38     |
| 1   | 2A    | 1939 | 5MU  | C6-N1   | -2.28 | 1.34        | 1.38     |
| 32  | 2a    | 1400 | 5MC  | C6-N1   | -2.26 | 1.34        | 1.38     |
| 1   | 1A    | 1942 | 5MC  | C6-N1   | -2.25 | 1.34        | 1.38     |
| 1   | 2A    | 1939 | 5MU  | C4-C5   | 2.24  | 1.48        | 1.44     |
| 1   | 2A    | 2251 | OMG  | C5-N7   | -2.22 | 1.34        | 1.39     |
| 1   | 1A    | 2503 | 2MA  | C5-C6   | 2.18  | 1.47        | 1.41     |
| 1   | 1A    | 2552 | OMU  | C5-C4   | -2.18 | 1.39        | 1.43     |
| 32  | 1a    | 1498 | UR3  | C6-C5   | 2.16  | 1.40        | 1.35     |
| 32  | 2a    | 1519 | MA6  | C4-N3   | 2.16  | 1.38        | 1.34     |
| 32  | 2a    | 967  | 5MC  | C6-N1   | -2.14 | 1.34        | 1.38     |
| 1   | 2A    | 2552 | OMU  | C2-N3   | -2.13 | 1.34        | 1.38     |
| 32  | 1a    | 967  | 5MC  | C6-N1   | -2.12 | 1.34        | 1.38     |
| 32  | 2a    | 1498 | UR3  | C6-C5   | 2.09  | 1.39        | 1.35     |
| 32  | 2a    | 516  | PSU  | O4'-C1' | -2.08 | 1.41        | 1.43     |
| 1   | 2A    | 2552 | OMU  | C6-C5   | 2.08  | 1.39        | 1.35     |
| 32  | 2a    | 527  | G7M  | C4-N9   | -2.06 | 1.32        | 1.38     |
| 1   | 1A    | 1917 | PSU  | C2-N3   | -2.06 | 1.34        | 1.37     |
| 1   | 1A    | 2503 | 2MA  | C8-N7   | 2.05  | 1.35        | 1.31     |
| 1   | 1A    | 1915 | 5MU  | C2-N3   | -2.05 | 1.34        | 1.38     |
| 32  | 2a    | 1407 | 5MC  | C6-N1   | -2.05 | 1.34        | 1.38     |
| 32  | 1a    | 1207 | 2MG  | C2-N3   | 2.04  | 1.35        | 1.32     |
| 32  | 2a    | 1207 | 2MG  | C5-N7   | -2.04 | 1.35        | 1.39     |
| 32  | 1a    | 966  | M2G  | C5-N7   | -2.01 | 1.35        | 1.39     |
| 1   | 1A    | 1939 | 5MU  | C4-C5   | 2.01  | 1.48        | 1.44     |
| 32  | 2a    | 1207 | 2MG  | C2-N3   | 2.00  | 1.35        | 1.32     |

All (224) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms     | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|--------|-------------|----------|
| 43  | 1l    | 92   | 0TD  | CSB-SB-CB | -17.51 | 70.89       | 102.36   |
| 1   | 2A    | 2503 | 2MA  | C5-C4-N3  | -8.92  | 117.78      | 127.18   |
| 1   | 1A    | 2503 | 2MA  | C5-C4-N3  | -8.54  | 118.19      | 127.18   |
| 32  | 1a    | 1207 | 2MG  | C2-N3-C4  | 7.19   | 120.99      | 112.00   |
| 32  | 2a    | 1498 | UR3  | C4-N3-C2  | -7.08  | 118.88      | 124.58   |
| 1   | 2A    | 2503 | 2MA  | N3-C4-N9  | 6.99   | 135.86      | 126.99   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1   | 1A    | 2503 | 2MA  | N3-C4-N9  | 6.99  | 135.86      | 126.99   |
| 1   | 2A    | 2251 | OMG  | C5-C4-N3  | -6.73 | 117.68      | 128.39   |
| 32  | 2a    | 516  | PSU  | N1-C2-N3  | 6.62  | 122.15      | 115.17   |
| 32  | 1a    | 1498 | UR3  | C4-N3-C2  | -6.53 | 119.33      | 124.58   |
| 1   | 1A    | 1917 | PSU  | N1-C2-N3  | 6.45  | 121.97      | 115.17   |
| 32  | 2a    | 1207 | 2MG  | C2-N3-C4  | 6.42  | 120.03      | 112.00   |
| 1   | 1A    | 1911 | PSU  | N1-C2-N3  | 6.27  | 121.78      | 115.17   |
| 1   | 1A    | 2251 | OMG  | C5-C4-N3  | -6.22 | 118.49      | 128.39   |
| 1   | 2A    | 1917 | PSU  | N1-C2-N3  | 6.19  | 121.69      | 115.17   |
| 1   | 2A    | 1911 | PSU  | N1-C2-N3  | 6.16  | 121.67      | 115.17   |
| 32  | 2a    | 966  | M2G  | C5-C4-N3  | -6.14 | 118.62      | 128.39   |
| 32  | 1a    | 966  | M2G  | C5-C4-N3  | -6.06 | 118.74      | 128.39   |
| 1   | 1A    | 2605 | PSU  | N1-C2-N3  | 5.99  | 121.49      | 115.17   |
| 32  | 1a    | 1207 | 2MG  | C5-C4-N3  | -5.98 | 118.87      | 128.39   |
| 32  | 1a    | 516  | PSU  | N1-C2-N3  | 5.72  | 121.21      | 115.17   |
| 1   | 2A    | 2605 | PSU  | N1-C2-N3  | 5.60  | 121.07      | 115.17   |
| 32  | 2a    | 1207 | 2MG  | C5-C4-N3  | -5.52 | 119.60      | 128.39   |
| 32  | 1a    | 527  | G7M  | C5-C4-N3  | -5.46 | 117.83      | 128.15   |
| 43  | 2l    | 92   | 0TD  | CSB-SB-CB | 5.46  | 112.18      | 102.36   |
| 1   | 2A    | 1939 | 5MU  | N3-C2-N1  | 5.46  | 121.99      | 114.89   |
| 32  | 1a    | 527  | G7M  | N9-C4-N3  | 5.41  | 136.78      | 125.95   |
| 32  | 1a    | 1518 | MA6  | N1-C2-N3  | -5.30 | 120.56      | 128.58   |
| 1   | 2A    | 2251 | OMG  | C2-N3-C4  | 5.27  | 121.38      | 112.30   |
| 1   | 1A    | 1939 | 5MU  | C4-N3-C2  | -5.24 | 120.47      | 127.34   |
| 32  | 2a    | 1519 | MA6  | C5-C4-N3  | -5.22 | 119.53      | 126.72   |
| 1   | 1A    | 2251 | OMG  | C2-N3-C4  | 5.14  | 121.15      | 112.30   |
| 1   | 2A    | 1939 | 5MU  | C4-N3-C2  | -5.13 | 120.62      | 127.34   |
| 1   | 1A    | 1939 | 5MU  | N3-C2-N1  | 4.95  | 121.34      | 114.89   |
| 1   | 1A    | 1915 | 5MU  | N3-C2-N1  | 4.92  | 121.29      | 114.89   |
| 32  | 2a    | 527  | G7M  | N9-C4-N3  | 4.91  | 135.78      | 125.95   |
| 32  | 2a    | 1519 | MA6  | N1-C2-N3  | -4.88 | 121.19      | 128.58   |
| 1   | 1A    | 1915 | 5MU  | C1'-N1-C2 | 4.87  | 126.33      | 117.59   |
| 1   | 2A    | 2251 | OMG  | N9-C4-N3  | 4.85  | 135.65      | 125.95   |
| 32  | 2a    | 527  | G7M  | C5-C4-N3  | -4.77 | 119.13      | 128.15   |
| 32  | 2a    | 1518 | MA6  | N1-C2-N3  | -4.77 | 121.36      | 128.58   |
| 1   | 1A    | 2552 | OMU  | C4-N3-C2  | -4.75 | 120.72      | 126.61   |
| 32  | 1a    | 966  | M2G  | N9-C4-N3  | 4.74  | 135.44      | 125.95   |
| 1   | 2A    | 2552 | OMU  | C4-N3-C2  | -4.74 | 120.73      | 126.61   |
| 1   | 2A    | 1915 | 5MU  | N3-C2-N1  | 4.73  | 121.05      | 114.89   |
| 1   | 2A    | 2552 | OMU  | N3-C2-N1  | 4.72  | 121.03      | 114.89   |
| 32  | 2a    | 527  | G7M  | C2-N3-C4  | 4.67  | 120.34      | 112.30   |
| 1   | 1A    | 2251 | OMG  | N9-C4-N3  | 4.65  | 135.25      | 125.95   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1   | 1A    | 1915 | 5MU  | C4-N3-C2  | -4.61 | 121.30      | 127.34   |
| 1   | 1A    | 1939 | 5MU  | C5-C4-N3  | 4.59  | 119.32      | 115.32   |
| 32  | 2a    | 966  | M2G  | C2-N3-C4  | 4.59  | 121.00      | 112.51   |
| 32  | 1a    | 1519 | MA6  | N1-C2-N3  | -4.57 | 121.66      | 128.58   |
| 32  | 2a    | 1519 | MA6  | C4-C5-N7  | -4.56 | 105.37      | 110.58   |
| 32  | 1a    | 527  | G7M  | C2-N3-C4  | 4.55  | 120.14      | 112.30   |
| 1   | 1A    | 1939 | 5MU  | C5-C6-N1  | -4.52 | 118.41      | 123.31   |
| 32  | 1a    | 1519 | MA6  | C5-C4-N3  | -4.45 | 120.59      | 126.72   |
| 1   | 2A    | 1915 | 5MU  | C4-N3-C2  | -4.44 | 121.53      | 127.34   |
| 32  | 2a    | 966  | M2G  | N9-C4-N3  | 4.37  | 134.69      | 125.95   |
| 1   | 1A    | 2605 | PSU  | C4-N3-C2  | -4.34 | 120.40      | 126.37   |
| 32  | 2a    | 516  | PSU  | C4-N3-C2  | -4.33 | 120.41      | 126.37   |
| 1   | 1A    | 1915 | 5MU  | C5-C4-N3  | 4.32  | 119.08      | 115.32   |
| 32  | 1a    | 1518 | MA6  | C2-N1-C6  | 4.27  | 122.26      | 111.83   |
| 1   | 1A    | 2552 | OMU  | N3-C2-N1  | 4.24  | 120.42      | 114.89   |
| 32  | 2a    | 1518 | MA6  | C5-C4-N3  | -4.22 | 120.91      | 126.72   |
| 1   | 2A    | 2605 | PSU  | C4-N3-C2  | -4.21 | 120.57      | 126.37   |
| 1   | 2A    | 1915 | 5MU  | C1'-N1-C2 | 4.18  | 125.09      | 117.59   |
| 32  | 1a    | 966  | M2G  | C2-N3-C4  | 4.17  | 120.22      | 112.51   |
| 1   | 1A    | 1915 | 5MU  | C1'-N1-C6 | -4.17 | 114.29      | 121.15   |
| 32  | 2a    | 1519 | MA6  | C2-N1-C6  | 4.16  | 122.00      | 111.83   |
| 1   | 2A    | 1911 | PSU  | C4-N3-C2  | -4.15 | 120.65      | 126.37   |
| 32  | 1a    | 1518 | MA6  | C5-N7-C8  | 4.11  | 109.91      | 103.45   |
| 1   | 1A    | 1939 | 5MU  | O4-C4-C5  | -4.11 | 120.22      | 124.92   |
| 1   | 1A    | 1911 | PSU  | C4-N3-C2  | -4.11 | 120.71      | 126.37   |
| 1   | 1A    | 2552 | OMU  | C5-C4-N3  | 4.06  | 120.48      | 114.80   |
| 32  | 2a    | 1518 | MA6  | C2-N1-C6  | 4.04  | 121.70      | 111.83   |
| 1   | 1A    | 1917 | PSU  | C4-N3-C2  | -4.04 | 120.81      | 126.37   |
| 1   | 2A    | 1939 | 5MU  | C5-C4-N3  | 4.02  | 118.82      | 115.32   |
| 1   | 2A    | 2552 | OMU  | O2-C2-N1  | -4.01 | 117.58      | 122.80   |
| 1   | 1A    | 2605 | PSU  | O2-C2-N1  | -4.00 | 118.67      | 122.79   |
| 1   | 2A    | 1917 | PSU  | C4-N3-C2  | -3.99 | 120.88      | 126.37   |
| 32  | 1a    | 516  | PSU  | C4-N3-C2  | -3.98 | 120.89      | 126.37   |
| 32  | 1a    | 1519 | MA6  | C2-N1-C6  | 3.97  | 121.52      | 111.83   |
| 32  | 1a    | 1207 | 2MG  | N9-C4-N3  | 3.90  | 133.76      | 125.95   |
| 32  | 2a    | 1207 | 2MG  | N9-C4-N3  | 3.90  | 133.74      | 125.95   |
| 32  | 2a    | 1519 | MA6  | N9-C8-N7  | -3.88 | 108.43      | 113.94   |
| 32  | 1a    | 1519 | MA6  | C5-N7-C8  | 3.87  | 109.54      | 103.45   |
| 32  | 2a    | 1519 | MA6  | C5-N7-C8  | 3.86  | 109.51      | 103.45   |
| 1   | 2A    | 1962 | 5MC  | C5-C6-N1  | -3.82 | 119.16      | 123.31   |
| 1   | 2A    | 1915 | 5MU  | C5-C4-N3  | 3.82  | 118.64      | 115.32   |
| 1   | 2A    | 1939 | 5MU  | O4-C4-C5  | -3.81 | 120.56      | 124.92   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 32  | 1a    | 1518 | MA6  | N9-C8-N7  | -3.80 | 108.55      | 113.94   |
| 32  | 2a    | 1518 | MA6  | C4-C5-N7  | -3.80 | 106.24      | 110.58   |
| 32  | 1a    | 1207 | 2MG  | C6-C5-N7  | 3.76  | 137.14      | 130.29   |
| 32  | 2a    | 516  | PSU  | O2-C2-N1  | -3.72 | 118.95      | 122.79   |
| 32  | 2a    | 1518 | MA6  | C5-N7-C8  | 3.70  | 109.26      | 103.45   |
| 1   | 1A    | 1942 | 5MC  | C5-C6-N1  | -3.65 | 119.35      | 123.31   |
| 1   | 2A    | 1915 | 5MU  | O4-C4-C5  | -3.61 | 120.78      | 124.92   |
| 32  | 1a    | 1400 | 5MC  | C5-C6-N1  | -3.60 | 119.40      | 123.31   |
| 1   | 2A    | 2503 | 2MA  | C4-C5-N7  | -3.60 | 106.46      | 110.58   |
| 1   | 1A    | 1917 | PSU  | O2-C2-N1  | -3.60 | 119.08      | 122.79   |
| 32  | 2a    | 967  | 5MC  | C5-C6-N1  | -3.59 | 119.41      | 123.31   |
| 1   | 1A    | 2503 | 2MA  | N6-C6-N1  | 3.57  | 121.84      | 117.03   |
| 1   | 2A    | 1915 | 5MU  | C1'-N1-C6 | -3.55 | 115.30      | 121.15   |
| 32  | 1a    | 1519 | MA6  | C4-C5-N7  | -3.54 | 106.53      | 110.58   |
| 32  | 2a    | 1400 | 5MC  | C5-C6-N1  | -3.52 | 119.48      | 123.31   |
| 1   | 2A    | 2552 | OMU  | C5-C4-N3  | 3.50  | 119.70      | 114.80   |
| 1   | 2A    | 1939 | 5MU  | C5-C6-N1  | -3.48 | 119.53      | 123.31   |
| 32  | 2a    | 966  | M2G  | C6-C5-N7  | 3.48  | 136.62      | 130.29   |
| 1   | 2A    | 1942 | 5MC  | C5-C6-N1  | -3.44 | 119.58      | 123.31   |
| 32  | 2a    | 1519 | MA6  | C2-N3-C4  | 3.43  | 120.21      | 111.83   |
| 32  | 1a    | 1518 | MA6  | C5-C4-N3  | -3.40 | 122.03      | 126.72   |
| 1   | 1A    | 2251 | OMG  | C6-C5-N7  | 3.34  | 136.38      | 130.29   |
| 32  | 1a    | 1404 | 5MC  | C5-C6-N1  | -3.32 | 119.71      | 123.31   |
| 32  | 1a    | 1518 | MA6  | C2-N3-C4  | 3.30  | 119.90      | 111.83   |
| 32  | 2a    | 1518 | MA6  | C2-N3-C4  | 3.30  | 119.89      | 111.83   |
| 32  | 1a    | 1519 | MA6  | C2-N3-C4  | 3.29  | 119.87      | 111.83   |
| 1   | 2A    | 1939 | 5MU  | O2-C2-N1  | -3.28 | 118.52      | 122.80   |
| 1   | 1A    | 1915 | 5MU  | O4-C4-C5  | -3.27 | 121.17      | 124.92   |
| 32  | 1a    | 1519 | MA6  | N9-C8-N7  | -3.27 | 109.30      | 113.94   |
| 32  | 1a    | 1518 | MA6  | C4-C5-N7  | -3.26 | 106.86      | 110.58   |
| 32  | 2a    | 1407 | 5MC  | C5-C6-N1  | -3.23 | 119.81      | 123.31   |
| 32  | 2a    | 1207 | 2MG  | C6-C5-N7  | 3.21  | 136.13      | 130.29   |
| 1   | 2A    | 1917 | PSU  | O2-C2-N1  | -3.20 | 119.49      | 122.79   |
| 1   | 1A    | 1911 | PSU  | O2-C2-N1  | -3.16 | 119.53      | 122.79   |
| 32  | 2a    | 1519 | MA6  | C4-C5-C6  | 3.13  | 119.14      | 115.91   |
| 1   | 1A    | 1939 | 5MU  | O2-C2-N1  | -3.10 | 118.76      | 122.80   |
| 32  | 1a    | 1207 | 2MG  | C4-C5-N7  | -3.08 | 105.79      | 110.67   |
| 1   | 1A    | 1962 | 5MC  | C5-C6-N1  | -3.07 | 119.98      | 123.31   |
| 1   | 2A    | 2605 | PSU  | O2-C2-N1  | -3.07 | 119.62      | 122.79   |
| 32  | 2a    | 1498 | UR3  | C5-C4-N3  | 3.05  | 119.06      | 115.04   |
| 32  | 2a    | 1404 | 5MC  | C5-C6-N1  | -3.05 | 120.00      | 123.31   |
| 32  | 2a    | 1404 | 5MC  | C5-C4-N3  | -3.03 | 118.65      | 121.75   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | 1A    | 1962 | 5MC  | C5-C4-N3    | -3.03 | 118.65      | 121.75   |
| 32  | 2a    | 1407 | 5MC  | C5-C4-N3    | -3.02 | 118.66      | 121.75   |
| 1   | 2A    | 1911 | PSU  | O2-C2-N1    | -3.02 | 119.67      | 122.79   |
| 1   | 1A    | 2503 | 2MA  | C4-C5-N7    | -3.00 | 107.15      | 110.58   |
| 32  | 1a    | 516  | PSU  | O2-C2-N1    | -2.99 | 119.71      | 122.79   |
| 32  | 2a    | 1519 | MA6  | C5-C4-N9    | 2.99  | 109.06      | 105.81   |
| 32  | 1a    | 967  | 5MC  | C5-C6-N1    | -2.97 | 120.09      | 123.31   |
| 1   | 1A    | 1915 | 5MU  | O2-C2-N3    | -2.97 | 116.02      | 121.49   |
| 32  | 1a    | 1519 | MA6  | N3-C4-N9    | 2.96  | 132.21      | 127.17   |
| 32  | 2a    | 1518 | MA6  | N9-C8-N7    | -2.96 | 109.73      | 113.94   |
| 43  | 2l    | 92   | 0TD  | OD2-CG-CB   | 2.95  | 119.52      | 113.15   |
| 32  | 1a    | 1498 | UR3  | C5-C4-N3    | 2.94  | 118.92      | 115.04   |
| 1   | 2A    | 2503 | 2MA  | N6-C6-N1    | 2.92  | 120.97      | 117.03   |
| 1   | 2A    | 2251 | OMG  | C6-C5-N7    | 2.90  | 135.57      | 130.29   |
| 32  | 1a    | 1519 | MA6  | C4-C5-C6    | 2.88  | 118.89      | 115.91   |
| 1   | 2A    | 1942 | 5MC  | C5-C4-N3    | -2.88 | 118.81      | 121.75   |
| 32  | 1a    | 1407 | 5MC  | C5-C4-N3    | -2.87 | 118.81      | 121.75   |
| 32  | 1a    | 1404 | 5MC  | C5-C4-N3    | -2.82 | 118.86      | 121.75   |
| 1   | 1A    | 2552 | OMU  | O4-C4-C5    | -2.81 | 120.31      | 125.16   |
| 32  | 2a    | 966  | M2G  | C4-C5-N7    | -2.79 | 106.25      | 110.67   |
| 32  | 1a    | 1207 | 2MG  | N1-C2-N2    | 2.73  | 119.35      | 116.56   |
| 32  | 1a    | 1407 | 5MC  | C5-C6-N1    | -2.72 | 120.36      | 123.31   |
| 1   | 2A    | 2503 | 2MA  | C5-N7-C8    | 2.70  | 107.70      | 103.45   |
| 1   | 1A    | 1915 | 5MU  | C5M-C5-C4   | 2.69  | 121.65      | 118.78   |
| 32  | 1a    | 1400 | 5MC  | C5-C4-N3    | -2.67 | 119.02      | 121.75   |
| 32  | 1a    | 966  | M2G  | C6-C5-N7    | 2.67  | 135.14      | 130.29   |
| 32  | 1a    | 967  | 5MC  | C5-C4-N3    | -2.66 | 119.03      | 121.75   |
| 32  | 2a    | 516  | PSU  | O4'-C1'-C2' | 2.66  | 108.83      | 105.15   |
| 32  | 1a    | 1518 | MA6  | N3-C4-N9    | 2.63  | 131.65      | 127.17   |
| 1   | 2A    | 2251 | OMG  | C4-C5-N7    | -2.59 | 106.56      | 110.67   |
| 32  | 2a    | 1207 | 2MG  | N1-C2-N2    | 2.56  | 119.17      | 116.56   |
| 32  | 2a    | 1207 | 2MG  | C4-C5-N7    | -2.55 | 106.63      | 110.67   |
| 1   | 2A    | 2503 | 2MA  | C4-N9-C8    | 2.55  | 108.41      | 105.74   |
| 1   | 2A    | 1920 | OMC  | O2-C2-N3    | -2.54 | 118.32      | 122.33   |
| 1   | 1A    | 2251 | OMG  | C4-C5-N7    | -2.54 | 106.64      | 110.67   |
| 1   | 1A    | 1920 | OMC  | O2-C2-N3    | -2.53 | 118.34      | 122.33   |
| 1   | 1A    | 2503 | 2MA  | C5-N7-C8    | 2.53  | 107.42      | 103.45   |
| 32  | 2a    | 1402 | 4OC  | C6-C5-C4    | 2.51  | 120.02      | 117.00   |
| 1   | 2A    | 2552 | OMU  | O4-C4-C5    | -2.51 | 120.84      | 125.16   |
| 32  | 1a    | 1518 | MA6  | C4-N9-C8    | 2.50  | 108.36      | 105.74   |
| 32  | 1a    | 1404 | 5MC  | CM5-C5-C6   | -2.49 | 119.48      | 122.85   |
| 32  | 2a    | 967  | 5MC  | C5-C4-N3    | -2.49 | 119.20      | 121.75   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 32  | 2a    | 1519 | MA6  | N3-C4-N9    | 2.49  | 131.40      | 127.17   |
| 1   | 1A    | 2605 | PSU  | C5-C6-N1    | -2.48 | 118.70      | 122.14   |
| 32  | 2a    | 1404 | 5MC  | CM5-C5-C6   | -2.47 | 119.51      | 122.85   |
| 1   | 1A    | 1942 | 5MC  | C5-C4-N3    | -2.46 | 119.24      | 121.75   |
| 1   | 1A    | 2503 | 2MA  | C4-N9-C8    | 2.45  | 108.31      | 105.74   |
| 32  | 2a    | 1400 | 5MC  | C5-C4-N3    | -2.43 | 119.26      | 121.75   |
| 1   | 1A    | 1915 | 5MU  | C5-C6-N1    | -2.41 | 120.69      | 123.31   |
| 32  | 1a    | 1400 | 5MC  | O2-C2-N3    | -2.40 | 118.55      | 122.33   |
| 32  | 2a    | 516  | PSU  | C5-C6-N1    | -2.39 | 118.82      | 122.14   |
| 1   | 2A    | 1915 | 5MU  | C5-C6-N1    | -2.38 | 120.73      | 123.31   |
| 1   | 2A    | 1915 | 5MU  | O2-C2-N3    | -2.38 | 117.11      | 121.49   |
| 32  | 2a    | 527  | G7M  | O6-C6-C5    | -2.37 | 122.73      | 128.01   |
| 32  | 2a    | 1518 | MA6  | N3-C4-N9    | 2.36  | 131.19      | 127.17   |
| 32  | 1a    | 1207 | 2MG  | O3'-C3'-C2' | 2.36  | 119.37      | 111.82   |
| 32  | 2a    | 1518 | MA6  | C4-C5-C6    | 2.34  | 118.33      | 115.91   |
| 32  | 2a    | 527  | G7M  | C5-C6-N1    | 2.30  | 116.59      | 111.84   |
| 1   | 1A    | 2503 | 2MA  | C2-N1-C6    | 2.29  | 121.62      | 118.10   |
| 32  | 1a    | 1402 | 4OC  | C6-C5-C4    | 2.28  | 119.75      | 117.00   |
| 32  | 2a    | 1407 | 5MC  | O2-C2-N3    | -2.27 | 118.76      | 122.33   |
| 32  | 1a    | 516  | PSU  | C6-C5-C4    | -2.25 | 116.65      | 118.17   |
| 43  | 2l    | 92   | 0TD  | OD1-CG-CB   | -2.22 | 117.79      | 122.44   |
| 32  | 1a    | 1207 | 2MG  | N2-C2-N3    | -2.21 | 117.70      | 120.51   |
| 1   | 1A    | 1962 | 5MC  | O2-C2-N3    | -2.21 | 118.85      | 122.33   |
| 32  | 1a    | 966  | M2G  | O6-C6-C5    | -2.21 | 120.71      | 126.53   |
| 1   | 1A    | 1911 | PSU  | C5-C6-N1    | -2.19 | 119.10      | 122.14   |
| 32  | 2a    | 1400 | 5MC  | C1'-N1-C6   | -2.18 | 117.57      | 121.15   |
| 1   | 2A    | 2251 | OMG  | O6-C6-C5    | -2.16 | 120.83      | 126.53   |
| 32  | 1a    | 516  | PSU  | O4'-C1'-C2' | 2.16  | 108.14      | 105.15   |
| 1   | 1A    | 2251 | OMG  | C5-C6-N1    | 2.15  | 118.73      | 113.25   |
| 32  | 1a    | 966  | M2G  | C4-C5-N7    | -2.15 | 107.26      | 110.67   |
| 1   | 1A    | 2552 | OMU  | CM2-O2'-C2' | -2.14 | 108.98      | 114.47   |
| 32  | 1a    | 1498 | UR3  | C6-N1-C2    | -2.13 | 120.06      | 121.80   |
| 1   | 2A    | 1962 | 5MC  | C5-C4-N3    | -2.12 | 119.58      | 121.75   |
| 1   | 1A    | 2552 | OMU  | O2-C2-N1    | -2.10 | 120.06      | 122.80   |
| 1   | 2A    | 1911 | PSU  | C5-C6-N1    | -2.10 | 119.23      | 122.14   |
| 32  | 1a    | 1407 | 5MC  | O2-C2-N3    | -2.09 | 119.04      | 122.33   |
| 32  | 1a    | 527  | G7M  | O6-C6-C5    | -2.09 | 123.35      | 128.01   |
| 32  | 1a    | 1498 | UR3  | C3U-N3-C4   | 2.08  | 120.75      | 117.87   |
| 32  | 2a    | 1207 | 2MG  | N2-C2-N3    | -2.08 | 117.86      | 120.51   |
| 32  | 2a    | 1400 | 5MC  | CM5-C5-C6   | -2.06 | 120.07      | 122.85   |
| 1   | 1A    | 1911 | PSU  | O4'-C1'-C2' | 2.05  | 107.99      | 105.15   |
| 1   | 1A    | 1917 | PSU  | C5-C6-N1    | -2.05 | 119.29      | 122.14   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1   | 2A    | 1917 | PSU  | C5-C6-N1  | -2.05 | 119.29      | 122.14   |
| 1   | 1A    | 2251 | OMG  | O6-C6-C5  | -2.05 | 121.13      | 126.53   |
| 1   | 2A    | 2605 | PSU  | C5-C6-N1  | -2.04 | 119.30      | 122.14   |
| 1   | 1A    | 1915 | 5MU  | C5M-C5-C6 | -2.04 | 120.10      | 122.85   |
| 1   | 2A    | 2503 | 2MA  | C2-N1-C6  | 2.03  | 121.22      | 118.10   |
| 1   | 2A    | 2503 | 2MA  | N9-C8-N7  | -2.03 | 111.06      | 113.94   |
| 1   | 2A    | 1942 | 5MC  | CM5-C5-C6 | -2.03 | 120.11      | 122.85   |
| 32  | 1a    | 1207 | 2MG  | C8-N7-C5  | 2.02  | 107.86      | 104.26   |

There are no chirality outliers.

All (36) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 1   | 1A    | 1915 | 5MU  | O4'-C1'-N1-C2   |
| 1   | 1A    | 1915 | 5MU  | O4'-C1'-N1-C6   |
| 32  | 1a    | 1207 | 2MG  | N1-C2-N2-CM2    |
| 32  | 1a    | 1207 | 2MG  | N3-C2-N2-CM2    |
| 43  | 1l    | 92   | 0TD  | O-C-CA-CB       |
| 1   | 2A    | 1915 | 5MU  | O4'-C1'-N1-C2   |
| 1   | 2A    | 1915 | 5MU  | O4'-C1'-N1-C6   |
| 1   | 1A    | 1915 | 5MU  | O4'-C4'-C5'-O5' |
| 1   | 1A    | 1917 | PSU  | O4'-C4'-C5'-O5' |
| 32  | 1a    | 1402 | 4OC  | O4'-C4'-C5'-O5' |
| 32  | 1a    | 1519 | MA6  | O4'-C4'-C5'-O5' |
| 32  | 2a    | 1402 | 4OC  | O4'-C4'-C5'-O5' |
| 32  | 2a    | 1519 | MA6  | O4'-C4'-C5'-O5' |
| 1   | 1A    | 1915 | 5MU  | C3'-C4'-C5'-O5' |
| 1   | 1A    | 1917 | PSU  | C3'-C4'-C5'-O5' |
| 32  | 1a    | 1402 | 4OC  | C3'-C4'-C5'-O5' |
| 32  | 2a    | 1402 | 4OC  | C3'-C4'-C5'-O5' |
| 32  | 1a    | 1519 | MA6  | C3'-C4'-C5'-O5' |
| 32  | 2a    | 527  | G7M  | C3'-C4'-C5'-O5' |
| 32  | 2a    | 1519 | MA6  | C3'-C4'-C5'-O5' |
| 43  | 2l    | 92   | 0TD  | CG-CB-SB-CSB    |
| 1   | 2A    | 1920 | OMC  | O4'-C4'-C5'-O5' |
| 43  | 1l    | 92   | 0TD  | SB-CB-CG-OD1    |
| 43  | 2l    | 92   | 0TD  | SB-CB-CG-OD1    |
| 32  | 2a    | 516  | PSU  | O4'-C1'-C5-C4   |
| 32  | 1a    | 1207 | 2MG  | C3'-C4'-C5'-O5' |
| 32  | 1a    | 527  | G7M  | C3'-C4'-C5'-O5' |
| 32  | 2a    | 1402 | 4OC  | C3'-C2'-O2'-CM2 |
| 1   | 2A    | 2503 | 2MA  | O4'-C4'-C5'-O5' |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 1   | 1A    | 2503 | 2MA  | O4'-C4'-C5'-O5' |
| 1   | 1A    | 2503 | 2MA  | C4'-C5'-O5'-P   |
| 43  | 1l    | 92   | 0TD  | CG-CB-SB-CSB    |
| 1   | 1A    | 1920 | OMC  | C2'-C1'-N1-C2   |
| 1   | 1A    | 2251 | OMG  | C4'-C5'-O5'-P   |
| 32  | 1a    | 527  | G7M  | C4'-C5'-O5'-P   |
| 1   | 2A    | 2503 | 2MA  | C4'-C5'-O5'-P   |

There are no ring outliers.

13 monomers are involved in 18 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 32  | 1a    | 1518 | MA6  | 2       | 0            |
| 32  | 1a    | 1402 | 4OC  | 1       | 0            |
| 1   | 1A    | 1939 | 5MU  | 2       | 0            |
| 32  | 2a    | 1519 | MA6  | 1       | 0            |
| 1   | 1A    | 1920 | OMC  | 1       | 0            |
| 32  | 2a    | 1400 | 5MC  | 1       | 0            |
| 32  | 1a    | 1519 | MA6  | 2       | 0            |
| 32  | 2a    | 1402 | 4OC  | 2       | 0            |
| 1   | 2A    | 1962 | 5MC  | 1       | 0            |
| 32  | 1a    | 966  | M2G  | 1       | 0            |
| 32  | 1a    | 1207 | 2MG  | 3       | 0            |
| 32  | 2a    | 1518 | MA6  | 3       | 0            |
| 1   | 1A    | 1962 | 5MC  | 1       | 0            |

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 2583 ligands modelled in this entry, 2571 are monoatomic - leaving 12 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 |
| 56  | MPD   | 2B    | 220  | -    | 7,7,7        | 0.33 | 0        | 9,10,10     | 0.29 | 0        |
| 59  | SF4   | 2d    | 501  | 35   | 0,12,12      | -    | -        | -           |      |          |
| 56  | MPD   | 18    | 104  | -    | 7,7,7        | 0.37 | 0        | 9,10,10     | 0.48 | 0        |
| 56  | MPD   | 1O    | 203  | -    | 7,7,7        | 0.35 | 0        | 9,10,10     | 0.25 | 0        |
| 56  | MPD   | 2A    | 3759 | -    | 7,7,7        | 0.34 | 0        | 9,10,10     | 0.25 | 0        |
| 59  | SF4   | 1d    | 306  | 35   | 0,12,12      | -    | -        | -           |      |          |
| 57  | ARG   | 1B    | 231  | -    | 10,11,11     | 0.74 | 1 (10%)  | 9,13,13     | 0.89 | 1 (11%)  |
| 56  | MPD   | 1a    | 1883 | 32   | 7,7,7        | 0.37 | 0        | 9,10,10     | 0.72 | 0        |
| 56  | MPD   | 1A    | 4051 | -    | 7,7,7        | 0.33 | 0        | 9,10,10     | 0.18 | 0        |
| 55  | A1CQ5 | 2A    | 3757 | -    | 48,49,49     | 2.67 | 10 (20%) | 64,73,73    | 2.19 | 20 (31%) |
| 56  | MPD   | 2A    | 3758 | -    | 7,7,7        | 0.30 | 0        | 9,10,10     | 0.38 | 0        |
| 55  | A1CQ5 | 1A    | 4050 | -    | 48,49,49     | 2.74 | 10 (20%) | 64,73,73    | 2.18 | 19 (29%) |

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   |
|-----|-------|-------|------|------|---------|------------|---------|
| 56  | MPD   | 2B    | 220  | -    | -       | 1/5/5/5    | -       |
| 59  | SF4   | 2d    | 501  | 35   | -       | -          | 0/6/5/5 |
| 56  | MPD   | 18    | 104  | -    | -       | 3/5/5/5    | -       |
| 56  | MPD   | 1O    | 203  | -    | -       | 3/5/5/5    | -       |
| 56  | MPD   | 2A    | 3759 | -    | -       | 3/5/5/5    | -       |
| 59  | SF4   | 1d    | 306  | 35   | -       | -          | 0/6/5/5 |
| 57  | ARG   | 1B    | 231  | -    | -       | 4/11/11/11 | -       |
| 56  | MPD   | 1a    | 1883 | 32   | -       | 2/5/5/5    | -       |
| 56  | MPD   | 1A    | 4051 | -    | -       | 1/5/5/5    | -       |
| 55  | A1CQ5 | 2A    | 3757 | -    | -       | 4/24/86/86 | 0/5/5/5 |
| 56  | MPD   | 2A    | 3758 | -    | -       | 1/5/5/5    | -       |
| 55  | A1CQ5 | 1A    | 4050 | -    | -       | 5/24/86/86 | 0/5/5/5 |

All (21) bond length outliers are listed below:

| Mol | Chain | Res  | Type  | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|-------|---------|--------|-------------|----------|
| 55  | 2A    | 3757 | A1CQ5 | CBG-CBE | -10.86 | 1.31        | 1.47     |
| 55  | 1A    | 4050 | A1CQ5 | CBG-CBE | -10.51 | 1.32        | 1.47     |
| 55  | 1A    | 4050 | A1CQ5 | CAA-CAQ | -8.83  | 1.40        | 1.53     |
| 55  | 1A    | 4050 | A1CQ5 | CAT-CAQ | -8.67  | 1.37        | 1.51     |
| 55  | 2A    | 3757 | A1CQ5 | CAA-CAQ | -7.99  | 1.41        | 1.53     |

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| Mol | Chain | Res  | Type  | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|-------|---------|-------|-------------|----------|
| 55  | 2A    | 3757 | A1CQ5 | CAT-CAQ | -7.82 | 1.38        | 1.51     |
| 55  | 1A    | 4050 | A1CQ5 | OAU-CAC | -4.65 | 1.38        | 1.46     |
| 55  | 2A    | 3757 | A1CQ5 | OAU-CAC | -3.80 | 1.40        | 1.46     |
| 55  | 2A    | 3757 | A1CQ5 | CBF-CBE | -3.36 | 1.31        | 1.37     |
| 55  | 2A    | 3757 | A1CQ5 | CAH-CAI | -3.33 | 1.52        | 1.56     |
| 55  | 1A    | 4050 | A1CQ5 | CBF-CBE | -3.29 | 1.31        | 1.37     |
| 55  | 2A    | 3757 | A1CQ5 | CAS-CAD | -3.16 | 1.48        | 1.54     |
| 55  | 1A    | 4050 | A1CQ5 | CAS-CAD | -3.15 | 1.48        | 1.54     |
| 55  | 2A    | 3757 | A1CQ5 | CAF-CAG | -3.11 | 1.49        | 1.53     |
| 55  | 1A    | 4050 | A1CQ5 | CAF-CAG | -3.02 | 1.49        | 1.53     |
| 55  | 1A    | 4050 | A1CQ5 | CAH-CAI | -2.89 | 1.53        | 1.56     |
| 55  | 2A    | 3757 | A1CQ5 | CBE-NBD | -2.84 | 1.31        | 1.36     |
| 55  | 1A    | 4050 | A1CQ5 | CBE-NBD | -2.79 | 1.31        | 1.36     |
| 55  | 2A    | 3757 | A1CQ5 | CAB-CAC | -2.68 | 1.54        | 1.56     |
| 55  | 1A    | 4050 | A1CQ5 | CAB-CAC | -2.38 | 1.54        | 1.56     |
| 57  | 1B    | 231  | ARG   | OXT-C   | -2.13 | 1.23        | 1.30     |

All (40) bond angle outliers are listed below:

| Mol | Chain | Res  | Type  | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|-------|-------------|-------|-------------|----------|
| 55  | 2A    | 3757 | A1CQ5 | CAK-CAC-CAB | -8.29 | 107.38      | 116.28   |
| 55  | 1A    | 4050 | A1CQ5 | CAK-CAC-CAB | -8.04 | 107.65      | 116.28   |
| 55  | 1A    | 4050 | A1CQ5 | CAZ-CAB-CAC | -5.15 | 103.55      | 108.81   |
| 55  | 2A    | 3757 | A1CQ5 | CAZ-CAB-CAC | -4.91 | 103.79      | 108.81   |
| 55  | 1A    | 4050 | A1CQ5 | CAC-OAU-CAV | -4.21 | 110.37      | 118.03   |
| 55  | 1A    | 4050 | A1CQ5 | CAD-CAA-CAB | -4.04 | 112.49      | 117.94   |
| 55  | 2A    | 3757 | A1CQ5 | CAD-CAA-CAB | -4.02 | 112.52      | 117.94   |
| 55  | 2A    | 3757 | A1CQ5 | CAE-CAF-CAG | -3.99 | 107.23      | 112.38   |
| 55  | 2A    | 3757 | A1CQ5 | CAG-CAB-CAC | 3.88  | 114.76      | 112.13   |
| 55  | 1A    | 4050 | A1CQ5 | CAE-CAF-CAG | -3.82 | 107.45      | 112.38   |
| 55  | 1A    | 4050 | A1CQ5 | CAF-CAG-CAB | -3.80 | 107.34      | 111.57   |
| 55  | 2A    | 3757 | A1CQ5 | CAF-CAG-CAB | -3.65 | 107.50      | 111.57   |
| 55  | 1A    | 4050 | A1CQ5 | CBG-CBE-CBF | -3.61 | 124.14      | 129.65   |
| 55  | 2A    | 3757 | A1CQ5 | CBF-CBE-NBD | 3.42  | 111.15      | 107.85   |
| 55  | 1A    | 4050 | A1CQ5 | CAE-CAD-CAA | 3.34  | 112.61      | 106.82   |
| 55  | 2A    | 3757 | A1CQ5 | CBG-CBE-CBF | -3.26 | 124.66      | 129.65   |
| 55  | 1A    | 4050 | A1CQ5 | CAG-CAB-CAC | 3.24  | 114.33      | 112.13   |
| 55  | 1A    | 4050 | A1CQ5 | CBE-NBD-NBC | -3.23 | 105.77      | 109.23   |
| 55  | 1A    | 4050 | A1CQ5 | CBF-CBE-NBD | 3.17  | 110.90      | 107.85   |
| 55  | 2A    | 3757 | A1CQ5 | CBE-NBD-NBC | -3.16 | 105.85      | 109.23   |
| 55  | 2A    | 3757 | A1CQ5 | OAR-CAQ-CAT | -3.11 | 121.07      | 125.52   |
| 55  | 2A    | 3757 | A1CQ5 | OAU-CAC-CAB | 3.11  | 111.17      | 106.32   |

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| Mol | Chain | Res  | Type  | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|-------|-------------|-------|-------------|----------|
| 55  | 1A    | 4050 | A1CQ5 | OAU-CAC-CAB | 3.00  | 111.00      | 106.32   |
| 55  | 2A    | 3757 | A1CQ5 | CBA-NBB-NBC | 2.97  | 126.75      | 120.78   |
| 55  | 2A    | 3757 | A1CQ5 | CAC-OAU-CAV | -2.90 | 112.75      | 118.03   |
| 55  | 2A    | 3757 | A1CQ5 | CAE-CAD-CAA | 2.88  | 111.80      | 106.82   |
| 55  | 1A    | 4050 | A1CQ5 | OAR-CAQ-CAT | -2.78 | 121.54      | 125.52   |
| 55  | 2A    | 3757 | A1CQ5 | CAT-CAQ-CAA | 2.68  | 111.38      | 108.53   |
| 55  | 1A    | 4050 | A1CQ5 | OAM-CAI-CAH | -2.57 | 107.54      | 110.91   |
| 55  | 1A    | 4050 | A1CQ5 | CBF-NBB-NBC | -2.55 | 108.28      | 110.75   |
| 55  | 1A    | 4050 | A1CQ5 | OAU-CAV-CAW | 2.54  | 114.70      | 110.52   |
| 57  | 1B    | 231  | ARG   | OXT-C-O     | -2.42 | 118.58      | 124.08   |
| 55  | 1A    | 4050 | A1CQ5 | CAD-CAH-CAI | -2.40 | 110.23      | 112.46   |
| 55  | 2A    | 3757 | A1CQ5 | CAL-CAH-CAI | -2.38 | 110.29      | 112.20   |
| 55  | 2A    | 3757 | A1CQ5 | CBF-NBB-NBC | -2.30 | 108.51      | 110.75   |
| 55  | 2A    | 3757 | A1CQ5 | CBA-NBB-CBF | -2.19 | 124.73      | 128.83   |
| 55  | 1A    | 4050 | A1CQ5 | CBA-NBB-NBC | 2.18  | 125.15      | 120.78   |
| 55  | 2A    | 3757 | A1CQ5 | OAU-CAV-CAW | 2.17  | 114.09      | 110.52   |
| 55  | 1A    | 4050 | A1CQ5 | CAT-CAQ-CAA | 2.11  | 110.77      | 108.53   |
| 55  | 2A    | 3757 | A1CQ5 | CAL-CAH-CAD | -2.11 | 108.51      | 111.23   |

There are no chirality outliers.

All (27) torsion outliers are listed below:

| Mol | Chain | Res  | Type  | Atoms           |
|-----|-------|------|-------|-----------------|
| 55  | 1A    | 4050 | A1CQ5 | CAV-CAW-SAY-CBM |
| 55  | 1A    | 4050 | A1CQ5 | CBN-CBM-SAY-CAW |
| 55  | 2A    | 3757 | A1CQ5 | CAV-CAW-SAY-CBM |
| 56  | 1O    | 203  | MPD   | CM-C2-C3-C4     |
| 56  | 1a    | 1883 | MPD   | C2-C3-C4-O4     |
| 57  | 1B    | 231  | ARG   | N-CA-CB-CG      |
| 55  | 1A    | 4050 | A1CQ5 | SAY-CBM-CBN-NBO |
| 55  | 2A    | 3757 | A1CQ5 | SAY-CBM-CBN-NBO |
| 55  | 2A    | 3757 | A1CQ5 | CBR-CBP-NBO-CBN |
| 55  | 2A    | 3757 | A1CQ5 | CBR-CBP-NBO-CBQ |
| 56  | 1O    | 203  | MPD   | O2-C2-C3-C4     |
| 56  | 2A    | 3759 | MPD   | O2-C2-C3-C4     |
| 56  | 1O    | 203  | MPD   | C1-C2-C3-C4     |
| 56  | 2A    | 3759 | MPD   | C1-C2-C3-C4     |
| 56  | 2A    | 3759 | MPD   | CM-C2-C3-C4     |
| 56  | 1A    | 4051 | MPD   | C2-C3-C4-C5     |
| 56  | 1a    | 1883 | MPD   | C2-C3-C4-C5     |
| 57  | 1B    | 231  | ARG   | O-C-CA-CB       |
| 57  | 1B    | 231  | ARG   | OXT-C-CA-CB     |

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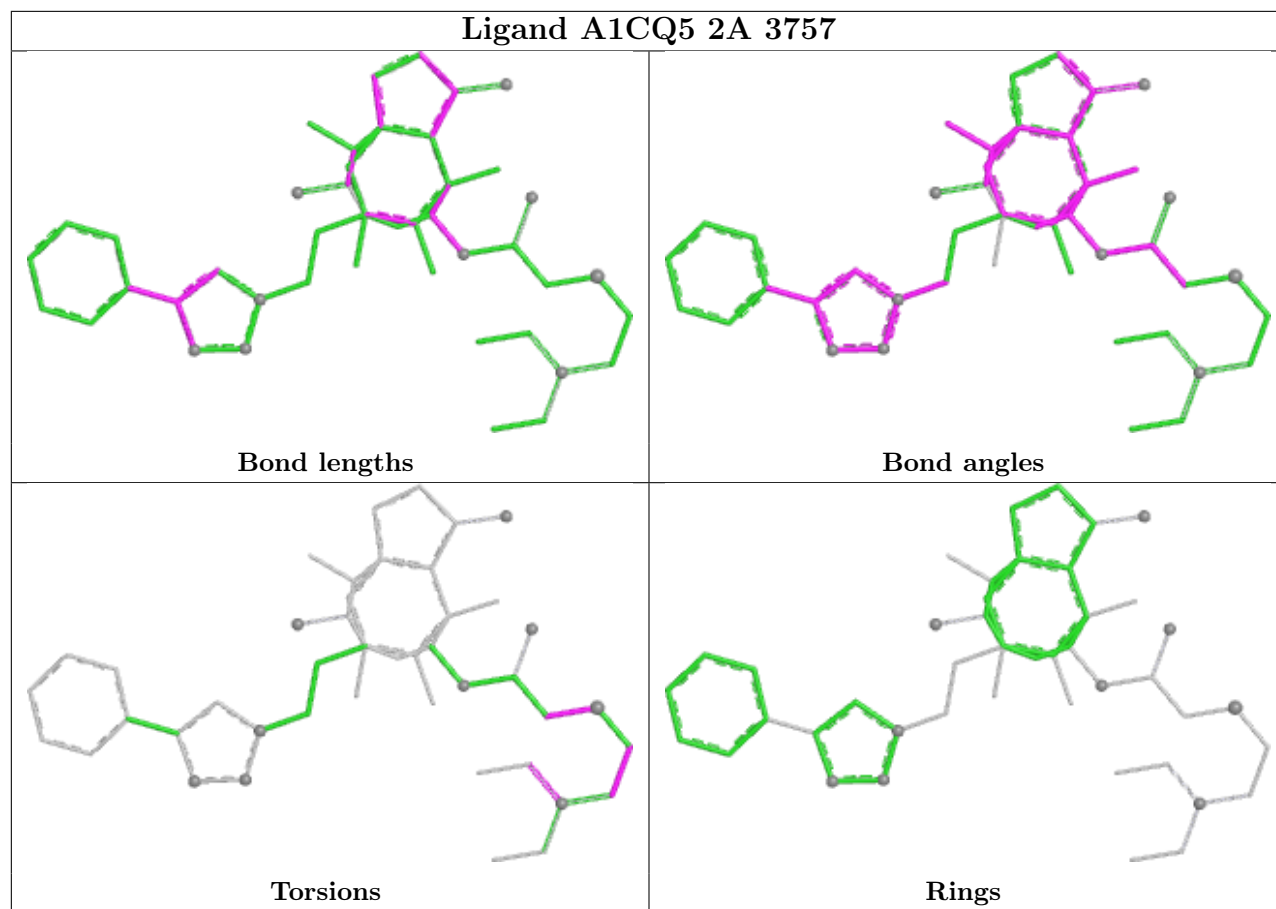
| Mol | Chain | Res  | Type  | Atoms           |
|-----|-------|------|-------|-----------------|
| 57  | 1B    | 231  | ARG   | C-CA-CB-CG      |
| 55  | 1A    | 4050 | A1CQ5 | CBM-CBN-NBO-CBP |
| 55  | 1A    | 4050 | A1CQ5 | CBM-CBN-NBO-CBQ |
| 56  | 18    | 104  | MPD   | C2-C3-C4-O4     |
| 56  | 2A    | 3758 | MPD   | C2-C3-C4-O4     |
| 56  | 2B    | 220  | MPD   | C2-C3-C4-O4     |
| 56  | 18    | 104  | MPD   | C1-C2-C3-C4     |
| 56  | 18    | 104  | MPD   | CM-C2-C3-C4     |

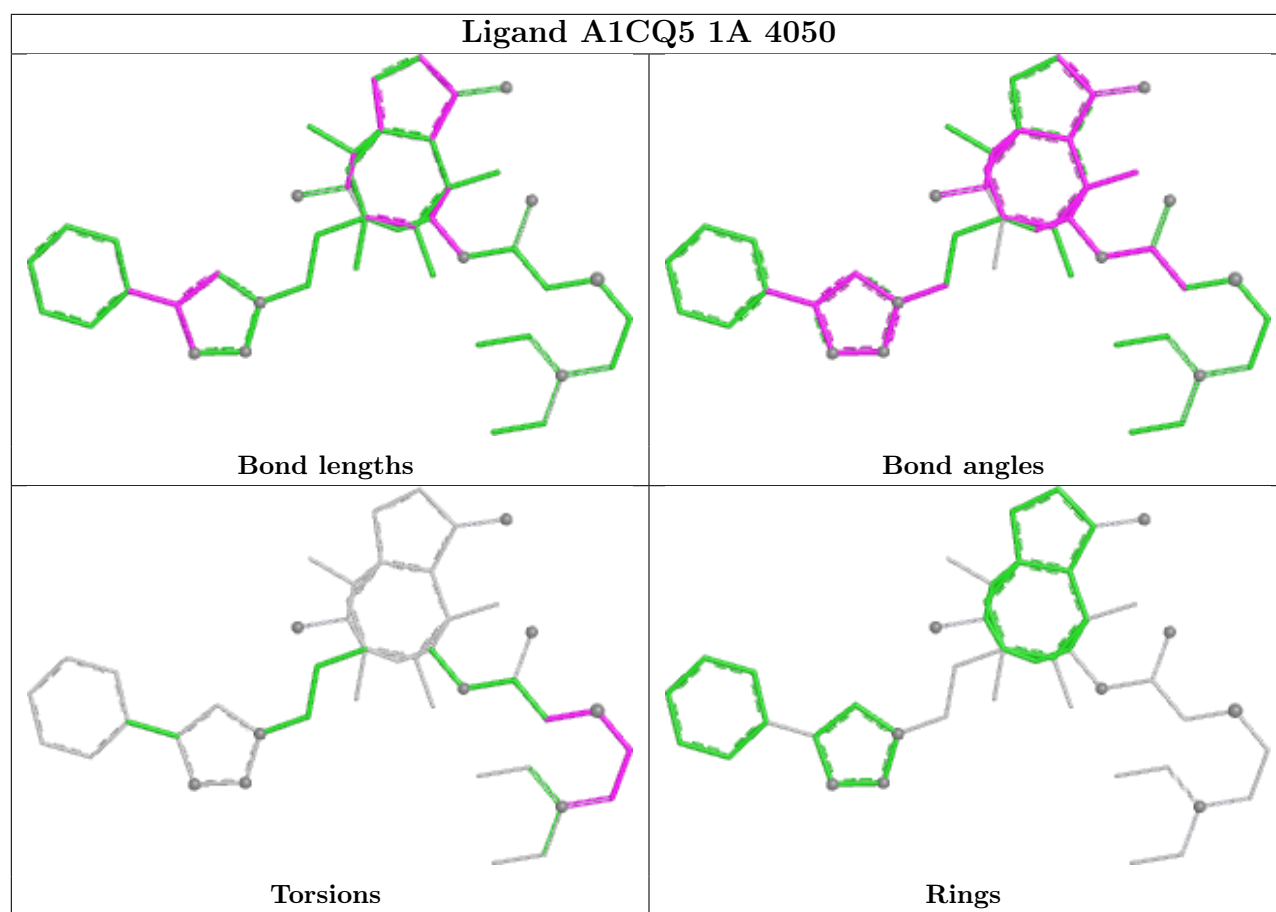
There are no ring outliers.

5 monomers are involved in 17 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 59  | 2d    | 501  | SF4  | 2       | 0            |
| 56  | 18    | 104  | MPD  | 4       | 0            |
| 57  | 1B    | 231  | ARG  | 3       | 0            |
| 56  | 1a    | 1883 | MPD  | 5       | 0            |
| 56  | 2A    | 3758 | MPD  | 3       | 0            |

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





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|----------------|-----------------------|-------|
| 1   | 1A    | 2861/2915 (98%) | -0.60  | 106 (3%) 45 35 | 12, 29, 92, 107       | 0     |
| 1   | 2A    | 2856/2915 (97%) | -0.22  | 119 (4%) 40 32 | 25, 49, 95, 110       | 0     |
| 2   | 1B    | 120/121 (99%)   | -0.52  | 0 100 100      | 24, 46, 60, 77        | 0     |
| 2   | 2B    | 120/121 (99%)   | 0.22   | 1 (0%) 82 78   | 53, 73, 83, 91        | 0     |
| 3   | 1D    | 275/276 (99%)   | -0.48  | 1 (0%) 88 87   | 13, 29, 44, 63        | 0     |
| 3   | 2D    | 275/276 (99%)   | -0.11  | 4 (1%) 72 65   | 24, 43, 56, 72        | 0     |
| 4   | 1E    | 204/206 (99%)   | -0.41  | 0 100 100      | 12, 32, 52, 66        | 0     |
| 4   | 2E    | 204/206 (99%)   | -0.01  | 2 (0%) 79 74   | 27, 49, 65, 77        | 0     |
| 5   | 1F    | 203/210 (96%)   | -0.34  | 1 (0%) 87 85   | 11, 32, 59, 78        | 0     |
| 5   | 2F    | 203/210 (96%)   | 0.04   | 0 100 100      | 26, 55, 73, 84        | 0     |
| 6   | 1G    | 181/182 (99%)   | 0.29   | 3 (1%) 69 63   | 42, 62, 77, 87        | 0     |
| 6   | 2G    | 181/182 (99%)   | 1.06   | 19 (10%) 11 9  | 68, 80, 88, 92        | 0     |
| 7   | 1H    | 174/180 (96%)   | -0.14  | 1 (0%) 85 82   | 30, 45, 60, 65        | 0     |
| 7   | 2H    | 173/180 (96%)   | 0.71   | 4 (2%) 61 52   | 62, 75, 85, 92        | 0     |
| 8   | 1I    | 147/148 (99%)   | 0.38   | 3 (2%) 65 57   | 37, 65, 75, 79        | 0     |
| 8   | 2I    | 146/148 (98%)   | 1.11   | 27 (18%) 3 3   | 45, 75, 90, 98        | 0     |
| 9   | 1N    | 140/140 (100%)  | -0.43  | 0 100 100      | 18, 30, 53, 69        | 0     |
| 9   | 2N    | 140/140 (100%)  | 0.10   | 0 100 100      | 36, 55, 70, 78        | 0     |
| 10  | 1O    | 122/122 (100%)  | -0.44  | 0 100 100      | 19, 30, 46, 55        | 0     |
| 10  | 2O    | 122/122 (100%)  | -0.16  | 0 100 100      | 35, 46, 59, 69        | 0     |
| 11  | 1P    | 149/150 (99%)   | -0.33  | 1 (0%) 84 80   | 14, 36, 58, 73        | 0     |
| 11  | 2P    | 149/150 (99%)   | 0.20   | 1 (0%) 84 80   | 30, 58, 78, 82        | 0     |
| 12  | 1Q    | 141/141 (100%)  | -0.41  | 0 100 100      | 17, 32, 47, 63        | 0     |
| 12  | 2Q    | 141/141 (100%)  | 0.21   | 3 (2%) 63 55   | 38, 55, 67, 75        | 0     |

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| Mol | Chain | Analysed       | <RSRZ> | #RSRZ>2      | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|----------------|--------|--------------|-----------------------|-------|
| 13  | 1R    | 118/118 (100%) | -0.49  | 0 100 100    | 17, 27, 40, 53        | 0     |
| 13  | 2R    | 118/118 (100%) | -0.15  | 0 100 100    | 32, 44, 56, 67        | 0     |
| 14  | 1S    | 110/112 (98%)  | -0.12  | 1 (0%) 81 76 | 32, 45, 57, 64        | 0     |
| 14  | 2S    | 110/112 (98%)  | 0.79   | 3 (2%) 56 47 | 59, 68, 78, 82        | 0     |
| 15  | 1T    | 131/146 (89%)  | -0.12  | 4 (3%) 51 43 | 27, 36, 61, 73        | 0     |
| 15  | 2T    | 131/146 (89%)  | 0.05   | 0 100 100    | 41, 51, 68, 75        | 0     |
| 16  | 1U    | 116/118 (98%)  | -0.50  | 1 (0%) 81 76 | 13, 23, 41, 60        | 0     |
| 16  | 2U    | 116/118 (98%)  | 0.17   | 1 (0%) 81 76 | 31, 51, 67, 72        | 0     |
| 17  | 1V    | 101/101 (100%) | -0.52  | 0 100 100    | 17, 32, 51, 61        | 0     |
| 17  | 2V    | 101/101 (100%) | 0.12   | 1 (0%) 79 74 | 30, 60, 72, 80        | 0     |
| 18  | 1W    | 112/113 (99%)  | -0.55  | 0 100 100    | 14, 21, 44, 79        | 0     |
| 18  | 2W    | 112/113 (99%)  | -0.17  | 0 100 100    | 30, 40, 58, 78        | 0     |
| 19  | 1X    | 95/96 (98%)    | -0.35  | 0 100 100    | 20, 29, 50, 62        | 0     |
| 19  | 2X    | 95/96 (98%)    | 0.26   | 1 (1%) 78 73 | 38, 51, 66, 75        | 0     |
| 20  | 1Y    | 107/110 (97%)  | -0.03  | 1 (0%) 81 76 | 28, 43, 62, 70        | 0     |
| 20  | 2Y    | 107/110 (97%)  | 0.73   | 6 (5%) 30 22 | 47, 63, 76, 85        | 0     |
| 21  | 1Z    | 203/206 (98%)  | 0.12   | 1 (0%) 87 85 | 34, 51, 69, 80        | 0     |
| 21  | 2Z    | 201/206 (97%)  | 0.52   | 1 (0%) 87 85 | 60, 70, 81, 88        | 0     |
| 22  | 10    | 77/85 (90%)    | -0.39  | 0 100 100    | 19, 31, 46, 64        | 0     |
| 22  | 20    | 77/85 (90%)    | 0.29   | 0 100 100    | 40, 54, 66, 70        | 0     |
| 23  | 11    | 97/98 (98%)    | -0.18  | 2 (2%) 63 55 | 20, 36, 62, 69        | 0     |
| 23  | 21    | 97/98 (98%)    | 0.09   | 2 (2%) 63 55 | 31, 49, 70, 76        | 0     |
| 24  | 12    | 70/72 (97%)    | -0.16  | 1 (1%) 73 67 | 26, 39, 50, 74        | 0     |
| 24  | 22    | 70/72 (97%)    | 0.31   | 2 (2%) 53 45 | 50, 61, 70, 74        | 0     |
| 25  | 13    | 59/60 (98%)    | -0.39  | 0 100 100    | 20, 28, 56, 74        | 0     |
| 25  | 23    | 59/60 (98%)    | 0.10   | 1 (1%) 69 63 | 44, 52, 70, 74        | 0     |
| 26  | 14    | 69/71 (97%)    | 0.67   | 5 (7%) 21 15 | 62, 79, 92, 97        | 0     |
| 26  | 24    | 69/71 (97%)    | 1.44   | 15 (21%) 2 2 | 78, 88, 98, 105       | 0     |
| 27  | 15    | 59/60 (98%)    | -0.41  | 0 100 100    | 13, 26, 56, 64        | 0     |
| 27  | 25    | 59/60 (98%)    | -0.19  | 0 100 100    | 27, 46, 67, 69        | 0     |
| 28  | 16    | 53/54 (98%)    | -0.34  | 0 100 100    | 27, 36, 50, 55        | 0     |

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| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 28  | 26    | 53/54 (98%)     | 0.16   | 0 100 100     | 46, 54, 64, 68        | 0     |
| 29  | 17    | 48/49 (97%)     | -0.36  | 2 (4%) 40 32  | 13, 19, 53, 63        | 0     |
| 29  | 27    | 48/49 (97%)     | -0.08  | 2 (4%) 40 32  | 23, 34, 60, 68        | 0     |
| 30  | 18    | 64/65 (98%)     | -0.46  | 0 100 100     | 18, 25, 34, 41        | 0     |
| 30  | 28    | 64/65 (98%)     | 0.21   | 1 (1%) 70 64  | 38, 45, 55, 61        | 0     |
| 31  | 19    | 37/37 (100%)    | -0.16  | 0 100 100     | 25, 35, 51, 61        | 0     |
| 31  | 29    | 37/37 (100%)    | 0.84   | 3 (8%) 18 13  | 52, 62, 69, 72        | 0     |
| 32  | 1a    | 1488/1521 (97%) | 0.22   | 37 (2%) 58 49 | 28, 70, 93, 108       | 0     |
| 32  | 2a    | 1492/1521 (98%) | 0.25   | 38 (2%) 58 49 | 38, 70, 94, 108       | 0     |
| 33  | 1b    | 231/256 (90%)   | 0.93   | 19 (8%) 17 13 | 61, 76, 86, 91        | 0     |
| 33  | 2b    | 231/256 (90%)   | 1.02   | 23 (9%) 12 10 | 62, 78, 87, 95        | 0     |
| 34  | 1c    | 206/239 (86%)   | 0.76   | 10 (4%) 35 27 | 62, 76, 85, 92        | 0     |
| 34  | 2c    | 206/239 (86%)   | 0.94   | 12 (5%) 29 21 | 68, 80, 86, 92        | 0     |
| 35  | 1d    | 208/209 (99%)   | 0.80   | 13 (6%) 26 19 | 53, 69, 79, 85        | 0     |
| 35  | 2d    | 208/209 (99%)   | 0.73   | 7 (3%) 48 38  | 56, 67, 77, 83        | 0     |
| 36  | 1e    | 148/162 (91%)   | 0.34   | 2 (1%) 73 67  | 42, 62, 71, 82        | 0     |
| 36  | 2e    | 148/162 (91%)   | 0.43   | 3 (2%) 65 57  | 54, 66, 75, 86        | 0     |
| 37  | 1f    | 100/101 (99%)   | 0.31   | 0 100 100     | 52, 65, 72, 79        | 0     |
| 37  | 2f    | 100/101 (99%)   | 0.23   | 1 (1%) 79 74  | 53, 65, 75, 76        | 0     |
| 38  | 1g    | 155/156 (99%)   | 0.52   | 6 (3%) 43 34  | 62, 72, 80, 86        | 0     |
| 38  | 2g    | 155/156 (99%)   | 0.72   | 8 (5%) 33 25  | 68, 75, 82, 88        | 0     |
| 39  | 1h    | 137/138 (99%)   | 0.38   | 1 (0%) 84 80  | 50, 64, 70, 80        | 0     |
| 39  | 2h    | 137/138 (99%)   | 0.42   | 2 (1%) 72 65  | 53, 65, 72, 75        | 0     |
| 40  | 1i    | 127/128 (99%)   | 1.41   | 30 (23%) 2 2  | 63, 80, 87, 89        | 0     |
| 40  | 2i    | 126/128 (98%)   | 1.62   | 38 (30%) 1 1  | 68, 82, 88, 90        | 0     |
| 41  | 1j    | 97/105 (92%)    | 1.45   | 22 (22%) 2 2  | 68, 81, 88, 92        | 0     |
| 41  | 2j    | 96/105 (91%)    | 1.58   | 27 (28%) 1 1  | 75, 82, 88, 91        | 0     |
| 42  | 1k    | 114/129 (88%)   | 0.16   | 2 (1%) 67 61  | 35, 57, 68, 74        | 0     |
| 42  | 2k    | 114/129 (88%)   | 0.29   | 2 (1%) 67 61  | 51, 64, 76, 79        | 0     |
| 43  | 1l    | 121/132 (91%)   | 0.27   | 3 (2%) 58 49  | 46, 56, 66, 74        | 0     |
| 43  | 2l    | 121/132 (91%)   | 0.44   | 3 (2%) 58 49  | 48, 61, 68, 75        | 0     |

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| Mol | Chain | Analysed          | <RSRZ> | #RSRZ>2        | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-------------------|--------|----------------|-----------------------|-------|
| 44  | 1m    | 116/126 (92%)     | 0.89   | 5 (4%) 40 31   | 66, 75, 82, 85        | 0     |
| 44  | 2m    | 114/126 (90%)     | 1.16   | 12 (10%) 11 9  | 69, 81, 87, 89        | 0     |
| 45  | 1n    | 60/61 (98%)       | 1.32   | 9 (15%) 5 4    | 65, 75, 81, 85        | 0     |
| 45  | 2n    | 60/61 (98%)       | 1.87   | 26 (43%) 0 0   | 70, 81, 87, 90        | 0     |
| 46  | 1o    | 88/89 (98%)       | 0.28   | 1 (1%) 78 73   | 45, 61, 73, 78        | 0     |
| 46  | 2o    | 88/89 (98%)       | 0.33   | 2 (2%) 61 52   | 46, 63, 74, 80        | 0     |
| 47  | 1p    | 82/88 (93%)       | 0.97   | 5 (6%) 27 20   | 52, 69, 81, 86        | 0     |
| 47  | 2p    | 82/88 (93%)       | 0.72   | 3 (3%) 45 35   | 55, 64, 74, 80        | 0     |
| 48  | 1q    | 99/105 (94%)      | 0.58   | 2 (2%) 65 57   | 47, 62, 70, 74        | 0     |
| 48  | 2q    | 99/105 (94%)      | 0.45   | 0 100 100      | 47, 62, 72, 76        | 0     |
| 49  | 1r    | 68/88 (77%)       | 0.29   | 0 100 100      | 48, 61, 73, 80        | 0     |
| 49  | 2r    | 68/88 (77%)       | 0.47   | 1 (1%) 72 65   | 56, 65, 74, 78        | 0     |
| 50  | 1s    | 83/93 (89%)       | 1.42   | 16 (19%) 3 3   | 68, 78, 86, 90        | 0     |
| 50  | 2s    | 83/93 (89%)       | 1.61   | 20 (24%) 2 1   | 73, 85, 92, 96        | 0     |
| 51  | 1t    | 96/106 (90%)      | 0.85   | 10 (10%) 11 9  | 53, 67, 76, 80        | 0     |
| 51  | 2t    | 98/106 (92%)      | 0.66   | 5 (5%) 33 26   | 53, 63, 75, 78        | 0     |
| 52  | 1u    | 23/27 (85%)       | 2.19   | 12 (52%) 0 0   | 69, 75, 80, 84        | 0     |
| 52  | 2u    | 23/27 (85%)       | 2.13   | 13 (56%) 0 0   | 74, 79, 85, 87        | 0     |
| 53  | 1y    | 97/113 (85%)      | 0.48   | 3 (3%) 51 43   | 48, 65, 74, 79        | 0     |
| 53  | 2y    | 96/113 (84%)      | 1.52   | 30 (31%) 1 1   | 67, 78, 87, 89        | 0     |
| All | All   | 20766/21468 (96%) | 0.11   | 837 (4%) 42 33 | 11, 57, 87, 110       | 0     |

All (837) RSRZ outliers are listed below:

| Mol | Chain | Res     | Type | RSRZ |
|-----|-------|---------|------|------|
| 1   | 1A    | 1076    | C    | 7.1  |
| 1   | 1A    | 1064    | C    | 6.4  |
| 32  | 2a    | 1030(B) | C    | 6.4  |
| 1   | 2A    | 2125    | G    | 6.3  |
| 1   | 1A    | 1087    | G    | 6.1  |
| 45  | 2n    | 30      | ALA  | 6.0  |
| 45  | 2n    | 2       | ALA  | 6.0  |
| 1   | 1A    | 2123    | G    | 5.8  |
| 1   | 1A    | 1063    | G    | 5.7  |
| 23  | 11    | 2       | SER  | 5.6  |

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| Mol | Chain | Res     | Type | RSRZ |
|-----|-------|---------|------|------|
| 1   | 2A    | 2173    | A    | 5.5  |
| 1   | 2A    | 2602    | A    | 5.5  |
| 32  | 1a    | 1036    | G    | 5.4  |
| 1   | 2A    | 2123    | G    | 5.2  |
| 1   | 2A    | 2174    | C    | 5.2  |
| 32  | 2a    | 1030(A) | G    | 5.2  |
| 44  | 2m    | 102     | ARG  | 5.1  |
| 1   | 1A    | 1080    | C    | 5.1  |
| 1   | 1A    | 1081    | U    | 5.1  |
| 1   | 1A    | 1091    | G    | 5.0  |
| 1   | 2A    | 2126    | A    | 5.0  |
| 1   | 2A    | 1076    | C    | 5.0  |
| 50  | 2s    | 71      | LEU  | 4.9  |
| 1   | 1A    | 1075    | C    | 4.9  |
| 1   | 1A    | 1089    | G    | 4.8  |
| 1   | 1A    | 1077    | A    | 4.8  |
| 1   | 2A    | 2162    | G    | 4.8  |
| 1   | 2A    | 2176    | A    | 4.8  |
| 40  | 2i    | 64      | THR  | 4.7  |
| 1   | 2A    | 2127    | G    | 4.7  |
| 8   | 2I    | 86      | THR  | 4.7  |
| 40  | 2i    | 102     | LEU  | 4.7  |
| 1   | 1A    | 1067    | A    | 4.7  |
| 1   | 2A    | 2169    | A    | 4.6  |
| 24  | 12    | 70      | GLN  | 4.6  |
| 50  | 1s    | 13      | ASP  | 4.5  |
| 1   | 1A    | 1088    | A    | 4.5  |
| 1   | 1A    | 1092    | C    | 4.4  |
| 51  | 1t    | 103     | GLY  | 4.4  |
| 1   | 2A    | 2124    | G    | 4.4  |
| 1   | 2A    | 2172    | U    | 4.4  |
| 50  | 2s    | 15      | LEU  | 4.4  |
| 1   | 1A    | 1072    | C    | 4.4  |
| 1   | 2A    | 1075    | C    | 4.4  |
| 1   | 2A    | 2147    | G    | 4.4  |
| 1   | 1A    | 1079    | C    | 4.4  |
| 53  | 2y    | 98      | ALA  | 4.3  |
| 1   | 2A    | 1083    | U    | 4.3  |
| 8   | 2I    | 77      | LEU  | 4.3  |
| 53  | 1y    | 98      | ALA  | 4.3  |
| 20  | 2Y    | 58      | GLY  | 4.3  |
| 1   | 1A    | 1062    | G    | 4.3  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 1          | 1A           | 1093       | G           | 4.3         |
| 8          | 2I           | 140        | LEU         | 4.3         |
| 33         | 1b           | 12         | GLU         | 4.3         |
| 1          | 1A           | 1086       | A           | 4.2         |
| 53         | 2y           | 42         | SER         | 4.2         |
| 40         | 1i           | 66         | ARG         | 4.2         |
| 1          | 1A           | 1103       | A           | 4.2         |
| 1          | 2A           | 2130       | U           | 4.2         |
| 50         | 2s           | 14         | HIS         | 4.2         |
| 1          | 1A           | 1066       | U           | 4.2         |
| 8          | 2I           | 92         | VAL         | 4.2         |
| 40         | 1i           | 15         | ALA         | 4.2         |
| 34         | 1c           | 13         | GLY         | 4.2         |
| 1          | 2A           | 2148       | G           | 4.2         |
| 40         | 2i           | 2          | GLU         | 4.2         |
| 1          | 2A           | 2128       | C           | 4.1         |
| 1          | 1A           | 2116       | G           | 4.1         |
| 1          | 2A           | 2119       | A           | 4.1         |
| 50         | 1s           | 9          | VAL         | 4.0         |
| 1          | 1A           | 1078       | U           | 4.0         |
| 1          | 1A           | 2125       | G           | 4.0         |
| 1          | 2A           | 2171       | A           | 4.0         |
| 45         | 2n           | 25         | VAL         | 4.0         |
| 45         | 1n           | 2          | ALA         | 4.0         |
| 40         | 2i           | 109        | VAL         | 4.0         |
| 20         | 2Y           | 57         | GLN         | 4.0         |
| 1          | 2A           | 652(B)     | A           | 3.9         |
| 1          | 2A           | 2118       | U           | 3.9         |
| 53         | 2y           | 9          | GLN         | 3.9         |
| 50         | 2s           | 2          | PRO         | 3.9         |
| 1          | 1A           | 2147       | G           | 3.9         |
| 1          | 2A           | 2129       | C           | 3.9         |
| 1          | 1A           | 1090       | U           | 3.9         |
| 1          | 1A           | 1102       | C           | 3.9         |
| 8          | 2I           | 3          | VAL         | 3.8         |
| 1          | 1A           | 2602       | A           | 3.8         |
| 1          | 2A           | 2896       | C           | 3.8         |
| 1          | 1A           | 2172       | U           | 3.8         |
| 1          | 1A           | 2173       | A           | 3.8         |
| 1          | 2A           | 2153       | G           | 3.8         |
| 41         | 1j           | 33         | GLN         | 3.8         |
| 51         | 2t           | 103        | GLY         | 3.8         |

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| Mol | Chain | Res    | Type | RSRZ |
|-----|-------|--------|------|------|
| 1   | 2A    | 2139   | C    | 3.7  |
| 1   | 2A    | 2146   | C    | 3.7  |
| 1   | 2A    | 1046   | A    | 3.7  |
| 32  | 1a    | 1286   | A    | 3.7  |
| 5   | 1F    | 208    | GLY  | 3.7  |
| 1   | 1A    | 2139   | C    | 3.7  |
| 1   | 1A    | 1104   | C    | 3.6  |
| 1   | 2A    | 2107   | C    | 3.6  |
| 53  | 2y    | 41     | LEU  | 3.6  |
| 1   | 1A    | 2117   | A    | 3.6  |
| 1   | 1A    | 1074   | G    | 3.6  |
| 52  | 1u    | 6      | ARG  | 3.6  |
| 23  | 2l    | 2      | SER  | 3.6  |
| 40  | 2i    | 9      | ARG  | 3.6  |
| 41  | 1j    | 4      | ILE  | 3.6  |
| 1   | 2A    | 1091   | G    | 3.6  |
| 32  | 2a    | 1036   | G    | 3.6  |
| 6   | 2G    | 53     | LEU  | 3.6  |
| 20  | 2Y    | 1      | MET  | 3.6  |
| 52  | 2u    | 6      | ARG  | 3.6  |
| 52  | 1u    | 16     | GLY  | 3.6  |
| 6   | 2G    | 88     | ILE  | 3.6  |
| 6   | 2G    | 50     | ALA  | 3.5  |
| 1   | 2A    | 614(B) | G    | 3.5  |
| 1   | 1A    | 2161   | C    | 3.5  |
| 47  | 2p    | 82     | GLN  | 3.5  |
| 6   | 2G    | 146    | TYR  | 3.5  |
| 26  | 24    | 56     | VAL  | 3.5  |
| 51  | 1t    | 10     | LEU  | 3.5  |
| 32  | 1a    | 1034   | G    | 3.5  |
| 1   | 1A    | 1082   | U    | 3.5  |
| 8   | 2l    | 143    | SER  | 3.5  |
| 52  | 1u    | 15     | ARG  | 3.5  |
| 41  | 1j    | 38     | ILE  | 3.4  |
| 1   | 2A    | 2157   | G    | 3.4  |
| 45  | 2n    | 18     | VAL  | 3.4  |
| 52  | 2u    | 11     | GLY  | 3.4  |
| 40  | 2i    | 126    | SER  | 3.4  |
| 51  | 2t    | 6      | PRO  | 3.4  |
| 40  | 2i    | 11     | LYS  | 3.4  |
| 1   | 1A    | 1071   | G    | 3.4  |
| 1   | 1A    | 1083   | U    | 3.4  |

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| Mol | Chain | Res     | Type | RSRZ |
|-----|-------|---------|------|------|
| 1   | 1A    | 1057    | A    | 3.4  |
| 1   | 2A    | 2170    | A    | 3.4  |
| 32  | 1a    | 1030(B) | C    | 3.4  |
| 8   | 2I    | 79      | ILE  | 3.4  |
| 41  | 2j    | 44      | VAL  | 3.4  |
| 1   | 2A    | 2165    | G    | 3.4  |
| 15  | 1T    | 131     | ALA  | 3.4  |
| 53  | 2y    | 50      | ALA  | 3.4  |
| 8   | 2I    | 144     | VAL  | 3.4  |
| 8   | 2I    | 145     | VAL  | 3.4  |
| 33  | 2b    | 200     | ILE  | 3.4  |
| 1   | 2A    | 1085    | A    | 3.4  |
| 1   | 2A    | 1089    | G    | 3.3  |
| 1   | 2A    | 2802    | G    | 3.3  |
| 15  | 1T    | 130     | ALA  | 3.3  |
| 20  | 1Y    | 1       | MET  | 3.3  |
| 1   | 2A    | 2175    | C    | 3.3  |
| 40  | 2i    | 5       | TYR  | 3.3  |
| 42  | 2k    | 117     | ASN  | 3.3  |
| 40  | 2i    | 127     | LYS  | 3.3  |
| 1   | 2A    | 2136    | C    | 3.3  |
| 40  | 2i    | 13      | ALA  | 3.3  |
| 1   | 1A    | 2153    | G    | 3.3  |
| 1   | 2A    | 2131    | G    | 3.3  |
| 45  | 2n    | 33      | VAL  | 3.3  |
| 51  | 1t    | 11      | SER  | 3.3  |
| 1   | 2A    | 1082    | U    | 3.2  |
| 38  | 1g    | 2       | ALA  | 3.2  |
| 8   | 2I    | 127     | VAL  | 3.2  |
| 40  | 1i    | 17      | VAL  | 3.2  |
| 45  | 1n    | 25      | VAL  | 3.2  |
| 1   | 2A    | 1064    | C    | 3.2  |
| 1   | 1A    | 2162    | G    | 3.2  |
| 1   | 2A    | 2133    | G    | 3.2  |
| 1   | 2A    | 2159    | G    | 3.2  |
| 38  | 1g    | 84      | ASN  | 3.2  |
| 1   | 2A    | 1079    | C    | 3.2  |
| 1   | 2A    | 2145    | C    | 3.2  |
| 50  | 1s    | 38      | SER  | 3.2  |
| 45  | 2n    | 3       | ARG  | 3.2  |
| 1   | 2A    | 2166    | G    | 3.2  |
| 32  | 1a    | 1030(A) | G    | 3.2  |

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| Mol | Chain | Res     | Type | RSRZ |
|-----|-------|---------|------|------|
| 1   | 1A    | 2126    | A    | 3.2  |
| 52  | 1u    | 14      | TRP  | 3.2  |
| 1   | 2A    | 1536    | C    | 3.2  |
| 1   | 2A    | 2138    | C    | 3.2  |
| 1   | 2A    | 2132    | U    | 3.2  |
| 50  | 1s    | 33      | THR  | 3.1  |
| 1   | 1A    | 2124    | G    | 3.1  |
| 1   | 1A    | 2154    | G    | 3.1  |
| 52  | 1u    | 18      | TYR  | 3.1  |
| 1   | 2A    | 2122    | U    | 3.1  |
| 1   | 2A    | 2161    | C    | 3.1  |
| 8   | 2I    | 122     | GLU  | 3.1  |
| 1   | 2A    | 2110    | G    | 3.1  |
| 1   | 2A    | 2168    | G    | 3.1  |
| 32  | 1a    | 1030(C) | G    | 3.1  |
| 32  | 2a    | 1030(C) | G    | 3.1  |
| 40  | 1i    | 108     | VAL  | 3.1  |
| 1   | 1A    | 2176    | A    | 3.1  |
| 1   | 2A    | 1070    | A    | 3.1  |
| 36  | 2e    | 20      | GLN  | 3.1  |
| 26  | 14    | 54      | GLY  | 3.1  |
| 26  | 24    | 45      | GLY  | 3.1  |
| 26  | 24    | 57      | GLU  | 3.1  |
| 1   | 1A    | 2174    | C    | 3.1  |
| 45  | 2n    | 15      | LYS  | 3.1  |
| 40  | 2i    | 15      | ALA  | 3.1  |
| 34  | 2c    | 207     | VAL  | 3.1  |
| 50  | 2s    | 11      | VAL  | 3.1  |
| 6   | 2G    | 44      | GLY  | 3.1  |
| 34  | 1c    | 2       | GLY  | 3.1  |
| 43  | 2l    | 87      | GLY  | 3.1  |
| 45  | 2n    | 7       | ILE  | 3.1  |
| 32  | 1a    | 1037    | C    | 3.1  |
| 45  | 2n    | 5       | ALA  | 3.0  |
| 51  | 1t    | 55      | ILE  | 3.0  |
| 1   | 2A    | 229     | A    | 3.0  |
| 1   | 2A    | 1067    | A    | 3.0  |
| 12  | 2Q    | 104     | PHE  | 3.0  |
| 32  | 2a    | 1027    | C    | 3.0  |
| 40  | 2i    | 62      | TYR  | 3.0  |
| 41  | 2j    | 78      | ASN  | 3.0  |
| 41  | 2j    | 55      | LYS  | 3.0  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 40  | 2i    | 7    | THR  | 3.0  |
| 1   | 1A    | 1095 | A    | 3.0  |
| 40  | 1i    | 13   | ALA  | 3.0  |
| 1   | 2A    | 2120 | G    | 3.0  |
| 1   | 1A    | 2108 | C    | 3.0  |
| 1   | 2A    | 2789 | C    | 3.0  |
| 40  | 1i    | 9    | ARG  | 3.0  |
| 40  | 2i    | 125  | TYR  | 3.0  |
| 1   | 1A    | 2112 | G    | 3.0  |
| 1   | 1A    | 2168 | G    | 3.0  |
| 1   | 1A    | 2129 | C    | 3.0  |
| 53  | 2y    | 48   | PHE  | 3.0  |
| 53  | 2y    | 60   | VAL  | 3.0  |
| 8   | 2I    | 101  | LEU  | 2.9  |
| 50  | 2s    | 16   | LEU  | 2.9  |
| 52  | 2u    | 5    | ASP  | 2.9  |
| 52  | 2u    | 23   | PRO  | 2.9  |
| 50  | 1s    | 35   | SER  | 2.9  |
| 1   | 1A    | 2127 | G    | 2.9  |
| 40  | 1i    | 106  | ALA  | 2.9  |
| 26  | 14    | 59   | PHE  | 2.9  |
| 26  | 24    | 49   | PHE  | 2.9  |
| 41  | 2j    | 75   | ILE  | 2.9  |
| 50  | 1s    | 15   | LEU  | 2.9  |
| 32  | 2a    | 1286 | A    | 2.9  |
| 41  | 1j    | 76   | ASN  | 2.9  |
| 4   | 2E    | 204  | ALA  | 2.9  |
| 1   | 2A    | 2121 | G    | 2.9  |
| 1   | 2A    | 1081 | U    | 2.9  |
| 35  | 1d    | 4    | TYR  | 2.9  |
| 34  | 2c    | 92   | ALA  | 2.9  |
| 41  | 1j    | 72   | VAL  | 2.9  |
| 34  | 1c    | 10   | PHE  | 2.9  |
| 41  | 1j    | 8    | LEU  | 2.9  |
| 32  | 2a    | 1037 | C    | 2.9  |
| 1   | 2A    | 2152 | G    | 2.9  |
| 53  | 2y    | 79   | ASN  | 2.9  |
| 41  | 1j    | 34   | VAL  | 2.9  |
| 1   | 1A    | 1073 | A    | 2.9  |
| 1   | 2A    | 2134 | A    | 2.9  |
| 38  | 2g    | 5    | ARG  | 2.9  |
| 52  | 1u    | 24   | ARG  | 2.9  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 41  | 2j    | 98   | ILE  | 2.9  |
| 52  | 1u    | 2    | GLY  | 2.8  |
| 1   | 1A    | 2107 | C    | 2.8  |
| 6   | 2G    | 48   | GLU  | 2.8  |
| 45  | 2n    | 8    | GLU  | 2.8  |
| 1   | 2A    | 2151 | G    | 2.8  |
| 40  | 2i    | 108  | VAL  | 2.8  |
| 41  | 2j    | 34   | VAL  | 2.8  |
| 38  | 2g    | 32   | ARG  | 2.8  |
| 45  | 2n    | 6    | LEU  | 2.8  |
| 47  | 1p    | 19   | ILE  | 2.8  |
| 32  | 1a    | 65   | U    | 2.8  |
| 1   | 2A    | 2143 | C    | 2.8  |
| 40  | 1i    | 18   | PHE  | 2.8  |
| 6   | 2G    | 52   | ILE  | 2.8  |
| 7   | 1H    | 2    | SER  | 2.8  |
| 1   | 2A    | 1096 | A    | 2.8  |
| 52  | 1u    | 11   | GLY  | 2.8  |
| 8   | 2I    | 139  | GLN  | 2.8  |
| 35  | 2d    | 39   | PRO  | 2.8  |
| 44  | 1m    | 102  | ARG  | 2.8  |
| 45  | 2n    | 20   | ALA  | 2.8  |
| 41  | 1j    | 96   | ILE  | 2.8  |
| 44  | 2m    | 22   | ILE  | 2.8  |
| 41  | 1j    | 78   | ASN  | 2.8  |
| 50  | 2s    | 53   | ASN  | 2.8  |
| 1   | 1A    | 888  | C    | 2.8  |
| 32  | 2a    | 89   | C    | 2.8  |
| 26  | 14    | 52   | THR  | 2.8  |
| 41  | 2j    | 42   | THR  | 2.8  |
| 1   | 2A    | 2106 | G    | 2.8  |
| 32  | 2a    | 1026 | G    | 2.8  |
| 34  | 1c    | 90   | GLU  | 2.8  |
| 44  | 2m    | 74   | VAL  | 2.8  |
| 26  | 24    | 67   | TYR  | 2.8  |
| 45  | 2n    | 34   | TYR  | 2.8  |
| 53  | 2y    | 21   | ALA  | 2.8  |
| 35  | 1d    | 5    | ILE  | 2.8  |
| 45  | 2n    | 44   | LEU  | 2.8  |
| 50  | 2s    | 63   | THR  | 2.8  |
| 1   | 1A    | 2177 | C    | 2.8  |
| 50  | 1s    | 34   | TRP  | 2.7  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | 1A    | 2148 | G    | 2.7  |
| 32  | 1a    | 1026 | G    | 2.7  |
| 33  | 1b    | 214  | ILE  | 2.7  |
| 44  | 2m    | 84   | ILE  | 2.7  |
| 50  | 1s    | 16   | LEU  | 2.7  |
| 1   | 1A    | 2142 | C    | 2.7  |
| 1   | 2A    | 34   | C    | 2.7  |
| 45  | 1n    | 18   | VAL  | 2.7  |
| 33  | 1b    | 123  | ALA  | 2.7  |
| 40  | 2i    | 101  | PHE  | 2.7  |
| 52  | 1u    | 13   | ILE  | 2.7  |
| 32  | 1a    | 1035 | A    | 2.7  |
| 1   | 1A    | 2160 | G    | 2.7  |
| 1   | 2A    | 1071 | G    | 2.7  |
| 1   | 2A    | 2160 | G    | 2.7  |
| 1   | 2A    | 2167 | U    | 2.7  |
| 53  | 2y    | 53   | THR  | 2.7  |
| 29  | 27    | 45   | ALA  | 2.7  |
| 32  | 1a    | 1027 | C    | 2.7  |
| 50  | 2s    | 55   | LYS  | 2.7  |
| 1   | 1A    | 2169 | A    | 2.7  |
| 1   | 2A    | 1088 | A    | 2.7  |
| 1   | 2A    | 2135 | A    | 2.7  |
| 2   | 2B    | 1    | U    | 2.7  |
| 15  | 1T    | 37   | GLY  | 2.7  |
| 33  | 1b    | 131  | PRO  | 2.7  |
| 40  | 2i    | 66   | ARG  | 2.7  |
| 50  | 2s    | 33   | THR  | 2.7  |
| 52  | 1u    | 17   | THR  | 2.7  |
| 53  | 2y    | 45   | PRO  | 2.7  |
| 53  | 2y    | 51   | ASP  | 2.7  |
| 50  | 2s    | 35   | SER  | 2.7  |
| 24  | 22    | 6    | VAL  | 2.7  |
| 33  | 1b    | 15   | VAL  | 2.7  |
| 40  | 1i    | 109  | VAL  | 2.7  |
| 41  | 1j    | 44   | VAL  | 2.7  |
| 8   | 2I    | 146  | ALA  | 2.7  |
| 14  | 2S    | 35   | ILE  | 2.7  |
| 33  | 2b    | 201  | ILE  | 2.7  |
| 35  | 1d    | 135  | LEU  | 2.7  |
| 3   | 1D    | 276  | LYS  | 2.7  |
| 52  | 2u    | 14   | TRP  | 2.7  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 53  | 2y    | 38   | HIS  | 2.7  |
| 1   | 1A    | 1509 | C    | 2.7  |
| 45  | 2n    | 31   | ARG  | 2.7  |
| 32  | 1a    | 1447 | A    | 2.7  |
| 32  | 2a    | 1531 | A    | 2.7  |
| 44  | 2m    | 60   | VAL  | 2.7  |
| 40  | 2i    | 96   | LEU  | 2.7  |
| 40  | 2i    | 99   | LEU  | 2.7  |
| 44  | 2m    | 4    | ILE  | 2.6  |
| 45  | 2n    | 11   | LYS  | 2.6  |
| 1   | 2A    | 1063 | G    | 2.6  |
| 52  | 2u    | 9    | ARG  | 2.6  |
| 1   | 2A    | 2137 | C    | 2.6  |
| 1   | 2A    | 2177 | C    | 2.6  |
| 36  | 1e    | 85   | GLY  | 2.6  |
| 53  | 2y    | 75   | ASN  | 2.6  |
| 1   | 1A    | 1065 | U    | 2.6  |
| 26  | 24    | 9    | LEU  | 2.6  |
| 40  | 1i    | 86   | VAL  | 2.6  |
| 43  | 1l    | 18   | VAL  | 2.6  |
| 32  | 1a    | 1001 | A    | 2.6  |
| 41  | 1j    | 32   | ALA  | 2.6  |
| 50  | 1s    | 14   | HIS  | 2.6  |
| 1   | 1A    | 2166 | G    | 2.6  |
| 1   | 2A    | 2154 | G    | 2.6  |
| 12  | 2Q    | 59   | ARG  | 2.6  |
| 31  | 29    | 37   | GLY  | 2.6  |
| 1   | 2A    | 1092 | C    | 2.6  |
| 31  | 29    | 8    | LYS  | 2.6  |
| 53  | 2y    | 66   | LYS  | 2.6  |
| 6   | 1G    | 43   | LEU  | 2.6  |
| 38  | 2g    | 9    | VAL  | 2.6  |
| 41  | 2j    | 85   | LEU  | 2.6  |
| 53  | 2y    | 54   | ILE  | 2.6  |
| 32  | 1a    | 1020 | U    | 2.6  |
| 41  | 2j    | 32   | ALA  | 2.6  |
| 29  | 17    | 47   | ARG  | 2.6  |
| 33  | 1b    | 97   | TRP  | 2.6  |
| 36  | 1e    | 22   | GLY  | 2.6  |
| 41  | 2j    | 80   | LYS  | 2.6  |
| 1   | 1A    | 2115 | G    | 2.6  |
| 1   | 2A    | 1533 | G    | 2.6  |

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| Mol | Chain | Res     | Type | RSRZ |
|-----|-------|---------|------|------|
| 41  | 2j    | 65      | LEU  | 2.6  |
| 44  | 1m    | 43      | THR  | 2.6  |
| 45  | 1n    | 6       | LEU  | 2.6  |
| 53  | 2y    | 24      | LEU  | 2.6  |
| 8   | 2I    | 94      | ALA  | 2.6  |
| 33  | 1b    | 237     | ALA  | 2.6  |
| 50  | 2s    | 10      | PHE  | 2.6  |
| 1   | 1A    | 1026    | U    | 2.6  |
| 6   | 2G    | 118     | ARG  | 2.6  |
| 35  | 1d    | 73      | ARG  | 2.6  |
| 20  | 2Y    | 93      | GLY  | 2.6  |
| 6   | 2G    | 139     | LEU  | 2.6  |
| 8   | 2I    | 68      | LEU  | 2.6  |
| 33  | 2b    | 121     | LEU  | 2.6  |
| 44  | 2m    | 19      | LEU  | 2.6  |
| 35  | 2d    | 5       | ILE  | 2.6  |
| 52  | 2u    | 13      | ILE  | 2.6  |
| 53  | 2y    | 70      | MET  | 2.6  |
| 8   | 2I    | 85      | GLU  | 2.6  |
| 1   | 1A    | 1058    | G    | 2.5  |
| 1   | 1A    | 2133    | G    | 2.5  |
| 32  | 1a    | 1001(A) | G    | 2.5  |
| 1   | 1A    | 2132    | U    | 2.5  |
| 1   | 2A    | 2113    | U    | 2.5  |
| 32  | 1a    | 63      | C    | 2.5  |
| 8   | 2I    | 87      | LYS  | 2.5  |
| 1   | 1A    | 548     | A    | 2.5  |
| 33  | 2b    | 236     | TYR  | 2.5  |
| 35  | 2d    | 4       | TYR  | 2.5  |
| 39  | 1h    | 112     | LEU  | 2.5  |
| 37  | 2f    | 6       | VAL  | 2.5  |
| 50  | 2s    | 9       | VAL  | 2.5  |
| 41  | 1j    | 42      | THR  | 2.5  |
| 30  | 28    | 46      | ARG  | 2.5  |
| 1   | 2A    | 2109    | U    | 2.5  |
| 3   | 2D    | 276     | LYS  | 2.5  |
| 1   | 2A    | 2116    | G    | 2.5  |
| 32  | 1a    | 1003    | G    | 2.5  |
| 32  | 2a    | 1034    | G    | 2.5  |
| 32  | 2a    | 1373    | G    | 2.5  |
| 8   | 2I    | 128     | LEU  | 2.5  |
| 33  | 2b    | 131     | PRO  | 2.5  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 33  | 2b    | 97   | TRP  | 2.5  |
| 38  | 1g    | 16   | LEU  | 2.5  |
| 6   | 2G    | 28   | VAL  | 2.5  |
| 33  | 2b    | 164  | VAL  | 2.5  |
| 32  | 2a    | 1035 | A    | 2.5  |
| 33  | 2b    | 189  | ASP  | 2.5  |
| 1   | 1A    | 2122 | U    | 2.5  |
| 1   | 2A    | 2150 | U    | 2.5  |
| 34  | 2c    | 12   | LEU  | 2.5  |
| 41  | 2j    | 10   | GLY  | 2.5  |
| 50  | 2s    | 49   | ILE  | 2.5  |
| 51  | 1t    | 96   | GLY  | 2.5  |
| 51  | 2t    | 69   | GLY  | 2.5  |
| 33  | 2b    | 136  | VAL  | 2.5  |
| 40  | 2i    | 14   | VAL  | 2.5  |
| 1   | 1A    | 2178 | C    | 2.5  |
| 1   | 2A    | 1080 | C    | 2.5  |
| 1   | 2A    | 2164 | C    | 2.5  |
| 1   | 2A    | 2803 | C    | 2.5  |
| 32  | 1a    | 1030 | C    | 2.5  |
| 1   | 1A    | 1068 | G    | 2.5  |
| 44  | 2m    | 21   | TYR  | 2.5  |
| 1   | 1A    | 2790 | A    | 2.5  |
| 19  | 2X    | 68   | ARG  | 2.5  |
| 32  | 2a    | 1183 | A    | 2.5  |
| 8   | 2I    | 95   | LYS  | 2.5  |
| 33  | 2b    | 133  | LYS  | 2.5  |
| 40  | 1i    | 105  | ASP  | 2.5  |
| 38  | 1g    | 12   | LEU  | 2.5  |
| 40  | 1i    | 21   | PRO  | 2.5  |
| 40  | 2i    | 6    | GLY  | 2.5  |
| 40  | 2i    | 63   | ILE  | 2.5  |
| 45  | 2n    | 32   | SER  | 2.5  |
| 46  | 1o    | 87   | ILE  | 2.5  |
| 53  | 2y    | 64   | SER  | 2.5  |
| 33  | 2b    | 7    | VAL  | 2.5  |
| 53  | 2y    | 44   | GLU  | 2.5  |
| 35  | 1d    | 153  | ARG  | 2.5  |
| 8   | 2I    | 78   | THR  | 2.5  |
| 29  | 17    | 48   | LYS  | 2.5  |
| 32  | 2a    | 1019 | C    | 2.5  |
| 32  | 2a    | 1029 | C    | 2.5  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | 1A    | 2152 | G    | 2.5  |
| 1   | 1A    | 2119 | A    | 2.5  |
| 1   | 2A    | 653  | A    | 2.5  |
| 32  | 1a    | 344  | A    | 2.5  |
| 41  | 1j    | 56   | HIS  | 2.5  |
| 33  | 1b    | 187  | LEU  | 2.4  |
| 33  | 2b    | 187  | LEU  | 2.4  |
| 34  | 2c    | 2    | GLY  | 2.4  |
| 34  | 1c    | 206  | GLU  | 2.4  |
| 41  | 2j    | 5    | ARG  | 2.4  |
| 29  | 27    | 48   | LYS  | 2.4  |
| 40  | 1i    | 78   | LYS  | 2.4  |
| 45  | 1n    | 30   | ALA  | 2.4  |
| 32  | 1a    | 1019 | C    | 2.4  |
| 32  | 1a    | 1029 | C    | 2.4  |
| 8   | 2I    | 116  | LEU  | 2.4  |
| 1   | 1A    | 1070 | A    | 2.4  |
| 1   | 2A    | 2117 | A    | 2.4  |
| 32  | 1a    | 1493 | A    | 2.4  |
| 1   | 1A    | 2159 | G    | 2.4  |
| 26  | 24    | 31   | ILE  | 2.4  |
| 53  | 2y    | 62   | VAL  | 2.4  |
| 40  | 1i    | 104  | ARG  | 2.4  |
| 40  | 2i    | 10   | ARG  | 2.4  |
| 6   | 1G    | 75   | LYS  | 2.4  |
| 16  | 2U    | 89   | GLU  | 2.4  |
| 40  | 2i    | 12   | GLU  | 2.4  |
| 34  | 2c    | 129  | ALA  | 2.4  |
| 38  | 2g    | 2    | ALA  | 2.4  |
| 40  | 1i    | 7    | THR  | 2.4  |
| 52  | 2u    | 17   | THR  | 2.4  |
| 7   | 2H    | 41   | MET  | 2.4  |
| 35  | 1d    | 37   | PRO  | 2.4  |
| 41  | 1j    | 75   | ILE  | 2.4  |
| 26  | 24    | 54   | GLY  | 2.4  |
| 44  | 1m    | 95   | GLY  | 2.4  |
| 1   | 2A    | 1098 | A    | 2.4  |
| 40  | 2i    | 104  | ARG  | 2.4  |
| 43  | 2l    | 23   | LYS  | 2.4  |
| 1   | 1A    | 2131 | G    | 2.4  |
| 1   | 1A    | 2156 | G    | 2.4  |
| 32  | 1a    | 1031 | G    | 2.4  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 33  | 1b    | 17   | PHE  | 2.4  |
| 40  | 2i    | 110  | GLU  | 2.4  |
| 44  | 1m    | 2    | ALA  | 2.4  |
| 16  | 1U    | 117  | GLN  | 2.4  |
| 1   | 1A    | 2167 | U    | 2.4  |
| 45  | 2n    | 21   | TYR  | 2.4  |
| 41  | 2j    | 81   | THR  | 2.4  |
| 50  | 1s    | 69   | HIS  | 2.4  |
| 8   | 2I    | 123  | LEU  | 2.4  |
| 34  | 2c    | 175  | LEU  | 2.4  |
| 41  | 1j    | 71   | LEU  | 2.4  |
| 45  | 1n    | 39   | LEU  | 2.4  |
| 33  | 2b    | 162  | ILE  | 2.4  |
| 41  | 1j    | 74   | ILE  | 2.4  |
| 26  | 24    | 35   | VAL  | 2.4  |
| 40  | 1i    | 42   | ARG  | 2.4  |
| 1   | 1A    | 2140 | C    | 2.4  |
| 1   | 2A    | 2140 | C    | 2.4  |
| 8   | 1I    | 10   | GLU  | 2.4  |
| 45  | 2n    | 10   | ALA  | 2.4  |
| 41  | 2j    | 19   | SER  | 2.4  |
| 47  | 1p    | 82   | GLN  | 2.4  |
| 1   | 1A    | 12   | U    | 2.4  |
| 1   | 1A    | 1176 | G    | 2.4  |
| 1   | 1A    | 2805 | G    | 2.4  |
| 1   | 2A    | 2149 | G    | 2.4  |
| 32  | 2a    | 1202 | G    | 2.4  |
| 33  | 1b    | 48   | MET  | 2.4  |
| 33  | 1b    | 236  | TYR  | 2.4  |
| 34  | 1c    | 193  | TYR  | 2.4  |
| 48  | 1q    | 7    | THR  | 2.4  |
| 11  | 2P    | 15   | ARG  | 2.3  |
| 23  | 2I    | 26   | ARG  | 2.3  |
| 33  | 1b    | 133  | LYS  | 2.3  |
| 36  | 2e    | 18   | ARG  | 2.3  |
| 52  | 1u    | 22   | ARG  | 2.3  |
| 1   | 2A    | 279  | C    | 2.3  |
| 1   | 2A    | 2163 | C    | 2.3  |
| 8   | 1I    | 147  | GLN  | 2.3  |
| 51  | 1t    | 18   | GLN  | 2.3  |
| 32  | 1a    | 202  | U    | 2.3  |
| 6   | 2G    | 75   | LYS  | 2.3  |

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| Mol | Chain | Res     | Type | RSRZ |
|-----|-------|---------|------|------|
| 1   | 2A    | 2155    | G    | 2.3  |
| 34  | 1c    | 11      | ARG  | 2.3  |
| 34  | 1c    | 179     | ARG  | 2.3  |
| 35  | 2d    | 198     | VAL  | 2.3  |
| 41  | 2j    | 46      | ARG  | 2.3  |
| 24  | 22    | 52      | ASP  | 2.3  |
| 40  | 2i    | 82      | ALA  | 2.3  |
| 53  | 2y    | 52      | ALA  | 2.3  |
| 33  | 2b    | 44      | LEU  | 2.3  |
| 1   | 2A    | 2111    | C    | 2.3  |
| 26  | 24    | 27      | THR  | 2.3  |
| 32  | 1a    | 1038    | C    | 2.3  |
| 45  | 1n    | 7       | ILE  | 2.3  |
| 45  | 2n    | 17      | LYS  | 2.3  |
| 1   | 1A    | 2144    | U    | 2.3  |
| 32  | 2a    | 1020    | U    | 2.3  |
| 41  | 2j    | 37      | PRO  | 2.3  |
| 26  | 14    | 56      | VAL  | 2.3  |
| 6   | 2G    | 46      | ALA  | 2.3  |
| 32  | 2a    | 971     | G    | 2.3  |
| 32  | 2a    | 1001(A) | G    | 2.3  |
| 32  | 2a    | 1031    | G    | 2.3  |
| 50  | 1s    | 27      | GLU  | 2.3  |
| 33  | 1b    | 213     | LEU  | 2.3  |
| 41  | 1j    | 65      | LEU  | 2.3  |
| 50  | 2s    | 38      | SER  | 2.3  |
| 53  | 2y    | 8       | LYS  | 2.3  |
| 50  | 1s    | 37      | ARG  | 2.3  |
| 52  | 2u    | 7       | ARG  | 2.3  |
| 52  | 2u    | 15      | ARG  | 2.3  |
| 6   | 2G    | 87      | PRO  | 2.3  |
| 1   | 1A    | 2171    | A    | 2.3  |
| 1   | 1A    | 2179    | C    | 2.3  |
| 1   | 2A    | 1095    | A    | 2.3  |
| 12  | 2Q    | 33      | GLY  | 2.3  |
| 44  | 1m    | 100     | GLY  | 2.3  |
| 52  | 2u    | 2       | GLY  | 2.3  |
| 33  | 2b    | 70      | PHE  | 2.3  |
| 33  | 2b    | 152     | PHE  | 2.3  |
| 41  | 2j    | 76      | ASN  | 2.3  |
| 33  | 2b    | 123     | ALA  | 2.3  |
| 53  | 2y    | 73      | ALA  | 2.3  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 33  | 2b    | 166  | ASP  | 2.3  |
| 41  | 2j    | 71   | LEU  | 2.3  |
| 50  | 2s    | 12   | ASP  | 2.3  |
| 45  | 2n    | 9    | LYS  | 2.3  |
| 32  | 2a    | 1002 | G    | 2.3  |
| 32  | 2a    | 1003 | G    | 2.3  |
| 34  | 2c    | 176  | HIS  | 2.3  |
| 38  | 1g    | 156  | TRP  | 2.3  |
| 14  | 2S    | 52   | SER  | 2.3  |
| 51  | 2t    | 11   | SER  | 2.3  |
| 33  | 1b    | 125  | PRO  | 2.3  |
| 38  | 1g    | 154  | TYR  | 2.3  |
| 40  | 2i    | 36   | TYR  | 2.3  |
| 6   | 2G    | 149  | VAL  | 2.3  |
| 33  | 1b    | 136  | VAL  | 2.3  |
| 40  | 1i    | 14   | VAL  | 2.3  |
| 4   | 2E    | 10   | GLY  | 2.3  |
| 1   | 2A    | 2105 | C    | 2.2  |
| 32  | 2a    | 1001 | A    | 2.2  |
| 32  | 2a    | 1129 | C    | 2.2  |
| 41  | 2j    | 47   | PHE  | 2.2  |
| 33  | 2b    | 134  | GLU  | 2.2  |
| 41  | 1j    | 27   | ALA  | 2.2  |
| 42  | 2k    | 13   | GLN  | 2.2  |
| 53  | 2y    | 46   | GLN  | 2.2  |
| 40  | 1i    | 128  | ARG  | 2.2  |
| 51  | 1t    | 79   | ARG  | 2.2  |
| 53  | 1y    | 95   | ARG  | 2.2  |
| 44  | 2m    | 43   | THR  | 2.2  |
| 26  | 24    | 63   | TYR  | 2.2  |
| 1   | 1A    | 2149 | G    | 2.2  |
| 1   | 1A    | 2155 | G    | 2.2  |
| 1   | 2A    | 1087 | G    | 2.2  |
| 1   | 2A    | 2104 | G    | 2.2  |
| 21  | 1Z    | 1    | MET  | 2.2  |
| 33  | 2b    | 48   | MET  | 2.2  |
| 1   | 2A    | 1066 | U    | 2.2  |
| 1   | 2A    | 2144 | U    | 2.2  |
| 32  | 2a    | 90   | U    | 2.2  |
| 3   | 2D    | 28   | GLU  | 2.2  |
| 35  | 2d    | 156  | GLU  | 2.2  |
| 38  | 2g    | 7    | ALA  | 2.2  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 40  | 2i    | 122  | ALA  | 2.2  |
| 1   | 1A    | 6    | A    | 2.2  |
| 3   | 2D    | 275  | LYS  | 2.2  |
| 6   | 2G    | 7    | LEU  | 2.2  |
| 6   | 2G    | 62   | LEU  | 2.2  |
| 8   | 2I    | 38   | LEU  | 2.2  |
| 1   | 1A    | 2111 | C    | 2.2  |
| 1   | 2A    | 1509 | C    | 2.2  |
| 15  | 1T    | 38   | ASN  | 2.2  |
| 32  | 1a    | 221  | C    | 2.2  |
| 32  | 2a    | 975  | A    | 2.2  |
| 35  | 1d    | 154  | ASN  | 2.2  |
| 40  | 1i    | 19   | LEU  | 2.2  |
| 8   | 2I    | 88   | ILE  | 2.2  |
| 49  | 2r    | 65   | ILE  | 2.2  |
| 50  | 1s    | 31   | ILE  | 2.2  |
| 14  | 1S    | 13   | ARG  | 2.2  |
| 36  | 2e    | 120  | THR  | 2.2  |
| 41  | 2j    | 77   | PRO  | 2.2  |
| 45  | 2n    | 22   | THR  | 2.2  |
| 40  | 1i    | 125  | TYR  | 2.2  |
| 47  | 1p    | 39   | TYR  | 2.2  |
| 8   | 1I    | 90   | GLY  | 2.2  |
| 34  | 2c    | 9    | GLY  | 2.2  |
| 40  | 1i    | 6    | GLY  | 2.2  |
| 40  | 1i    | 61   | ALA  | 2.2  |
| 40  | 2i    | 19   | LEU  | 2.2  |
| 48  | 1q    | 98   | LEU  | 2.2  |
| 33  | 1b    | 94   | ASN  | 2.2  |
| 11  | 1P    | 15   | ARG  | 2.2  |
| 33  | 2b    | 127  | ILE  | 2.2  |
| 44  | 2m    | 104  | ARG  | 2.2  |
| 51  | 2t    | 100  | ILE  | 2.2  |
| 1   | 1A    | 1084 | A    | 2.2  |
| 1   | 2A    | 1084 | A    | 2.2  |
| 32  | 2a    | 1014 | A    | 2.2  |
| 1   | 1A    | 2136 | C    | 2.2  |
| 7   | 2H    | 173  | PRO  | 2.2  |
| 33  | 1b    | 165  | VAL  | 2.2  |
| 40  | 2i    | 49   | PRO  | 2.2  |
| 40  | 2i    | 103  | THR  | 2.2  |
| 42  | 1k    | 42   | TRP  | 2.2  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 52  | 1u    | 8    | THR  | 2.2  |
| 38  | 2g    | 154  | TYR  | 2.2  |
| 40  | 1i    | 126  | SER  | 2.2  |
| 50  | 2s    | 4    | SER  | 2.2  |
| 52  | 2u    | 4    | GLY  | 2.2  |
| 26  | 24    | 59   | PHE  | 2.2  |
| 34  | 2c    | 186  | PHE  | 2.2  |
| 40  | 1i    | 102  | LEU  | 2.2  |
| 40  | 2i    | 40   | LEU  | 2.2  |
| 51  | 1t    | 62   | LEU  | 2.2  |
| 45  | 1n    | 5    | ALA  | 2.2  |
| 31  | 29    | 17   | ILE  | 2.2  |
| 1   | 1A    | 2109 | U    | 2.2  |
| 1   | 2A    | 1090 | U    | 2.2  |
| 1   | 2A    | 2180 | U    | 2.2  |
| 1   | 2A    | 1059 | G    | 2.2  |
| 32  | 1a    | 306  | G    | 2.2  |
| 50  | 1s    | 47   | HIS  | 2.2  |
| 1   | 1A    | 1085 | A    | 2.2  |
| 1   | 2A    | 1077 | A    | 2.2  |
| 8   | 2I    | 81   | VAL  | 2.2  |
| 25  | 23    | 2    | PRO  | 2.2  |
| 32  | 1a    | 1492 | A    | 2.2  |
| 40  | 1i    | 49   | PRO  | 2.2  |
| 47  | 1p    | 68   | ASP  | 2.2  |
| 1   | 2A    | 2179 | C    | 2.2  |
| 32  | 2a    | 1028 | C    | 2.2  |
| 32  | 2a    | 1030 | C    | 2.2  |
| 26  | 24    | 52   | THR  | 2.2  |
| 45  | 1n    | 17   | LYS  | 2.2  |
| 33  | 1b    | 33   | TYR  | 2.2  |
| 33  | 2b    | 199  | TYR  | 2.2  |
| 35  | 1d    | 162  | LEU  | 2.2  |
| 20  | 2Y    | 48   | ALA  | 2.2  |
| 50  | 2s    | 75   | ALA  | 2.2  |
| 47  | 2p    | 19   | ILE  | 2.1  |
| 1   | 1A    | 2150 | U    | 2.1  |
| 6   | 2G    | 159  | VAL  | 2.1  |
| 47  | 2p    | 2    | VAL  | 2.1  |
| 1   | 2A    | 1074 | G    | 2.1  |
| 32  | 1a    | 79   | G    | 2.1  |
| 44  | 2m    | 65   | LYS  | 2.1  |

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| Mol | Chain | Res    | Type | RSRZ |
|-----|-------|--------|------|------|
| 1   | 2A    | 2178   | C    | 2.1  |
| 53  | 2y    | 61     | LEU  | 2.1  |
| 42  | 1k    | 25     | TYR  | 2.1  |
| 21  | 2Z    | 164    | ALA  | 2.1  |
| 23  | 1l    | 26     | ARG  | 2.1  |
| 45  | 2n    | 12     | ARG  | 2.1  |
| 6   | 2G    | 39     | ILE  | 2.1  |
| 53  | 2y    | 40     | ILE  | 2.1  |
| 53  | 2y    | 74     | ILE  | 2.1  |
| 47  | 1p    | 13     | HIS  | 2.1  |
| 1   | 1A    | 271(K) | U    | 2.1  |
| 1   | 2A    | 2897   | U    | 2.1  |
| 41  | 1j    | 39     | PRO  | 2.1  |
| 41  | 2j    | 91     | PRO  | 2.1  |
| 40  | 1i    | 103    | THR  | 2.1  |
| 45  | 2n    | 39     | LEU  | 2.1  |
| 52  | 2u    | 24     | ARG  | 2.1  |
| 32  | 1a    | 1002   | G    | 2.1  |
| 34  | 2c    | 8      | ILE  | 2.1  |
| 41  | 2j    | 6      | ILE  | 2.1  |
| 50  | 1s    | 21     | GLU  | 2.1  |
| 1   | 1A    | 34     | C    | 2.1  |
| 32  | 2a    | 1038   | C    | 2.1  |
| 40  | 2i    | 117    | HIS  | 2.1  |
| 34  | 1c    | 86     | VAL  | 2.1  |
| 32  | 2a    | 1040   | U    | 2.1  |
| 6   | 2G    | 43     | LEU  | 2.1  |
| 14  | 2S    | 32     | LEU  | 2.1  |
| 38  | 2g    | 34     | GLY  | 2.1  |
| 46  | 2o    | 86     | GLY  | 2.1  |
| 40  | 1i    | 64     | THR  | 2.1  |
| 41  | 2j    | 63     | PHE  | 2.1  |
| 41  | 2j    | 100    | THR  | 2.1  |
| 7   | 2H    | 60     | ARG  | 2.1  |
| 20  | 2Y    | 73     | ARG  | 2.1  |
| 26  | 24    | 58     | ARG  | 2.1  |
| 46  | 2o    | 68     | ARG  | 2.1  |
| 53  | 2y    | 76     | GLU  | 2.1  |
| 1   | 1A    | 229    | A    | 2.1  |
| 1   | 1A    | 2134   | A    | 2.1  |
| 6   | 1G    | 76     | SER  | 2.1  |
| 1   | 1A    | 2137   | C    | 2.1  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | 1A    | 2157 | G    | 2.1  |
| 1   | 1A    | 2165 | G    | 2.1  |
| 1   | 2A    | 1062 | G    | 2.1  |
| 1   | 2A    | 1093 | G    | 2.1  |
| 1   | 2A    | 2141 | G    | 2.1  |
| 32  | 1a    | 630  | G    | 2.1  |
| 32  | 1a    | 1018 | C    | 2.1  |
| 40  | 1i    | 117  | HIS  | 2.1  |
| 32  | 2a    | 976  | G    | 2.1  |
| 43  | 1l    | 126  | LYS  | 2.1  |
| 45  | 2n    | 4    | LYS  | 2.1  |
| 8   | 2I    | 75   | LEU  | 2.1  |
| 35  | 2d    | 11   | LEU  | 2.1  |
| 53  | 2y    | 81   | LEU  | 2.1  |
| 50  | 1s    | 84   | GLY  | 2.1  |
| 39  | 2h    | 3    | THR  | 2.1  |
| 40  | 2i    | 42   | ARG  | 2.1  |
| 43  | 2l    | 89   | ARG  | 2.1  |
| 53  | 1y    | 2    | THR  | 2.1  |
| 7   | 2H    | 58   | GLU  | 2.1  |
| 33  | 1b    | 148  | TYR  | 2.1  |
| 17  | 2V    | 73   | SER  | 2.0  |
| 26  | 24    | 66   | SER  | 2.0  |
| 35  | 1d    | 181  | MET  | 2.0  |
| 40  | 1i    | 11   | LYS  | 2.0  |
| 41  | 1j    | 30   | SER  | 2.0  |
| 1   | 1A    | 2170 | A    | 2.0  |
| 32  | 1a    | 1183 | A    | 2.0  |
| 1   | 2A    | 1104 | C    | 2.0  |
| 32  | 1a    | 345  | C    | 2.0  |
| 1   | 1A    | 2141 | G    | 2.0  |
| 1   | 2A    | 2112 | G    | 2.0  |
| 35  | 1d    | 3    | ARG  | 2.0  |
| 35  | 1d    | 171  | GLY  | 2.0  |
| 35  | 2d    | 2    | GLY  | 2.0  |
| 1   | 1A    | 2113 | U    | 2.0  |
| 1   | 2A    | 362  | U    | 2.0  |
| 50  | 2s    | 48   | THR  | 2.0  |
| 34  | 2c    | 206  | GLU  | 2.0  |
| 35  | 1d    | 163  | GLU  | 2.0  |
| 51  | 1t    | 65   | LYS  | 2.0  |
| 40  | 2i    | 124  | GLN  | 2.0  |

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| Mol | Chain | Res     | Type | RSRZ |
|-----|-------|---------|------|------|
| 41  | 2j    | 49      | VAL  | 2.0  |
| 44  | 2m    | 41      | PRO  | 2.0  |
| 32  | 1a    | 1030(D) | A    | 2.0  |
| 32  | 2a    | 1363(A) | A    | 2.0  |
| 33  | 2b    | 98      | LEU  | 2.0  |
| 34  | 1c    | 87      | LEU  | 2.0  |
| 39  | 2h    | 2       | LEU  | 2.0  |
| 40  | 1i    | 85      | LEU  | 2.0  |
| 41  | 1j    | 85      | LEU  | 2.0  |
| 41  | 2j    | 40      | LEU  | 2.0  |
| 43  | 1l    | 89      | ARG  | 2.0  |
| 45  | 2n    | 41      | ARG  | 2.0  |
| 51  | 1t    | 9       | ASN  | 2.0  |
| 35  | 1d    | 44      | GLY  | 2.0  |
| 32  | 1a    | 1028    | C    | 2.0  |
| 32  | 2a    | 995     | C    | 2.0  |
| 40  | 2i    | 27      | THR  | 2.0  |
| 1   | 2A    | 2100    | G    | 2.0  |
| 3   | 2D    | 38      | LYS  | 2.0  |
| 26  | 14    | 69      | LYS  | 2.0  |
| 32  | 1a    | 1021    | G    | 2.0  |
| 32  | 2a    | 630     | G    | 2.0  |
| 32  | 2a    | 1032    | G    | 2.0  |
| 32  | 2a    | 1224    | G    | 2.0  |
| 41  | 1j    | 55      | LYS  | 2.0  |
| 38  | 2g    | 156     | TRP  | 2.0  |
| 50  | 2s    | 34      | TRP  | 2.0  |
| 34  | 2c    | 173     | VAL  | 2.0  |
| 40  | 2i    | 44      | VAL  | 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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 32  | 2MG  | 2a    | 1207 | 24/25 | 0.80 | 0.12 | 74,84,88,89                | 0     |
| 1   | 5MU  | 2A    | 1915 | 21/22 | 0.84 | 0.09 | 77,83,88,92                | 0     |
| 32  | 2MG  | 1a    | 1207 | 24/25 | 0.86 | 0.11 | 68,77,80,88                | 0     |
| 32  | 5MC  | 2a    | 967  | 21/22 | 0.88 | 0.14 | 60,69,79,87                | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 1   | PSU  | 1A    | 1917 | 20/21 | 0.89 | 0.10 | 49,67,76,78                 | 0     |
| 32  | PSU  | 2a    | 516  | 20/21 | 0.89 | 0.09 | 68,77,84,84                 | 0     |
| 1   | 5MU  | 1A    | 1915 | 21/22 | 0.89 | 0.10 | 68,77,87,96                 | 0     |
| 1   | PSU  | 2A    | 1911 | 20/21 | 0.89 | 0.10 | 66,70,79,80                 | 0     |
| 32  | M2G  | 2a    | 966  | 25/26 | 0.90 | 0.13 | 51,67,80,82                 | 0     |
| 32  | G7M  | 2a    | 527  | 24/25 | 0.91 | 0.11 | 56,63,68,69                 | 0     |
| 32  | 5MC  | 1a    | 967  | 21/22 | 0.91 | 0.10 | 51,63,73,79                 | 0     |
| 1   | PSU  | 1A    | 1911 | 20/21 | 0.91 | 0.10 | 54,63,68,70                 | 0     |
| 43  | 0TD  | 1l    | 92   | 10/11 | 0.91 | 0.12 | 50,56,61,71                 | 0     |
| 1   | PSU  | 2A    | 1917 | 20/21 | 0.92 | 0.08 | 69,76,83,86                 | 0     |
| 32  | M2G  | 1a    | 966  | 25/26 | 0.93 | 0.10 | 46,62,71,74                 | 0     |
| 32  | G7M  | 1a    | 527  | 24/25 | 0.93 | 0.10 | 51,59,63,64                 | 0     |
| 32  | 5MC  | 2a    | 1400 | 21/22 | 0.93 | 0.11 | 59,64,66,68                 | 0     |
| 43  | 0TD  | 2l    | 92   | 10/11 | 0.93 | 0.10 | 61,63,67,77                 | 0     |
| 32  | 5MC  | 1a    | 1407 | 21/22 | 0.94 | 0.09 | 39,47,52,54                 | 0     |
| 32  | PSU  | 1a    | 516  | 20/21 | 0.94 | 0.09 | 52,66,70,71                 | 0     |
| 32  | MA6  | 1a    | 1519 | 24/25 | 0.95 | 0.10 | 37,43,51,55                 | 0     |
| 1   | OMC  | 2A    | 1920 | 21/22 | 0.95 | 0.09 | 51,62,69,74                 | 0     |
| 32  | 4OC  | 2a    | 1402 | 22/23 | 0.95 | 0.09 | 53,60,64,66                 | 0     |
| 32  | 5MC  | 2a    | 1404 | 21/22 | 0.95 | 0.08 | 41,51,56,59                 | 0     |
| 32  | 5MC  | 2a    | 1407 | 21/22 | 0.95 | 0.09 | 53,59,64,68                 | 0     |
| 32  | UR3  | 2a    | 1498 | 21/22 | 0.95 | 0.09 | 48,54,60,63                 | 0     |
| 32  | MA6  | 2a    | 1518 | 24/25 | 0.95 | 0.10 | 42,56,58,60                 | 0     |
| 1   | OMC  | 1A    | 1920 | 21/22 | 0.95 | 0.10 | 40,52,56,57                 | 0     |
| 32  | 5MC  | 1a    | 1404 | 21/22 | 0.96 | 0.08 | 40,44,47,52                 | 0     |
| 32  | 5MC  | 1a    | 1400 | 21/22 | 0.96 | 0.08 | 48,53,56,58                 | 0     |
| 32  | UR3  | 1a    | 1498 | 21/22 | 0.96 | 0.09 | 38,45,50,57                 | 0     |
| 32  | MA6  | 2a    | 1519 | 24/25 | 0.96 | 0.10 | 44,53,57,58                 | 0     |
| 1   | 5MC  | 2A    | 1942 | 21/22 | 0.96 | 0.07 | 38,45,48,50                 | 0     |
| 32  | MA6  | 1a    | 1518 | 24/25 | 0.97 | 0.08 | 32,40,43,46                 | 0     |
| 32  | 4OC  | 1a    | 1402 | 22/23 | 0.97 | 0.08 | 43,49,56,60                 | 0     |
| 1   | 5MU  | 2A    | 1939 | 21/22 | 0.97 | 0.08 | 26,35,38,39                 | 0     |
| 1   | 5MC  | 1A    | 1942 | 21/22 | 0.97 | 0.07 | 20,29,33,34                 | 0     |
| 1   | 5MC  | 2A    | 1962 | 21/22 | 0.97 | 0.08 | 32,37,43,48                 | 0     |
| 1   | OMG  | 2A    | 2251 | 24/25 | 0.97 | 0.08 | 30,35,42,45                 | 0     |
| 1   | 2MA  | 2A    | 2503 | 23/24 | 0.97 | 0.07 | 23,27,32,36                 | 0     |
| 1   | OMU  | 2A    | 2552 | 21/22 | 0.97 | 0.07 | 24,33,38,41                 | 0     |
| 1   | PSU  | 2A    | 2605 | 20/21 | 0.97 | 0.07 | 25,31,34,34                 | 0     |
| 1   | 5MC  | 1A    | 1962 | 21/22 | 0.97 | 0.07 | 24,29,32,42                 | 0     |
| 1   | OMG  | 1A    | 2251 | 24/25 | 0.97 | 0.07 | 13,16,21,26                 | 0     |
| 1   | 2MA  | 1A    | 2503 | 23/24 | 0.98 | 0.06 | 11,14,16,17                 | 0     |
| 1   | OMU  | 1A    | 2552 | 21/22 | 0.98 | 0.06 | 17,23,26,27                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 1   | PSU  | 1A    | 2605 | 20/21 | 0.98 | 0.07 | 18,21,28,29                 | 0     |
| 1   | 5MU  | 1A    | 1939 | 21/22 | 0.98 | 0.07 | 17,22,24,28                 | 0     |

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 2a    | 3186 | 1/1   | 0.42 | 0.24 | 82,82,82,82                 | 0     |
| 54  | MG   | 1a    | 1759 | 1/1   | 0.47 | 0.30 | 72,72,72,72                 | 0     |
| 54  | MG   | 1a    | 1850 | 1/1   | 0.49 | 0.23 | 58,58,58,58                 | 0     |
| 54  | MG   | 2a    | 3146 | 1/1   | 0.57 | 0.31 | 94,94,94,94                 | 0     |
| 54  | MG   | 2j    | 201  | 1/1   | 0.57 | 0.14 | 85,85,85,85                 | 0     |
| 54  | MG   | 1a    | 1764 | 1/1   | 0.59 | 0.20 | 75,75,75,75                 | 0     |
| 54  | MG   | 1A    | 3905 | 1/1   | 0.59 | 0.20 | 41,41,41,41                 | 0     |
| 54  | MG   | 1b    | 301  | 1/1   | 0.59 | 0.17 | 74,74,74,74                 | 0     |
| 54  | MG   | 2a    | 3117 | 1/1   | 0.60 | 0.27 | 66,66,66,66                 | 0     |
| 54  | MG   | 1a    | 1834 | 1/1   | 0.60 | 0.31 | 73,73,73,73                 | 0     |
| 54  | MG   | 1S    | 202  | 1/1   | 0.62 | 0.27 | 68,68,68,68                 | 0     |
| 54  | MG   | 1a    | 1778 | 1/1   | 0.63 | 0.15 | 89,89,89,89                 | 0     |
| 54  | MG   | 1a    | 1638 | 1/1   | 0.64 | 0.16 | 78,78,78,78                 | 0     |
| 54  | MG   | 1a    | 1641 | 1/1   | 0.64 | 0.25 | 73,73,73,73                 | 0     |
| 54  | MG   | 2A    | 3374 | 1/1   | 0.64 | 0.21 | 75,75,75,75                 | 0     |
| 54  | MG   | 2A    | 3501 | 1/1   | 0.64 | 0.26 | 61,61,61,61                 | 0     |
| 56  | MPD  | 2B    | 220  | 8/8   | 0.64 | 0.31 | 57,64,69,72                 | 0     |
| 54  | MG   | 1A    | 3377 | 1/1   | 0.65 | 0.15 | 37,37,37,37                 | 0     |
| 54  | MG   | 1A    | 3380 | 1/1   | 0.65 | 0.09 | 10,10,10,10                 | 0     |
| 54  | MG   | 1A    | 3642 | 1/1   | 0.65 | 0.21 | 61,61,61,61                 | 0     |
| 54  | MG   | 2a    | 3006 | 1/1   | 0.65 | 0.23 | 60,60,60,60                 | 0     |
| 54  | MG   | 2a    | 3063 | 1/1   | 0.65 | 0.14 | 70,70,70,70                 | 0     |
| 54  | MG   | 2A    | 3754 | 1/1   | 0.66 | 0.20 | 67,67,67,67                 | 0     |
| 54  | MG   | 2A    | 3448 | 1/1   | 0.66 | 0.18 | 71,71,71,71                 | 0     |
| 54  | MG   | 1T    | 203  | 1/1   | 0.66 | 0.11 | 68,68,68,68                 | 0     |
| 54  | MG   | 2A    | 3680 | 1/1   | 0.66 | 0.18 | 68,68,68,68                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 54  | MG   | 2A    | 3497 | 1/1   | 0.67 | 0.17 | 29,29,29,29                | 0     |
| 54  | MG   | 2A    | 3405 | 1/1   | 0.67 | 0.12 | 66,66,66,66                | 0     |
| 54  | MG   | 2a    | 3048 | 1/1   | 0.67 | 0.21 | 74,74,74,74                | 0     |
| 54  | MG   | 2a    | 3061 | 1/1   | 0.67 | 0.26 | 74,74,74,74                | 0     |
| 54  | MG   | 1A    | 3680 | 1/1   | 0.67 | 0.19 | 70,70,70,70                | 0     |
| 54  | MG   | 2a    | 3118 | 1/1   | 0.68 | 0.26 | 61,61,61,61                | 0     |
| 54  | MG   | 1a    | 1849 | 1/1   | 0.68 | 0.24 | 77,77,77,77                | 0     |
| 54  | MG   | 1A    | 3599 | 1/1   | 0.68 | 0.14 | 64,64,64,64                | 0     |
| 54  | MG   | 1a    | 1612 | 1/1   | 0.68 | 0.24 | 57,57,57,57                | 0     |
| 54  | MG   | 1f    | 201  | 1/1   | 0.68 | 0.33 | 70,70,70,70                | 0     |
| 54  | MG   | 1A    | 3750 | 1/1   | 0.69 | 0.22 | 64,64,64,64                | 0     |
| 54  | MG   | 1d    | 301  | 1/1   | 0.69 | 0.22 | 64,64,64,64                | 0     |
| 54  | MG   | 2a    | 3064 | 1/1   | 0.69 | 0.15 | 62,62,62,62                | 0     |
| 54  | MG   | 1A    | 3148 | 1/1   | 0.70 | 0.16 | 64,64,64,64                | 0     |
| 54  | MG   | 1a    | 1708 | 1/1   | 0.71 | 0.12 | 82,82,82,82                | 0     |
| 54  | MG   | 1A    | 3810 | 1/1   | 0.71 | 0.15 | 63,63,63,63                | 0     |
| 54  | MG   | 1a    | 1863 | 1/1   | 0.71 | 0.20 | 67,67,67,67                | 0     |
| 54  | MG   | 1A    | 3725 | 1/1   | 0.71 | 0.24 | 60,60,60,60                | 0     |
| 54  | MG   | 1A    | 3538 | 1/1   | 0.71 | 0.15 | 30,30,30,30                | 0     |
| 54  | MG   | 2A    | 3700 | 1/1   | 0.71 | 0.19 | 63,63,63,63                | 0     |
| 54  | MG   | 1a    | 1819 | 1/1   | 0.71 | 0.15 | 68,68,68,68                | 0     |
| 54  | MG   | 2A    | 3071 | 1/1   | 0.71 | 0.28 | 57,57,57,57                | 0     |
| 56  | MPD  | 1O    | 203  | 8/8   | 0.71 | 0.24 | 58,70,76,77                | 0     |
| 54  | MG   | 1T    | 201  | 1/1   | 0.71 | 0.16 | 57,57,57,57                | 0     |
| 54  | MG   | 2Q    | 202  | 1/1   | 0.72 | 0.23 | 47,47,47,47                | 0     |
| 54  | MG   | 1A    | 3199 | 1/1   | 0.72 | 0.37 | 62,62,62,62                | 0     |
| 54  | MG   | 1A    | 3533 | 1/1   | 0.72 | 0.16 | 30,30,30,30                | 0     |
| 54  | MG   | 2A    | 3444 | 1/1   | 0.72 | 0.14 | 65,65,65,65                | 0     |
| 54  | MG   | 1a    | 1845 | 1/1   | 0.72 | 0.13 | 58,58,58,58                | 0     |
| 54  | MG   | 1A    | 4027 | 1/1   | 0.72 | 0.09 | 66,66,66,66                | 0     |
| 54  | MG   | 1p    | 101  | 1/1   | 0.72 | 0.16 | 71,71,71,71                | 0     |
| 54  | MG   | 2A    | 3643 | 1/1   | 0.72 | 0.15 | 79,79,79,79                | 0     |
| 54  | MG   | 1t    | 202  | 1/1   | 0.72 | 0.12 | 62,62,62,62                | 0     |
| 54  | MG   | 2a    | 3180 | 1/1   | 0.72 | 0.18 | 75,75,75,75                | 0     |
| 54  | MG   | 1a    | 1684 | 1/1   | 0.72 | 0.21 | 61,61,61,61                | 0     |
| 54  | MG   | 2a    | 3190 | 1/1   | 0.72 | 0.20 | 64,64,64,64                | 0     |
| 54  | MG   | 2A    | 3337 | 1/1   | 0.72 | 0.13 | 76,76,76,76                | 0     |
| 54  | MG   | 2B    | 202  | 1/1   | 0.72 | 0.19 | 67,67,67,67                | 0     |
| 54  | MG   | 2G    | 203  | 1/1   | 0.72 | 0.15 | 73,73,73,73                | 0     |
| 54  | MG   | 1A    | 4010 | 1/1   | 0.73 | 0.12 | 68,68,68,68                | 0     |
| 54  | MG   | 2A    | 3108 | 1/1   | 0.73 | 0.09 | 64,64,64,64                | 0     |
| 54  | MG   | 2F    | 301  | 1/1   | 0.73 | 0.26 | 65,65,65,65                | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 2A    | 3491 | 1/1   | 0.73 | 0.19 | 63,63,63,63                 | 0     |
| 54  | MG   | 1A    | 3625 | 1/1   | 0.73 | 0.18 | 62,62,62,62                 | 0     |
| 54  | MG   | 1A    | 3931 | 1/1   | 0.73 | 0.12 | 51,51,51,51                 | 0     |
| 54  | MG   | 2a    | 3012 | 1/1   | 0.73 | 0.14 | 56,56,56,56                 | 0     |
| 54  | MG   | 2A    | 3382 | 1/1   | 0.73 | 0.17 | 56,56,56,56                 | 0     |
| 54  | MG   | 1A    | 3980 | 1/1   | 0.73 | 0.20 | 52,52,52,52                 | 0     |
| 54  | MG   | 2A    | 3427 | 1/1   | 0.73 | 0.18 | 54,54,54,54                 | 0     |
| 54  | MG   | 1A    | 3859 | 1/1   | 0.74 | 0.10 | 28,28,28,28                 | 0     |
| 54  | MG   | 2A    | 3157 | 1/1   | 0.74 | 0.36 | 62,62,62,62                 | 0     |
| 54  | MG   | 2B    | 212  | 1/1   | 0.74 | 0.13 | 96,96,96,96                 | 0     |
| 54  | MG   | 1A    | 3867 | 1/1   | 0.74 | 0.34 | 32,32,32,32                 | 0     |
| 54  | MG   | 2A    | 3350 | 1/1   | 0.74 | 0.22 | 59,59,59,59                 | 0     |
| 54  | MG   | 1A    | 3524 | 1/1   | 0.74 | 0.19 | 29,29,29,29                 | 0     |
| 54  | MG   | 2T    | 203  | 1/1   | 0.74 | 0.21 | 63,63,63,63                 | 0     |
| 54  | MG   | 2A    | 3517 | 1/1   | 0.74 | 0.13 | 61,61,61,61                 | 0     |
| 54  | MG   | 1A    | 3608 | 1/1   | 0.74 | 0.30 | 62,62,62,62                 | 0     |
| 54  | MG   | 1A    | 3220 | 1/1   | 0.74 | 0.16 | 39,39,39,39                 | 0     |
| 54  | MG   | 1A    | 3270 | 1/1   | 0.74 | 0.10 | 44,44,44,44                 | 0     |
| 54  | MG   | 1A    | 3878 | 1/1   | 0.75 | 0.13 | 41,41,41,41                 | 0     |
| 54  | MG   | 2A    | 3364 | 1/1   | 0.75 | 0.17 | 55,55,55,55                 | 0     |
| 54  | MG   | 2A    | 3559 | 1/1   | 0.75 | 0.14 | 79,79,79,79                 | 0     |
| 54  | MG   | 1A    | 3975 | 1/1   | 0.75 | 0.15 | 64,64,64,64                 | 0     |
| 54  | MG   | 1a    | 1729 | 1/1   | 0.75 | 0.35 | 75,75,75,75                 | 0     |
| 54  | MG   | 1a    | 1734 | 1/1   | 0.75 | 0.23 | 80,80,80,80                 | 0     |
| 54  | MG   | 2A    | 3753 | 1/1   | 0.75 | 0.20 | 72,72,72,72                 | 0     |
| 54  | MG   | 2A    | 3410 | 1/1   | 0.75 | 0.20 | 60,60,60,60                 | 0     |
| 54  | MG   | 1E    | 303  | 1/1   | 0.75 | 0.25 | 59,59,59,59                 | 0     |
| 54  | MG   | 1a    | 1856 | 1/1   | 0.75 | 0.14 | 63,63,63,63                 | 0     |
| 54  | MG   | 2A    | 3447 | 1/1   | 0.75 | 0.21 | 56,56,56,56                 | 0     |
| 54  | MG   | 1G    | 201  | 1/1   | 0.75 | 0.14 | 78,78,78,78                 | 0     |
| 54  | MG   | 2O    | 202  | 1/1   | 0.75 | 0.23 | 73,73,73,73                 | 0     |
| 54  | MG   | 2A    | 3329 | 1/1   | 0.75 | 0.16 | 62,62,62,62                 | 0     |
| 54  | MG   | 1A    | 3914 | 1/1   | 0.75 | 0.14 | 27,27,27,27                 | 0     |
| 54  | MG   | 1a    | 1705 | 1/1   | 0.76 | 0.16 | 85,85,85,85                 | 0     |
| 54  | MG   | 1A    | 3579 | 1/1   | 0.76 | 0.16 | 23,23,23,23                 | 0     |
| 54  | MG   | 1A    | 3737 | 1/1   | 0.76 | 0.13 | 72,72,72,72                 | 0     |
| 54  | MG   | 1A    | 3993 | 1/1   | 0.76 | 0.28 | 56,56,56,56                 | 0     |
| 54  | MG   | 1a    | 1750 | 1/1   | 0.76 | 0.29 | 67,67,67,67                 | 0     |
| 54  | MG   | 1A    | 3998 | 1/1   | 0.76 | 0.22 | 62,62,62,62                 | 0     |
| 54  | MG   | 2a    | 3066 | 1/1   | 0.76 | 0.10 | 60,60,60,60                 | 0     |
| 54  | MG   | 1A    | 3519 | 1/1   | 0.76 | 0.29 | 53,53,53,53                 | 0     |
| 54  | MG   | 1a    | 1621 | 1/1   | 0.76 | 0.15 | 68,68,68,68                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 2A    | 3426 | 1/1   | 0.76 | 0.14 | 49,49,49,49                 | 0     |
| 54  | MG   | 1A    | 3658 | 1/1   | 0.76 | 0.21 | 24,24,24,24                 | 0     |
| 54  | MG   | 1y    | 3102 | 1/1   | 0.76 | 0.15 | 71,71,71,71                 | 0     |
| 54  | MG   | 1a    | 1831 | 1/1   | 0.76 | 0.31 | 63,63,63,63                 | 0     |
| 54  | MG   | 2A    | 3090 | 1/1   | 0.76 | 0.27 | 63,63,63,63                 | 0     |
| 54  | MG   | 1D    | 314  | 1/1   | 0.76 | 0.21 | 35,35,35,35                 | 0     |
| 54  | MG   | 1A    | 3162 | 1/1   | 0.76 | 0.14 | 45,45,45,45                 | 0     |
| 58  | ZN   | 14    | 501  | 1/1   | 0.76 | 0.19 | 150,150,150,150             | 0     |
| 54  | MG   | 2B    | 207  | 1/1   | 0.77 | 0.29 | 69,69,69,69                 | 0     |
| 54  | MG   | 1a    | 1814 | 1/1   | 0.77 | 0.13 | 71,71,71,71                 | 0     |
| 54  | MG   | 2A    | 3089 | 1/1   | 0.77 | 0.25 | 66,66,66,66                 | 0     |
| 54  | MG   | 1A    | 3630 | 1/1   | 0.77 | 0.35 | 32,32,32,32                 | 0     |
| 54  | MG   | 2A    | 3574 | 1/1   | 0.77 | 0.16 | 48,48,48,48                 | 0     |
| 54  | MG   | 1G    | 202  | 1/1   | 0.77 | 0.19 | 55,55,55,55                 | 0     |
| 54  | MG   | 2A    | 3394 | 1/1   | 0.78 | 0.21 | 56,56,56,56                 | 0     |
| 54  | MG   | 1a    | 1677 | 1/1   | 0.78 | 0.19 | 67,67,67,67                 | 0     |
| 54  | MG   | 2A    | 3512 | 1/1   | 0.78 | 0.17 | 73,73,73,73                 | 0     |
| 54  | MG   | 2A    | 3231 | 1/1   | 0.78 | 0.37 | 59,59,59,59                 | 0     |
| 54  | MG   | 2A    | 3525 | 1/1   | 0.78 | 0.17 | 65,65,65,65                 | 0     |
| 54  | MG   | 1a    | 1878 | 1/1   | 0.78 | 0.13 | 46,46,46,46                 | 0     |
| 54  | MG   | 1y    | 3104 | 1/1   | 0.78 | 0.13 | 78,78,78,78                 | 0     |
| 54  | MG   | 2A    | 3609 | 1/1   | 0.78 | 0.12 | 53,53,53,53                 | 0     |
| 54  | MG   | 1a    | 1800 | 1/1   | 0.78 | 0.21 | 69,69,69,69                 | 0     |
| 54  | MG   | 1H    | 202  | 1/1   | 0.78 | 0.10 | 53,53,53,53                 | 0     |
| 54  | MG   | 1A    | 3783 | 1/1   | 0.78 | 0.13 | 47,47,47,47                 | 0     |
| 54  | MG   | 2A    | 3701 | 1/1   | 0.78 | 0.19 | 66,66,66,66                 | 0     |
| 54  | MG   | 1a    | 1766 | 1/1   | 0.78 | 0.16 | 69,69,69,69                 | 0     |
| 54  | MG   | 1A    | 3835 | 1/1   | 0.79 | 0.12 | 38,38,38,38                 | 0     |
| 54  | MG   | 1a    | 1781 | 1/1   | 0.79 | 0.12 | 70,70,70,70                 | 0     |
| 54  | MG   | 1A    | 3336 | 1/1   | 0.79 | 0.13 | 36,36,36,36                 | 0     |
| 54  | MG   | 1a    | 1703 | 1/1   | 0.79 | 0.25 | 66,66,66,66                 | 0     |
| 54  | MG   | 1A    | 3864 | 1/1   | 0.79 | 0.14 | 73,73,73,73                 | 0     |
| 54  | MG   | 2a    | 3019 | 1/1   | 0.79 | 0.20 | 66,66,66,66                 | 0     |
| 54  | MG   | 1A    | 3084 | 1/1   | 0.79 | 0.20 | 57,57,57,57                 | 0     |
| 54  | MG   | 1a    | 1716 | 1/1   | 0.79 | 0.23 | 80,80,80,80                 | 0     |
| 54  | MG   | 2A    | 3046 | 1/1   | 0.79 | 0.10 | 54,54,54,54                 | 0     |
| 54  | MG   | 2A    | 3688 | 1/1   | 0.79 | 0.12 | 27,27,27,27                 | 0     |
| 54  | MG   | 1A    | 3778 | 1/1   | 0.79 | 0.14 | 56,56,56,56                 | 0     |
| 54  | MG   | 2a    | 3102 | 1/1   | 0.79 | 0.10 | 55,55,55,55                 | 0     |
| 54  | MG   | 2a    | 3103 | 1/1   | 0.79 | 0.24 | 74,74,74,74                 | 0     |
| 54  | MG   | 1A    | 3143 | 1/1   | 0.79 | 0.17 | 47,47,47,47                 | 0     |
| 54  | MG   | 2A    | 3717 | 1/1   | 0.79 | 0.20 | 59,59,59,59                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 2A    | 3752 | 1/1   | 0.79 | 0.16 | 61,61,61,61                 | 0     |
| 54  | MG   | 1B    | 215  | 1/1   | 0.79 | 0.13 | 59,59,59,59                 | 0     |
| 54  | MG   | 1A    | 3802 | 1/1   | 0.79 | 0.28 | 30,30,30,30                 | 0     |
| 54  | MG   | 1A    | 3191 | 1/1   | 0.79 | 0.16 | 69,69,69,69                 | 0     |
| 54  | MG   | 2A    | 3457 | 1/1   | 0.79 | 0.13 | 51,51,51,51                 | 0     |
| 54  | MG   | 2q    | 201  | 1/1   | 0.79 | 0.13 | 48,48,48,48                 | 0     |
| 54  | MG   | 1a    | 1867 | 1/1   | 0.79 | 0.13 | 93,93,93,93                 | 0     |
| 54  | MG   | 2A    | 3312 | 1/1   | 0.79 | 0.19 | 64,64,64,64                 | 0     |
| 54  | MG   | 1F    | 315  | 1/1   | 0.79 | 0.27 | 41,41,41,41                 | 0     |
| 54  | MG   | 1A    | 4045 | 1/1   | 0.80 | 0.24 | 59,59,59,59                 | 0     |
| 54  | MG   | 2a    | 3007 | 1/1   | 0.80 | 0.16 | 68,68,68,68                 | 0     |
| 54  | MG   | 1A    | 3412 | 1/1   | 0.80 | 0.15 | 57,57,57,57                 | 0     |
| 54  | MG   | 1A    | 3976 | 1/1   | 0.80 | 0.12 | 48,48,48,48                 | 0     |
| 54  | MG   | 1A    | 3705 | 1/1   | 0.80 | 0.14 | 27,27,27,27                 | 0     |
| 54  | MG   | 2A    | 3703 | 1/1   | 0.80 | 0.29 | 52,52,52,52                 | 0     |
| 54  | MG   | 1A    | 3710 | 1/1   | 0.80 | 0.31 | 40,40,40,40                 | 0     |
| 54  | MG   | 2A    | 3746 | 1/1   | 0.80 | 0.18 | 58,58,58,58                 | 0     |
| 54  | MG   | 2a    | 3065 | 1/1   | 0.80 | 0.19 | 65,65,65,65                 | 0     |
| 54  | MG   | 1A    | 3593 | 1/1   | 0.80 | 0.09 | 24,24,24,24                 | 0     |
| 54  | MG   | 2A    | 3051 | 1/1   | 0.80 | 0.22 | 70,70,70,70                 | 0     |
| 54  | MG   | 2A    | 3055 | 1/1   | 0.80 | 0.19 | 62,62,62,62                 | 0     |
| 54  | MG   | 2A    | 3375 | 1/1   | 0.80 | 0.26 | 74,74,74,74                 | 0     |
| 54  | MG   | 2A    | 3379 | 1/1   | 0.80 | 0.26 | 54,54,54,54                 | 0     |
| 54  | MG   | 2a    | 3143 | 1/1   | 0.80 | 0.15 | 61,61,61,61                 | 0     |
| 54  | MG   | 1A    | 3439 | 1/1   | 0.80 | 0.19 | 57,57,57,57                 | 0     |
| 54  | MG   | 2B    | 217  | 1/1   | 0.80 | 0.20 | 80,80,80,80                 | 0     |
| 54  | MG   | 2a    | 3182 | 1/1   | 0.80 | 0.20 | 53,53,53,53                 | 0     |
| 54  | MG   | 2D    | 311  | 1/1   | 0.80 | 0.23 | 64,64,64,64                 | 0     |
| 54  | MG   | 1a    | 1657 | 1/1   | 0.80 | 0.17 | 69,69,69,69                 | 0     |
| 54  | MG   | 2G    | 202  | 1/1   | 0.80 | 0.16 | 76,76,76,76                 | 0     |
| 54  | MG   | 2A    | 3403 | 1/1   | 0.80 | 0.12 | 48,48,48,48                 | 0     |
| 54  | MG   | 2r    | 101  | 1/1   | 0.80 | 0.10 | 74,74,74,74                 | 0     |
| 56  | MPD  | 1A    | 4051 | 8/8   | 0.80 | 0.34 | 46,52,59,63                 | 0     |
| 54  | MG   | 1A    | 3281 | 1/1   | 0.80 | 0.14 | 52,52,52,52                 | 0     |
| 54  | MG   | 1e    | 201  | 1/1   | 0.80 | 0.23 | 51,51,51,51                 | 0     |
| 54  | MG   | 2A    | 3417 | 1/1   | 0.80 | 0.20 | 32,32,32,32                 | 0     |
| 54  | MG   | 1a    | 1740 | 1/1   | 0.81 | 0.18 | 63,63,63,63                 | 0     |
| 54  | MG   | 2A    | 3557 | 1/1   | 0.81 | 0.19 | 48,48,48,48                 | 0     |
| 54  | MG   | 1a    | 1872 | 1/1   | 0.81 | 0.22 | 65,65,65,65                 | 0     |
| 54  | MG   | 1a    | 1749 | 1/1   | 0.81 | 0.22 | 67,67,67,67                 | 0     |
| 54  | MG   | 2A    | 3588 | 1/1   | 0.81 | 0.16 | 78,78,78,78                 | 0     |
| 54  | MG   | 2a    | 3026 | 1/1   | 0.81 | 0.35 | 67,67,67,67                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 2a    | 3030 | 1/1   | 0.81 | 0.27 | 57,57,57,57                 | 0     |
| 54  | MG   | 2a    | 3037 | 1/1   | 0.81 | 0.18 | 71,71,71,71                 | 0     |
| 54  | MG   | 2a    | 3038 | 1/1   | 0.81 | 0.14 | 55,55,55,55                 | 0     |
| 54  | MG   | 1A    | 3299 | 1/1   | 0.81 | 0.22 | 59,59,59,59                 | 0     |
| 54  | MG   | 1a    | 1639 | 1/1   | 0.81 | 0.23 | 70,70,70,70                 | 0     |
| 54  | MG   | 1A    | 3826 | 1/1   | 0.81 | 0.17 | 59,59,59,59                 | 0     |
| 54  | MG   | 1a    | 1653 | 1/1   | 0.81 | 0.15 | 73,73,73,73                 | 0     |
| 54  | MG   | 1A    | 4038 | 1/1   | 0.81 | 0.11 | 49,49,49,49                 | 0     |
| 54  | MG   | 1A    | 3659 | 1/1   | 0.81 | 0.18 | 67,67,67,67                 | 0     |
| 54  | MG   | 1a    | 1793 | 1/1   | 0.81 | 0.17 | 70,70,70,70                 | 0     |
| 54  | MG   | 1a    | 1681 | 1/1   | 0.81 | 0.16 | 53,53,53,53                 | 0     |
| 54  | MG   | 2a    | 3114 | 1/1   | 0.81 | 0.19 | 72,72,72,72                 | 0     |
| 54  | MG   | 2A    | 3740 | 1/1   | 0.81 | 0.17 | 63,63,63,63                 | 0     |
| 54  | MG   | 1A    | 3893 | 1/1   | 0.81 | 0.13 | 70,70,70,70                 | 0     |
| 54  | MG   | 1a    | 1689 | 1/1   | 0.81 | 0.27 | 66,66,66,66                 | 0     |
| 54  | MG   | 2A    | 3421 | 1/1   | 0.81 | 0.14 | 52,52,52,52                 | 0     |
| 54  | MG   | 1B    | 217  | 1/1   | 0.81 | 0.13 | 48,48,48,48                 | 0     |
| 54  | MG   | 1B    | 220  | 1/1   | 0.81 | 0.10 | 37,37,37,37                 | 0     |
| 54  | MG   | 1T    | 204  | 1/1   | 0.81 | 0.10 | 52,52,52,52                 | 0     |
| 54  | MG   | 1A    | 3847 | 1/1   | 0.81 | 0.21 | 36,36,36,36                 | 0     |
| 54  | MG   | 1A    | 3773 | 1/1   | 0.81 | 0.20 | 32,32,32,32                 | 0     |
| 54  | MG   | 1a    | 1633 | 1/1   | 0.81 | 0.12 | 57,57,57,57                 | 0     |
| 54  | MG   | 2A    | 3224 | 1/1   | 0.81 | 0.13 | 62,62,62,62                 | 0     |
| 54  | MG   | 1a    | 1736 | 1/1   | 0.81 | 0.20 | 52,52,52,52                 | 0     |
| 54  | MG   | 2A    | 3285 | 1/1   | 0.81 | 0.18 | 43,43,43,43                 | 0     |
| 56  | MPD  | 1a    | 1883 | 8/8   | 0.81 | 0.15 | 49,64,76,80                 | 0     |
| 56  | MPD  | 2A    | 3759 | 8/8   | 0.81 | 0.25 | 55,58,70,70                 | 0     |
| 54  | MG   | 2A    | 3289 | 1/1   | 0.81 | 0.14 | 51,51,51,51                 | 0     |
| 54  | MG   | 1a    | 1864 | 1/1   | 0.81 | 0.12 | 67,67,67,67                 | 0     |
| 54  | MG   | 2A    | 3683 | 1/1   | 0.82 | 0.13 | 58,58,58,58                 | 0     |
| 54  | MG   | 1P    | 205  | 1/1   | 0.82 | 0.10 | 75,75,75,75                 | 0     |
| 54  | MG   | 1A    | 3933 | 1/1   | 0.82 | 0.09 | 49,49,49,49                 | 0     |
| 54  | MG   | 1A    | 3940 | 1/1   | 0.82 | 0.17 | 48,48,48,48                 | 0     |
| 54  | MG   | 2a    | 3059 | 1/1   | 0.82 | 0.27 | 73,73,73,73                 | 0     |
| 54  | MG   | 1a    | 1763 | 1/1   | 0.82 | 0.15 | 65,65,65,65                 | 0     |
| 54  | MG   | 1T    | 202  | 1/1   | 0.82 | 0.10 | 43,43,43,43                 | 0     |
| 54  | MG   | 2A    | 3193 | 1/1   | 0.82 | 0.40 | 69,69,69,69                 | 0     |
| 54  | MG   | 1A    | 3796 | 1/1   | 0.82 | 0.43 | 41,41,41,41                 | 0     |
| 54  | MG   | 1a    | 1769 | 1/1   | 0.82 | 0.16 | 68,68,68,68                 | 0     |
| 54  | MG   | 2a    | 3082 | 1/1   | 0.82 | 0.13 | 52,52,52,52                 | 0     |
| 54  | MG   | 2A    | 3238 | 1/1   | 0.82 | 0.10 | 47,47,47,47                 | 0     |
| 54  | MG   | 1A    | 3584 | 1/1   | 0.82 | 0.14 | 25,25,25,25                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 1A    | 3509 | 1/1   | 0.82 | 0.11 | 44,44,44,44                 | 0     |
| 54  | MG   | 1A    | 3881 | 1/1   | 0.82 | 0.16 | 45,45,45,45                 | 0     |
| 54  | MG   | 1A    | 3772 | 1/1   | 0.82 | 0.27 | 36,36,36,36                 | 0     |
| 54  | MG   | 2A    | 3506 | 1/1   | 0.82 | 0.22 | 68,68,68,68                 | 0     |
| 54  | MG   | 2D    | 304  | 1/1   | 0.82 | 0.38 | 51,51,51,51                 | 0     |
| 54  | MG   | 2a    | 3157 | 1/1   | 0.82 | 0.17 | 67,67,67,67                 | 0     |
| 54  | MG   | 1a    | 1806 | 1/1   | 0.82 | 0.11 | 102,102,102,102             | 0     |
| 54  | MG   | 2A    | 3515 | 1/1   | 0.82 | 0.21 | 66,66,66,66                 | 0     |
| 54  | MG   | 2a    | 3184 | 1/1   | 0.82 | 0.21 | 67,67,67,67                 | 0     |
| 54  | MG   | 1a    | 1721 | 1/1   | 0.82 | 0.12 | 73,73,73,73                 | 0     |
| 54  | MG   | 2a    | 3189 | 1/1   | 0.82 | 0.19 | 46,46,46,46                 | 0     |
| 54  | MG   | 1F    | 316  | 1/1   | 0.82 | 0.12 | 52,52,52,52                 | 0     |
| 54  | MG   | 2A    | 3530 | 1/1   | 0.82 | 0.10 | 53,53,53,53                 | 0     |
| 54  | MG   | 2A    | 3371 | 1/1   | 0.82 | 0.12 | 42,42,42,42                 | 0     |
| 54  | MG   | 1A    | 3633 | 1/1   | 0.82 | 0.43 | 31,31,31,31                 | 0     |
| 54  | MG   | 2a    | 3004 | 1/1   | 0.82 | 0.12 | 62,62,62,62                 | 0     |
| 54  | MG   | 2A    | 3031 | 1/1   | 0.82 | 0.17 | 58,58,58,58                 | 0     |
| 54  | MG   | 2A    | 3036 | 1/1   | 0.82 | 0.23 | 53,53,53,53                 | 0     |
| 54  | MG   | 1A    | 3188 | 1/1   | 0.82 | 0.20 | 58,58,58,58                 | 0     |
| 54  | MG   | 1A    | 3155 | 1/1   | 0.82 | 0.18 | 39,39,39,39                 | 0     |
| 54  | MG   | 1a    | 1748 | 1/1   | 0.82 | 0.10 | 51,51,51,51                 | 0     |
| 54  | MG   | 1A    | 3382 | 1/1   | 0.83 | 0.11 | 37,37,37,37                 | 0     |
| 54  | MG   | 2A    | 3544 | 1/1   | 0.83 | 0.12 | 72,72,72,72                 | 0     |
| 54  | MG   | 1A    | 4005 | 1/1   | 0.83 | 0.19 | 44,44,44,44                 | 0     |
| 54  | MG   | 1A    | 3634 | 1/1   | 0.83 | 0.14 | 57,57,57,57                 | 0     |
| 54  | MG   | 2a    | 3027 | 1/1   | 0.83 | 0.20 | 65,65,65,65                 | 0     |
| 54  | MG   | 2A    | 3569 | 1/1   | 0.83 | 0.12 | 98,98,98,98                 | 0     |
| 54  | MG   | 2A    | 3572 | 1/1   | 0.83 | 0.16 | 61,61,61,61                 | 0     |
| 54  | MG   | 1a    | 1679 | 1/1   | 0.83 | 0.23 | 55,55,55,55                 | 0     |
| 54  | MG   | 1A    | 3594 | 1/1   | 0.83 | 0.17 | 33,33,33,33                 | 0     |
| 54  | MG   | 1A    | 3195 | 1/1   | 0.83 | 0.15 | 33,33,33,33                 | 0     |
| 54  | MG   | 1e    | 203  | 1/1   | 0.83 | 0.13 | 63,63,63,63                 | 0     |
| 54  | MG   | 1a    | 1775 | 1/1   | 0.83 | 0.18 | 81,81,81,81                 | 0     |
| 54  | MG   | 1a    | 1686 | 1/1   | 0.83 | 0.18 | 48,48,48,48                 | 0     |
| 54  | MG   | 1A    | 3340 | 1/1   | 0.83 | 0.12 | 39,39,39,39                 | 0     |
| 54  | MG   | 1B    | 207  | 1/1   | 0.83 | 0.19 | 55,55,55,55                 | 0     |
| 54  | MG   | 1a    | 1798 | 1/1   | 0.83 | 0.18 | 68,68,68,68                 | 0     |
| 54  | MG   | 1a    | 1799 | 1/1   | 0.83 | 0.21 | 69,69,69,69                 | 0     |
| 54  | MG   | 2A    | 3716 | 1/1   | 0.83 | 0.11 | 58,58,58,58                 | 0     |
| 54  | MG   | 2A    | 3034 | 1/1   | 0.83 | 0.21 | 82,82,82,82                 | 0     |
| 54  | MG   | 2A    | 3735 | 1/1   | 0.83 | 0.26 | 72,72,72,72                 | 0     |
| 54  | MG   | 1B    | 209  | 1/1   | 0.83 | 0.10 | 41,41,41,41                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 1A    | 3282 | 1/1   | 0.83 | 0.10 | 45,45,45,45                 | 0     |
| 54  | MG   | 15    | 106  | 1/1   | 0.83 | 0.11 | 42,42,42,42                 | 0     |
| 54  | MG   | 2a    | 3156 | 1/1   | 0.83 | 0.12 | 70,70,70,70                 | 0     |
| 54  | MG   | 1A    | 3687 | 1/1   | 0.83 | 0.16 | 55,55,55,55                 | 0     |
| 54  | MG   | 2a    | 3162 | 1/1   | 0.83 | 0.15 | 40,40,40,40                 | 0     |
| 54  | MG   | 1a    | 1824 | 1/1   | 0.83 | 0.15 | 56,56,56,56                 | 0     |
| 54  | MG   | 1A    | 3970 | 1/1   | 0.83 | 0.17 | 48,48,48,48                 | 0     |
| 54  | MG   | 1a    | 1731 | 1/1   | 0.83 | 0.22 | 49,49,49,49                 | 0     |
| 54  | MG   | 1a    | 1835 | 1/1   | 0.83 | 0.13 | 59,59,59,59                 | 0     |
| 54  | MG   | 2A    | 3452 | 1/1   | 0.83 | 0.18 | 60,60,60,60                 | 0     |
| 54  | MG   | 2A    | 3118 | 1/1   | 0.83 | 0.16 | 42,42,42,42                 | 0     |
| 54  | MG   | 2a    | 3191 | 1/1   | 0.83 | 0.25 | 76,76,76,76                 | 0     |
| 54  | MG   | 2A    | 3141 | 1/1   | 0.83 | 0.13 | 60,60,60,60                 | 0     |
| 54  | MG   | 1A    | 3862 | 1/1   | 0.83 | 0.07 | 33,33,33,33                 | 0     |
| 54  | MG   | 1A    | 3780 | 1/1   | 0.83 | 0.17 | 55,55,55,55                 | 0     |
| 54  | MG   | 1A    | 3190 | 1/1   | 0.83 | 0.12 | 45,45,45,45                 | 0     |
| 54  | MG   | 1a    | 1747 | 1/1   | 0.83 | 0.16 | 58,58,58,58                 | 0     |
| 54  | MG   | 1A    | 3789 | 1/1   | 0.83 | 0.18 | 54,54,54,54                 | 0     |
| 54  | MG   | 2A    | 3516 | 1/1   | 0.83 | 0.11 | 58,58,58,58                 | 0     |
| 54  | MG   | 2A    | 3270 | 1/1   | 0.83 | 0.14 | 47,47,47,47                 | 0     |
| 54  | MG   | 1a    | 1648 | 1/1   | 0.83 | 0.23 | 57,57,57,57                 | 0     |
| 54  | MG   | 1a    | 1722 | 1/1   | 0.84 | 0.16 | 45,45,45,45                 | 0     |
| 54  | MG   | 2A    | 3412 | 1/1   | 0.84 | 0.29 | 64,64,64,64                 | 0     |
| 54  | MG   | 1A    | 3852 | 1/1   | 0.84 | 0.13 | 55,55,55,55                 | 0     |
| 54  | MG   | 1A    | 3293 | 1/1   | 0.84 | 0.18 | 39,39,39,39                 | 0     |
| 54  | MG   | 2a    | 3049 | 1/1   | 0.84 | 0.24 | 50,50,50,50                 | 0     |
| 54  | MG   | 2A    | 3215 | 1/1   | 0.84 | 0.22 | 49,49,49,49                 | 0     |
| 54  | MG   | 1a    | 1656 | 1/1   | 0.84 | 0.31 | 69,69,69,69                 | 0     |
| 54  | MG   | 2A    | 3437 | 1/1   | 0.84 | 0.10 | 61,61,61,61                 | 0     |
| 54  | MG   | 1A    | 3706 | 1/1   | 0.84 | 0.29 | 23,23,23,23                 | 0     |
| 54  | MG   | 1a    | 1672 | 1/1   | 0.84 | 0.26 | 71,71,71,71                 | 0     |
| 54  | MG   | 1A    | 4018 | 1/1   | 0.84 | 0.11 | 43,43,43,43                 | 0     |
| 54  | MG   | 2A    | 3275 | 1/1   | 0.84 | 0.15 | 58,58,58,58                 | 0     |
| 54  | MG   | 2a    | 3099 | 1/1   | 0.84 | 0.16 | 74,74,74,74                 | 0     |
| 54  | MG   | 2A    | 3284 | 1/1   | 0.84 | 0.22 | 52,52,52,52                 | 0     |
| 54  | MG   | 1Z    | 301  | 1/1   | 0.84 | 0.12 | 50,50,50,50                 | 0     |
| 54  | MG   | 1A    | 3264 | 1/1   | 0.84 | 0.18 | 62,62,62,62                 | 0     |
| 54  | MG   | 18    | 102  | 1/1   | 0.84 | 0.14 | 36,36,36,36                 | 0     |
| 54  | MG   | 2A    | 3756 | 1/1   | 0.84 | 0.34 | 55,55,55,55                 | 0     |
| 54  | MG   | 2A    | 3503 | 1/1   | 0.84 | 0.35 | 61,61,61,61                 | 0     |
| 54  | MG   | 1a    | 1602 | 1/1   | 0.84 | 0.18 | 65,65,65,65                 | 0     |
| 54  | MG   | 2a    | 3152 | 1/1   | 0.84 | 0.12 | 71,71,71,71                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 2a    | 3155 | 1/1   | 0.84 | 0.10 | 57,57,57,57                 | 0     |
| 54  | MG   | 1A    | 3679 | 1/1   | 0.84 | 0.15 | 57,57,57,57                 | 0     |
| 54  | MG   | 2A    | 3338 | 1/1   | 0.84 | 0.17 | 43,43,43,43                 | 0     |
| 54  | MG   | 1A    | 4041 | 1/1   | 0.84 | 0.15 | 61,61,61,61                 | 0     |
| 54  | MG   | 2a    | 3176 | 1/1   | 0.84 | 0.11 | 62,62,62,62                 | 0     |
| 54  | MG   | 1A    | 3621 | 1/1   | 0.84 | 0.12 | 51,51,51,51                 | 0     |
| 54  | MG   | 2A    | 3367 | 1/1   | 0.84 | 0.13 | 42,42,42,42                 | 0     |
| 54  | MG   | 2G    | 201  | 1/1   | 0.84 | 0.10 | 70,70,70,70                 | 0     |
| 54  | MG   | 2a    | 3185 | 1/1   | 0.84 | 0.14 | 54,54,54,54                 | 0     |
| 54  | MG   | 1a    | 1851 | 1/1   | 0.84 | 0.12 | 55,55,55,55                 | 0     |
| 54  | MG   | 1a    | 1706 | 1/1   | 0.84 | 0.17 | 50,50,50,50                 | 0     |
| 54  | MG   | 1A    | 3840 | 1/1   | 0.84 | 0.11 | 42,42,42,42                 | 0     |
| 54  | MG   | 2A    | 3082 | 1/1   | 0.84 | 0.11 | 45,45,45,45                 | 0     |
| 54  | MG   | 1A    | 3843 | 1/1   | 0.84 | 0.16 | 37,37,37,37                 | 0     |
| 54  | MG   | 2n    | 101  | 1/1   | 0.84 | 0.17 | 60,60,60,60                 | 0     |
| 54  | MG   | 2A    | 3392 | 1/1   | 0.84 | 0.24 | 66,66,66,66                 | 0     |
| 54  | MG   | 1A    | 3170 | 1/1   | 0.84 | 0.18 | 49,49,49,49                 | 0     |
| 54  | MG   | 1a    | 1783 | 1/1   | 0.84 | 0.07 | 57,57,57,57                 | 0     |
| 54  | MG   | 2a    | 3010 | 1/1   | 0.84 | 0.22 | 55,55,55,55                 | 0     |
| 54  | MG   | 2A    | 3593 | 1/1   | 0.84 | 0.14 | 45,45,45,45                 | 0     |
| 54  | MG   | 2A    | 3606 | 1/1   | 0.84 | 0.18 | 34,34,34,34                 | 0     |
| 54  | MG   | 1a    | 1876 | 1/1   | 0.84 | 0.10 | 70,70,70,70                 | 0     |
| 54  | MG   | 2A    | 3637 | 1/1   | 0.84 | 0.15 | 49,49,49,49                 | 0     |
| 54  | MG   | 1B    | 226  | 1/1   | 0.85 | 0.10 | 49,49,49,49                 | 0     |
| 54  | MG   | 28    | 102  | 1/1   | 0.85 | 0.15 | 44,44,44,44                 | 0     |
| 54  | MG   | 1A    | 3431 | 1/1   | 0.85 | 0.24 | 60,60,60,60                 | 0     |
| 54  | MG   | 1E    | 302  | 1/1   | 0.85 | 0.10 | 16,16,16,16                 | 0     |
| 54  | MG   | 1A    | 3977 | 1/1   | 0.85 | 0.11 | 28,28,28,28                 | 0     |
| 54  | MG   | 1a    | 1753 | 1/1   | 0.85 | 0.14 | 72,72,72,72                 | 0     |
| 54  | MG   | 1a    | 1755 | 1/1   | 0.85 | 0.16 | 44,44,44,44                 | 0     |
| 54  | MG   | 1a    | 1880 | 1/1   | 0.85 | 0.26 | 79,79,79,79                 | 0     |
| 54  | MG   | 1E    | 305  | 1/1   | 0.85 | 0.11 | 44,44,44,44                 | 0     |
| 54  | MG   | 2A    | 3307 | 1/1   | 0.85 | 0.10 | 27,27,27,27                 | 0     |
| 54  | MG   | 1F    | 314  | 1/1   | 0.85 | 0.20 | 62,62,62,62                 | 0     |
| 54  | MG   | 1a    | 1654 | 1/1   | 0.85 | 0.27 | 42,42,42,42                 | 0     |
| 54  | MG   | 1A    | 3739 | 1/1   | 0.85 | 0.14 | 53,53,53,53                 | 0     |
| 54  | MG   | 2a    | 3046 | 1/1   | 0.85 | 0.13 | 61,61,61,61                 | 0     |
| 54  | MG   | 1A    | 3989 | 1/1   | 0.85 | 0.09 | 65,65,65,65                 | 0     |
| 54  | MG   | 2A    | 3343 | 1/1   | 0.85 | 0.14 | 63,63,63,63                 | 0     |
| 54  | MG   | 1i    | 201  | 1/1   | 0.85 | 0.09 | 74,74,74,74                 | 0     |
| 54  | MG   | 2A    | 3601 | 1/1   | 0.85 | 0.12 | 33,33,33,33                 | 0     |
| 54  | MG   | 1A    | 3557 | 1/1   | 0.85 | 0.11 | 43,43,43,43                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 1A    | 3573 | 1/1   | 0.85 | 0.30 | 32,32,32,32                 | 0     |
| 54  | MG   | 2A    | 3617 | 1/1   | 0.85 | 0.26 | 56,56,56,56                 | 0     |
| 54  | MG   | 1A    | 3250 | 1/1   | 0.85 | 0.10 | 65,65,65,65                 | 0     |
| 54  | MG   | 1A    | 3582 | 1/1   | 0.85 | 0.13 | 61,61,61,61                 | 0     |
| 54  | MG   | 2a    | 3093 | 1/1   | 0.85 | 0.26 | 56,56,56,56                 | 0     |
| 54  | MG   | 2a    | 3098 | 1/1   | 0.85 | 0.18 | 67,67,67,67                 | 0     |
| 54  | MG   | 2A    | 3006 | 1/1   | 0.85 | 0.14 | 46,46,46,46                 | 0     |
| 54  | MG   | 1A    | 3458 | 1/1   | 0.85 | 0.09 | 44,44,44,44                 | 0     |
| 54  | MG   | 1A    | 4022 | 1/1   | 0.85 | 0.11 | 57,57,57,57                 | 0     |
| 54  | MG   | 1A    | 3663 | 1/1   | 0.85 | 0.17 | 62,62,62,62                 | 0     |
| 54  | MG   | 1A    | 3463 | 1/1   | 0.85 | 0.12 | 36,36,36,36                 | 0     |
| 54  | MG   | 2A    | 3402 | 1/1   | 0.85 | 0.08 | 70,70,70,70                 | 0     |
| 54  | MG   | 2a    | 3131 | 1/1   | 0.85 | 0.11 | 67,67,67,67                 | 0     |
| 54  | MG   | 2A    | 3050 | 1/1   | 0.85 | 0.17 | 57,57,57,57                 | 0     |
| 54  | MG   | 1A    | 3490 | 1/1   | 0.85 | 0.08 | 67,67,67,67                 | 0     |
| 54  | MG   | 2A    | 3728 | 1/1   | 0.85 | 0.11 | 54,54,54,54                 | 0     |
| 54  | MG   | 1V    | 203  | 1/1   | 0.85 | 0.28 | 51,51,51,51                 | 0     |
| 54  | MG   | 2A    | 3739 | 1/1   | 0.85 | 0.15 | 60,60,60,60                 | 0     |
| 54  | MG   | 1A    | 3273 | 1/1   | 0.85 | 0.25 | 53,53,53,53                 | 0     |
| 54  | MG   | 2A    | 3742 | 1/1   | 0.85 | 0.11 | 55,55,55,55                 | 0     |
| 54  | MG   | 1I    | 101  | 1/1   | 0.85 | 0.39 | 46,46,46,46                 | 0     |
| 54  | MG   | 1A    | 3230 | 1/1   | 0.85 | 0.58 | 37,37,37,37                 | 0     |
| 54  | MG   | 1A    | 3613 | 1/1   | 0.85 | 0.13 | 18,18,18,18                 | 0     |
| 54  | MG   | 18    | 103  | 1/1   | 0.85 | 0.39 | 37,37,37,37                 | 0     |
| 54  | MG   | 1A    | 3384 | 1/1   | 0.85 | 0.12 | 19,19,19,19                 | 0     |
| 54  | MG   | 2A    | 3134 | 1/1   | 0.85 | 0.20 | 70,70,70,70                 | 0     |
| 54  | MG   | 2a    | 3188 | 1/1   | 0.85 | 0.21 | 71,71,71,71                 | 0     |
| 54  | MG   | 1a    | 1607 | 1/1   | 0.85 | 0.30 | 61,61,61,61                 | 0     |
| 54  | MG   | 1A    | 3711 | 1/1   | 0.85 | 0.12 | 26,26,26,26                 | 0     |
| 54  | MG   | 2A    | 3166 | 1/1   | 0.85 | 0.11 | 55,55,55,55                 | 0     |
| 54  | MG   | 2D    | 303  | 1/1   | 0.85 | 0.64 | 39,39,39,39                 | 0     |
| 54  | MG   | 2A    | 3454 | 1/1   | 0.85 | 0.11 | 26,26,26,26                 | 0     |
| 54  | MG   | 2D    | 305  | 1/1   | 0.85 | 0.44 | 40,40,40,40                 | 0     |
| 54  | MG   | 2A    | 3176 | 1/1   | 0.85 | 0.11 | 64,64,64,64                 | 0     |
| 54  | MG   | 2t    | 201  | 1/1   | 0.85 | 0.16 | 50,50,50,50                 | 0     |
| 54  | MG   | 2A    | 3464 | 1/1   | 0.85 | 0.10 | 60,60,60,60                 | 0     |
| 54  | MG   | 2A    | 3183 | 1/1   | 0.85 | 0.34 | 61,61,61,61                 | 0     |
| 54  | MG   | 1A    | 3268 | 1/1   | 0.85 | 0.15 | 51,51,51,51                 | 0     |
| 56  | MPD  | 2A    | 3758 | 8/8   | 0.85 | 0.27 | 36,41,48,53                 | 0     |
| 54  | MG   | 2A    | 3499 | 1/1   | 0.85 | 0.14 | 50,50,50,50                 | 0     |
| 54  | MG   | 2A    | 3198 | 1/1   | 0.85 | 0.21 | 53,53,53,53                 | 0     |
| 54  | MG   | 1a    | 1744 | 1/1   | 0.85 | 0.09 | 61,61,61,61                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 1a    | 1655 | 1/1   | 0.86 | 0.16 | 67,67,67,67                 | 0     |
| 54  | MG   | 1A    | 3279 | 1/1   | 0.86 | 0.19 | 84,84,84,84                 | 0     |
| 54  | MG   | 2W    | 203  | 1/1   | 0.86 | 0.09 | 48,48,48,48                 | 0     |
| 54  | MG   | 25    | 102  | 1/1   | 0.86 | 0.19 | 56,56,56,56                 | 0     |
| 54  | MG   | 1A    | 3562 | 1/1   | 0.86 | 0.16 | 70,70,70,70                 | 0     |
| 54  | MG   | 2A    | 3236 | 1/1   | 0.86 | 0.10 | 55,55,55,55                 | 0     |
| 54  | MG   | 2A    | 3510 | 1/1   | 0.86 | 0.17 | 62,62,62,62                 | 0     |
| 54  | MG   | 1a    | 1660 | 1/1   | 0.86 | 0.14 | 78,78,78,78                 | 0     |
| 54  | MG   | 2a    | 3008 | 1/1   | 0.86 | 0.10 | 71,71,71,71                 | 0     |
| 54  | MG   | 2A    | 3242 | 1/1   | 0.86 | 0.15 | 65,65,65,65                 | 0     |
| 54  | MG   | 1A    | 3569 | 1/1   | 0.86 | 0.12 | 40,40,40,40                 | 0     |
| 54  | MG   | 2a    | 3016 | 1/1   | 0.86 | 0.09 | 61,61,61,61                 | 0     |
| 54  | MG   | 2A    | 3272 | 1/1   | 0.86 | 0.16 | 61,61,61,61                 | 0     |
| 54  | MG   | 1A    | 3198 | 1/1   | 0.86 | 0.14 | 39,39,39,39                 | 0     |
| 54  | MG   | 1A    | 3574 | 1/1   | 0.86 | 0.24 | 47,47,47,47                 | 0     |
| 54  | MG   | 1A    | 3987 | 1/1   | 0.86 | 0.23 | 46,46,46,46                 | 0     |
| 54  | MG   | 2A    | 3547 | 1/1   | 0.86 | 0.11 | 69,69,69,69                 | 0     |
| 54  | MG   | 1f    | 202  | 1/1   | 0.86 | 0.11 | 49,49,49,49                 | 0     |
| 54  | MG   | 2A    | 3302 | 1/1   | 0.86 | 0.12 | 45,45,45,45                 | 0     |
| 54  | MG   | 1h    | 201  | 1/1   | 0.86 | 0.12 | 65,65,65,65                 | 0     |
| 54  | MG   | 1A    | 3873 | 1/1   | 0.86 | 0.11 | 40,40,40,40                 | 0     |
| 54  | MG   | 2a    | 3057 | 1/1   | 0.86 | 0.24 | 66,66,66,66                 | 0     |
| 54  | MG   | 1B    | 228  | 1/1   | 0.86 | 0.12 | 71,71,71,71                 | 0     |
| 54  | MG   | 1A    | 3456 | 1/1   | 0.86 | 0.12 | 34,34,34,34                 | 0     |
| 54  | MG   | 1a    | 1691 | 1/1   | 0.86 | 0.17 | 48,48,48,48                 | 0     |
| 54  | MG   | 15    | 108  | 1/1   | 0.86 | 0.10 | 62,62,62,62                 | 0     |
| 54  | MG   | 1A    | 3457 | 1/1   | 0.86 | 0.12 | 40,40,40,40                 | 0     |
| 54  | MG   | 2A    | 3359 | 1/1   | 0.86 | 0.19 | 53,53,53,53                 | 0     |
| 54  | MG   | 2a    | 3074 | 1/1   | 0.86 | 0.24 | 50,50,50,50                 | 0     |
| 54  | MG   | 1A    | 3278 | 1/1   | 0.86 | 0.23 | 67,67,67,67                 | 0     |
| 54  | MG   | 2A    | 3622 | 1/1   | 0.86 | 0.11 | 79,79,79,79                 | 0     |
| 54  | MG   | 1A    | 3635 | 1/1   | 0.86 | 0.19 | 47,47,47,47                 | 0     |
| 54  | MG   | 1A    | 4013 | 1/1   | 0.86 | 0.10 | 41,41,41,41                 | 0     |
| 54  | MG   | 2a    | 3100 | 1/1   | 0.86 | 0.11 | 56,56,56,56                 | 0     |
| 54  | MG   | 1a    | 1610 | 1/1   | 0.86 | 0.13 | 63,63,63,63                 | 0     |
| 54  | MG   | 2A    | 3049 | 1/1   | 0.86 | 0.23 | 46,46,46,46                 | 0     |
| 54  | MG   | 2a    | 3113 | 1/1   | 0.86 | 0.14 | 54,54,54,54                 | 0     |
| 54  | MG   | 1a    | 1823 | 1/1   | 0.86 | 0.12 | 60,60,60,60                 | 0     |
| 54  | MG   | 2A    | 3691 | 1/1   | 0.86 | 0.15 | 66,66,66,66                 | 0     |
| 54  | MG   | 1A    | 3430 | 1/1   | 0.86 | 0.09 | 47,47,47,47                 | 0     |
| 54  | MG   | 2a    | 3119 | 1/1   | 0.86 | 0.12 | 47,47,47,47                 | 0     |
| 54  | MG   | 1a    | 1726 | 1/1   | 0.86 | 0.19 | 53,53,53,53                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 2a    | 3137 | 1/1   | 0.86 | 0.12 | 53,53,53,53                 | 0     |
| 54  | MG   | 2A    | 3058 | 1/1   | 0.86 | 0.16 | 57,57,57,57                 | 0     |
| 54  | MG   | 1a    | 1615 | 1/1   | 0.86 | 0.15 | 74,74,74,74                 | 0     |
| 54  | MG   | 2A    | 3074 | 1/1   | 0.86 | 0.28 | 69,69,69,69                 | 0     |
| 54  | MG   | 2A    | 3726 | 1/1   | 0.86 | 0.13 | 71,71,71,71                 | 0     |
| 54  | MG   | 1A    | 4019 | 1/1   | 0.86 | 0.13 | 41,41,41,41                 | 0     |
| 54  | MG   | 2A    | 3729 | 1/1   | 0.86 | 0.12 | 48,48,48,48                 | 0     |
| 54  | MG   | 1a    | 1839 | 1/1   | 0.86 | 0.13 | 64,64,64,64                 | 0     |
| 54  | MG   | 1a    | 1629 | 1/1   | 0.86 | 0.17 | 44,44,44,44                 | 0     |
| 54  | MG   | 2A    | 3414 | 1/1   | 0.86 | 0.18 | 62,62,62,62                 | 0     |
| 54  | MG   | 1A    | 3645 | 1/1   | 0.86 | 0.18 | 54,54,54,54                 | 0     |
| 54  | MG   | 1A    | 3553 | 1/1   | 0.86 | 0.20 | 48,48,48,48                 | 0     |
| 54  | MG   | 1A    | 3596 | 1/1   | 0.86 | 0.13 | 58,58,58,58                 | 0     |
| 54  | MG   | 1a    | 1854 | 1/1   | 0.86 | 0.16 | 48,48,48,48                 | 0     |
| 54  | MG   | 1H    | 203  | 1/1   | 0.86 | 0.13 | 47,47,47,47                 | 0     |
| 54  | MG   | 2A    | 3160 | 1/1   | 0.86 | 0.12 | 44,44,44,44                 | 0     |
| 54  | MG   | 2A    | 3446 | 1/1   | 0.86 | 0.13 | 75,75,75,75                 | 0     |
| 54  | MG   | 2B    | 204  | 1/1   | 0.86 | 0.10 | 74,74,74,74                 | 0     |
| 54  | MG   | 2A    | 3161 | 1/1   | 0.86 | 0.10 | 52,52,52,52                 | 0     |
| 54  | MG   | 1N    | 201  | 1/1   | 0.86 | 0.12 | 56,56,56,56                 | 0     |
| 54  | MG   | 2A    | 3451 | 1/1   | 0.86 | 0.14 | 61,61,61,61                 | 0     |
| 54  | MG   | 1P    | 203  | 1/1   | 0.86 | 0.25 | 31,31,31,31                 | 0     |
| 54  | MG   | 2A    | 3178 | 1/1   | 0.86 | 0.13 | 59,59,59,59                 | 0     |
| 54  | MG   | 1A    | 3949 | 1/1   | 0.86 | 0.22 | 38,38,38,38                 | 0     |
| 54  | MG   | 2A    | 3459 | 1/1   | 0.86 | 0.10 | 55,55,55,55                 | 0     |
| 54  | MG   | 1a    | 1869 | 1/1   | 0.86 | 0.23 | 62,62,62,62                 | 0     |
| 54  | MG   | 2A    | 3473 | 1/1   | 0.86 | 0.17 | 53,53,53,53                 | 0     |
| 54  | MG   | 2A    | 3481 | 1/1   | 0.86 | 0.26 | 57,57,57,57                 | 0     |
| 54  | MG   | 1a    | 1752 | 1/1   | 0.86 | 0.18 | 76,76,76,76                 | 0     |
| 54  | MG   | 2A    | 3199 | 1/1   | 0.86 | 0.21 | 49,49,49,49                 | 0     |
| 54  | MG   | 2A    | 3220 | 1/1   | 0.87 | 0.11 | 50,50,50,50                 | 0     |
| 54  | MG   | 1A    | 3547 | 1/1   | 0.87 | 0.09 | 39,39,39,39                 | 0     |
| 54  | MG   | 2a    | 3044 | 1/1   | 0.87 | 0.20 | 60,60,60,60                 | 0     |
| 54  | MG   | 1A    | 3572 | 1/1   | 0.87 | 0.15 | 44,44,44,44                 | 0     |
| 54  | MG   | 2A    | 3705 | 1/1   | 0.87 | 0.15 | 67,67,67,67                 | 0     |
| 54  | MG   | 2A    | 3709 | 1/1   | 0.87 | 0.12 | 74,74,74,74                 | 0     |
| 54  | MG   | 1A    | 3829 | 1/1   | 0.87 | 0.07 | 34,34,34,34                 | 0     |
| 54  | MG   | 2A    | 3022 | 1/1   | 0.87 | 0.10 | 60,60,60,60                 | 0     |
| 54  | MG   | 2A    | 3723 | 1/1   | 0.87 | 0.13 | 59,59,59,59                 | 0     |
| 54  | MG   | 1A    | 3762 | 1/1   | 0.87 | 0.07 | 21,21,21,21                 | 0     |
| 54  | MG   | 2A    | 3254 | 1/1   | 0.87 | 0.17 | 61,61,61,61                 | 0     |
| 54  | MG   | 2A    | 3255 | 1/1   | 0.87 | 0.20 | 59,59,59,59                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 2A    | 3268 | 1/1   | 0.87 | 0.17 | 38,38,38,38                 | 0     |
| 54  | MG   | 2a    | 3070 | 1/1   | 0.87 | 0.23 | 53,53,53,53                 | 0     |
| 54  | MG   | 1A    | 3919 | 1/1   | 0.87 | 0.09 | 51,51,51,51                 | 0     |
| 54  | MG   | 2a    | 3075 | 1/1   | 0.87 | 0.31 | 53,53,53,53                 | 0     |
| 54  | MG   | 2a    | 3081 | 1/1   | 0.87 | 0.24 | 53,53,53,53                 | 0     |
| 54  | MG   | 1a    | 1671 | 1/1   | 0.87 | 0.20 | 61,61,61,61                 | 0     |
| 54  | MG   | 2A    | 3040 | 1/1   | 0.87 | 0.14 | 55,55,55,55                 | 0     |
| 54  | MG   | 1A    | 3771 | 1/1   | 0.87 | 0.12 | 18,18,18,18                 | 0     |
| 54  | MG   | 1a    | 1673 | 1/1   | 0.87 | 0.14 | 65,65,65,65                 | 0     |
| 54  | MG   | 1A    | 3841 | 1/1   | 0.87 | 0.14 | 30,30,30,30                 | 0     |
| 54  | MG   | 2a    | 3101 | 1/1   | 0.87 | 0.09 | 63,63,63,63                 | 0     |
| 54  | MG   | 2A    | 3291 | 1/1   | 0.87 | 0.26 | 70,70,70,70                 | 0     |
| 54  | MG   | 1A    | 3552 | 1/1   | 0.87 | 0.09 | 41,41,41,41                 | 0     |
| 54  | MG   | 1a    | 1604 | 1/1   | 0.87 | 0.16 | 76,76,76,76                 | 0     |
| 54  | MG   | 2B    | 203  | 1/1   | 0.87 | 0.10 | 63,63,63,63                 | 0     |
| 54  | MG   | 1A    | 3945 | 1/1   | 0.87 | 0.17 | 22,22,22,22                 | 0     |
| 54  | MG   | 1A    | 4030 | 1/1   | 0.87 | 0.33 | 54,54,54,54                 | 0     |
| 54  | MG   | 2A    | 3073 | 1/1   | 0.87 | 0.09 | 39,39,39,39                 | 0     |
| 54  | MG   | 2a    | 3125 | 1/1   | 0.87 | 0.13 | 75,75,75,75                 | 0     |
| 54  | MG   | 1A    | 3946 | 1/1   | 0.87 | 0.08 | 14,14,14,14                 | 0     |
| 54  | MG   | 1a    | 1866 | 1/1   | 0.87 | 0.12 | 66,66,66,66                 | 0     |
| 54  | MG   | 1a    | 1767 | 1/1   | 0.87 | 0.11 | 70,70,70,70                 | 0     |
| 54  | MG   | 1A    | 3700 | 1/1   | 0.87 | 0.09 | 39,39,39,39                 | 0     |
| 54  | MG   | 2D    | 308  | 1/1   | 0.87 | 0.17 | 66,66,66,66                 | 0     |
| 54  | MG   | 2A    | 3362 | 1/1   | 0.87 | 0.09 | 24,24,24,24                 | 0     |
| 54  | MG   | 2A    | 3092 | 1/1   | 0.87 | 0.15 | 59,59,59,59                 | 0     |
| 54  | MG   | 1a    | 1772 | 1/1   | 0.87 | 0.09 | 87,87,87,87                 | 0     |
| 54  | MG   | 1a    | 1619 | 1/1   | 0.87 | 0.20 | 76,76,76,76                 | 0     |
| 54  | MG   | 2a    | 3172 | 1/1   | 0.87 | 0.17 | 59,59,59,59                 | 0     |
| 54  | MG   | 1A    | 3653 | 1/1   | 0.87 | 0.09 | 17,17,17,17                 | 0     |
| 54  | MG   | 2a    | 3177 | 1/1   | 0.87 | 0.16 | 80,80,80,80                 | 0     |
| 54  | MG   | 1A    | 3657 | 1/1   | 0.87 | 0.29 | 69,69,69,69                 | 0     |
| 54  | MG   | 2A    | 3148 | 1/1   | 0.87 | 0.16 | 50,50,50,50                 | 0     |
| 54  | MG   | 1A    | 3492 | 1/1   | 0.87 | 0.12 | 31,31,31,31                 | 0     |
| 54  | MG   | 2A    | 3158 | 1/1   | 0.87 | 0.08 | 51,51,51,51                 | 0     |
| 54  | MG   | 1a    | 1787 | 1/1   | 0.87 | 0.12 | 73,73,73,73                 | 0     |
| 54  | MG   | 2a    | 3187 | 1/1   | 0.87 | 0.17 | 47,47,47,47                 | 0     |
| 54  | MG   | 1A    | 3312 | 1/1   | 0.87 | 0.15 | 53,53,53,53                 | 0     |
| 54  | MG   | 2a    | 3002 | 1/1   | 0.87 | 0.22 | 57,57,57,57                 | 0     |
| 54  | MG   | 1A    | 3794 | 1/1   | 0.87 | 0.15 | 49,49,49,49                 | 0     |
| 54  | MG   | 2A    | 3175 | 1/1   | 0.87 | 0.22 | 55,55,55,55                 | 0     |
| 54  | MG   | 2A    | 3407 | 1/1   | 0.87 | 0.10 | 25,25,25,25                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 1A    | 3126 | 1/1   | 0.87 | 0.10 | 48,48,48,48                 | 0     |
| 54  | MG   | 1a    | 1644 | 1/1   | 0.87 | 0.14 | 60,60,60,60                 | 0     |
| 54  | MG   | 1B    | 225  | 1/1   | 0.87 | 0.10 | 46,46,46,46                 | 0     |
| 54  | MG   | 2A    | 3651 | 1/1   | 0.87 | 0.10 | 29,29,29,29                 | 0     |
| 54  | MG   | 1a    | 1809 | 1/1   | 0.87 | 0.11 | 50,50,50,50                 | 0     |
| 54  | MG   | 2a    | 3021 | 1/1   | 0.87 | 0.24 | 38,38,38,38                 | 0     |
| 54  | MG   | 1n    | 101  | 1/1   | 0.87 | 0.12 | 60,60,60,60                 | 0     |
| 54  | MG   | 1a    | 1652 | 1/1   | 0.87 | 0.18 | 63,63,63,63                 | 0     |
| 54  | MG   | 1A    | 3670 | 1/1   | 0.87 | 0.10 | 69,69,69,69                 | 0     |
| 54  | MG   | 2a    | 3033 | 1/1   | 0.87 | 0.18 | 57,57,57,57                 | 0     |
| 54  | MG   | 2a    | 3035 | 1/1   | 0.87 | 0.17 | 55,55,55,55                 | 0     |
| 54  | MG   | 2A    | 3319 | 1/1   | 0.88 | 0.12 | 46,46,46,46                 | 0     |
| 54  | MG   | 2A    | 3326 | 1/1   | 0.88 | 0.20 | 73,73,73,73                 | 0     |
| 54  | MG   | 1A    | 4008 | 1/1   | 0.88 | 0.29 | 35,35,35,35                 | 0     |
| 54  | MG   | 2A    | 3331 | 1/1   | 0.88 | 0.12 | 45,45,45,45                 | 0     |
| 54  | MG   | 1a    | 1779 | 1/1   | 0.88 | 0.09 | 77,77,77,77                 | 0     |
| 54  | MG   | 2A    | 3590 | 1/1   | 0.88 | 0.11 | 45,45,45,45                 | 0     |
| 54  | MG   | 2A    | 3592 | 1/1   | 0.88 | 0.09 | 30,30,30,30                 | 0     |
| 54  | MG   | 1a    | 1870 | 1/1   | 0.88 | 0.12 | 40,40,40,40                 | 0     |
| 54  | MG   | 1a    | 1871 | 1/1   | 0.88 | 0.22 | 58,58,58,58                 | 0     |
| 54  | MG   | 1A    | 3860 | 1/1   | 0.88 | 0.23 | 44,44,44,44                 | 0     |
| 54  | MG   | 1a    | 1873 | 1/1   | 0.88 | 0.16 | 58,58,58,58                 | 0     |
| 54  | MG   | 2a    | 3040 | 1/1   | 0.88 | 0.28 | 55,55,55,55                 | 0     |
| 54  | MG   | 1a    | 1874 | 1/1   | 0.88 | 0.12 | 57,57,57,57                 | 0     |
| 54  | MG   | 2A    | 3107 | 1/1   | 0.88 | 0.09 | 61,61,61,61                 | 0     |
| 54  | MG   | 2a    | 3047 | 1/1   | 0.88 | 0.23 | 62,62,62,62                 | 0     |
| 54  | MG   | 2A    | 3626 | 1/1   | 0.88 | 0.12 | 79,79,79,79                 | 0     |
| 54  | MG   | 2A    | 3365 | 1/1   | 0.88 | 0.18 | 66,66,66,66                 | 0     |
| 54  | MG   | 1A    | 3039 | 1/1   | 0.88 | 0.13 | 50,50,50,50                 | 0     |
| 54  | MG   | 2A    | 3117 | 1/1   | 0.88 | 0.33 | 49,49,49,49                 | 0     |
| 54  | MG   | 2A    | 3654 | 1/1   | 0.88 | 0.08 | 22,22,22,22                 | 0     |
| 54  | MG   | 1a    | 1647 | 1/1   | 0.88 | 0.15 | 64,64,64,64                 | 0     |
| 54  | MG   | 2A    | 3124 | 1/1   | 0.88 | 0.17 | 54,54,54,54                 | 0     |
| 54  | MG   | 2A    | 3132 | 1/1   | 0.88 | 0.12 | 58,58,58,58                 | 0     |
| 54  | MG   | 1a    | 1879 | 1/1   | 0.88 | 0.12 | 57,57,57,57                 | 0     |
| 54  | MG   | 2A    | 3139 | 1/1   | 0.88 | 0.13 | 55,55,55,55                 | 0     |
| 54  | MG   | 1D    | 321  | 1/1   | 0.88 | 0.10 | 43,43,43,43                 | 0     |
| 54  | MG   | 1A    | 3146 | 1/1   | 0.88 | 0.11 | 45,45,45,45                 | 0     |
| 54  | MG   | 2a    | 3078 | 1/1   | 0.88 | 0.26 | 58,58,58,58                 | 0     |
| 54  | MG   | 1A    | 3133 | 1/1   | 0.88 | 0.27 | 27,27,27,27                 | 0     |
| 54  | MG   | 1d    | 303  | 1/1   | 0.88 | 0.19 | 63,63,63,63                 | 0     |
| 54  | MG   | 1A    | 3448 | 1/1   | 0.88 | 0.12 | 38,38,38,38                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 54  | MG   | 2A    | 3409 | 1/1   | 0.88 | 0.12 | 55,55,55,55                | 0     |
| 54  | MG   | 1F    | 301  | 1/1   | 0.88 | 0.15 | 26,26,26,26                | 0     |
| 54  | MG   | 1F    | 306  | 1/1   | 0.88 | 0.14 | 22,22,22,22                | 0     |
| 54  | MG   | 2A    | 3174 | 1/1   | 0.88 | 0.22 | 56,56,56,56                | 0     |
| 54  | MG   | 1A    | 3455 | 1/1   | 0.88 | 0.10 | 44,44,44,44                | 0     |
| 54  | MG   | 1g    | 202  | 1/1   | 0.88 | 0.06 | 44,44,44,44                | 0     |
| 54  | MG   | 1a    | 1658 | 1/1   | 0.88 | 0.17 | 78,78,78,78                | 0     |
| 54  | MG   | 2A    | 3182 | 1/1   | 0.88 | 0.16 | 49,49,49,49                | 0     |
| 54  | MG   | 1A    | 3309 | 1/1   | 0.88 | 0.21 | 27,27,27,27                | 0     |
| 54  | MG   | 2A    | 3438 | 1/1   | 0.88 | 0.17 | 70,70,70,70                | 0     |
| 54  | MG   | 2A    | 3747 | 1/1   | 0.88 | 0.12 | 49,49,49,49                | 0     |
| 54  | MG   | 2A    | 3184 | 1/1   | 0.88 | 0.19 | 47,47,47,47                | 0     |
| 54  | MG   | 1A    | 3591 | 1/1   | 0.88 | 0.13 | 48,48,48,48                | 0     |
| 54  | MG   | 1a    | 1825 | 1/1   | 0.88 | 0.21 | 69,69,69,69                | 0     |
| 54  | MG   | 1t    | 201  | 1/1   | 0.88 | 0.14 | 61,61,61,61                | 0     |
| 54  | MG   | 1a    | 1828 | 1/1   | 0.88 | 0.10 | 75,75,75,75                | 0     |
| 54  | MG   | 1y    | 3101 | 1/1   | 0.88 | 0.10 | 72,72,72,72                | 0     |
| 54  | MG   | 1A    | 3184 | 1/1   | 0.88 | 0.20 | 58,58,58,58                | 0     |
| 54  | MG   | 1a    | 1609 | 1/1   | 0.88 | 0.14 | 69,69,69,69                | 0     |
| 54  | MG   | 2A    | 3458 | 1/1   | 0.88 | 0.15 | 55,55,55,55                | 0     |
| 54  | MG   | 1A    | 3984 | 1/1   | 0.88 | 0.39 | 46,46,46,46                | 0     |
| 54  | MG   | 2B    | 219  | 1/1   | 0.88 | 0.20 | 64,64,64,64                | 0     |
| 54  | MG   | 2A    | 3013 | 1/1   | 0.88 | 0.13 | 45,45,45,45                | 0     |
| 54  | MG   | 2A    | 3016 | 1/1   | 0.88 | 0.11 | 43,43,43,43                | 0     |
| 54  | MG   | 2A    | 3017 | 1/1   | 0.88 | 0.20 | 47,47,47,47                | 0     |
| 54  | MG   | 1B    | 202  | 1/1   | 0.88 | 0.19 | 55,55,55,55                | 0     |
| 54  | MG   | 2A    | 3261 | 1/1   | 0.88 | 0.18 | 68,68,68,68                | 0     |
| 54  | MG   | 1a    | 1613 | 1/1   | 0.88 | 0.16 | 56,56,56,56                | 0     |
| 54  | MG   | 1a    | 1760 | 1/1   | 0.88 | 0.17 | 77,77,77,77                | 0     |
| 54  | MG   | 1A    | 3318 | 1/1   | 0.88 | 0.16 | 60,60,60,60                | 0     |
| 54  | MG   | 1A    | 3918 | 1/1   | 0.88 | 0.11 | 52,52,52,52                | 0     |
| 54  | MG   | 1A    | 3406 | 1/1   | 0.88 | 0.18 | 52,52,52,52                | 0     |
| 54  | MG   | 2P    | 202  | 1/1   | 0.88 | 0.17 | 61,61,61,61                | 0     |
| 54  | MG   | 2P    | 203  | 1/1   | 0.88 | 0.11 | 39,39,39,39                | 0     |
| 54  | MG   | 2a    | 3192 | 1/1   | 0.88 | 0.28 | 59,59,59,59                | 0     |
| 54  | MG   | 1a    | 1626 | 1/1   | 0.88 | 0.07 | 50,50,50,50                | 0     |
| 54  | MG   | 2A    | 3513 | 1/1   | 0.88 | 0.13 | 49,49,49,49                | 0     |
| 54  | MG   | 2A    | 3287 | 1/1   | 0.88 | 0.10 | 37,37,37,37                | 0     |
| 54  | MG   | 2I    | 102  | 1/1   | 0.88 | 0.15 | 70,70,70,70                | 0     |
| 54  | MG   | 2A    | 3288 | 1/1   | 0.88 | 0.08 | 25,25,25,25                | 0     |
| 54  | MG   | 1a    | 1858 | 1/1   | 0.88 | 0.12 | 90,90,90,90                | 0     |
| 54  | MG   | 1A    | 3994 | 1/1   | 0.88 | 0.09 | 45,45,45,45                | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 2A    | 3526 | 1/1   | 0.88 | 0.11 | 75,75,75,75                 | 0     |
| 54  | MG   | 2A    | 3293 | 1/1   | 0.88 | 0.14 | 60,60,60,60                 | 0     |
| 54  | MG   | 1A    | 3321 | 1/1   | 0.88 | 0.12 | 16,16,16,16                 | 0     |
| 54  | MG   | 1A    | 3427 | 1/1   | 0.88 | 0.16 | 44,44,44,44                 | 0     |
| 54  | MG   | 2A    | 3060 | 1/1   | 0.88 | 0.35 | 62,62,62,62                 | 0     |
| 54  | MG   | 2A    | 3460 | 1/1   | 0.89 | 0.17 | 57,57,57,57                 | 0     |
| 54  | MG   | 1A    | 3105 | 1/1   | 0.89 | 0.32 | 38,38,38,38                 | 0     |
| 54  | MG   | 2A    | 3191 | 1/1   | 0.89 | 0.14 | 50,50,50,50                 | 0     |
| 54  | MG   | 1A    | 3692 | 1/1   | 0.89 | 0.10 | 50,50,50,50                 | 0     |
| 54  | MG   | 1a    | 1741 | 1/1   | 0.89 | 0.13 | 56,56,56,56                 | 0     |
| 54  | MG   | 1A    | 3698 | 1/1   | 0.89 | 0.09 | 44,44,44,44                 | 0     |
| 54  | MG   | 2A    | 3211 | 1/1   | 0.89 | 0.15 | 46,46,46,46                 | 0     |
| 54  | MG   | 1A    | 3595 | 1/1   | 0.89 | 0.11 | 45,45,45,45                 | 0     |
| 54  | MG   | 1d    | 302  | 1/1   | 0.89 | 0.28 | 63,63,63,63                 | 0     |
| 54  | MG   | 1a    | 1606 | 1/1   | 0.89 | 0.16 | 55,55,55,55                 | 0     |
| 54  | MG   | 2a    | 3005 | 1/1   | 0.89 | 0.14 | 62,62,62,62                 | 0     |
| 54  | MG   | 1A    | 3848 | 1/1   | 0.89 | 0.13 | 11,11,11,11                 | 0     |
| 54  | MG   | 1e    | 202  | 1/1   | 0.89 | 0.18 | 58,58,58,58                 | 0     |
| 54  | MG   | 1A    | 4028 | 1/1   | 0.89 | 0.20 | 42,42,42,42                 | 0     |
| 54  | MG   | 1A    | 3214 | 1/1   | 0.89 | 0.09 | 50,50,50,50                 | 0     |
| 54  | MG   | 2A    | 3244 | 1/1   | 0.89 | 0.15 | 48,48,48,48                 | 0     |
| 54  | MG   | 2A    | 3249 | 1/1   | 0.89 | 0.17 | 44,44,44,44                 | 0     |
| 54  | MG   | 1A    | 3365 | 1/1   | 0.89 | 0.18 | 44,44,44,44                 | 0     |
| 54  | MG   | 1A    | 3076 | 1/1   | 0.89 | 0.28 | 29,29,29,29                 | 0     |
| 54  | MG   | 2A    | 3527 | 1/1   | 0.89 | 0.07 | 65,65,65,65                 | 0     |
| 54  | MG   | 1A    | 3611 | 1/1   | 0.89 | 0.13 | 48,48,48,48                 | 0     |
| 54  | MG   | 2a    | 3029 | 1/1   | 0.89 | 0.25 | 44,44,44,44                 | 0     |
| 54  | MG   | 1A    | 3713 | 1/1   | 0.89 | 0.10 | 42,42,42,42                 | 0     |
| 54  | MG   | 2A    | 3545 | 1/1   | 0.89 | 0.11 | 55,55,55,55                 | 0     |
| 54  | MG   | 1A    | 3717 | 1/1   | 0.89 | 0.11 | 33,33,33,33                 | 0     |
| 54  | MG   | 2A    | 3553 | 1/1   | 0.89 | 0.11 | 24,24,24,24                 | 0     |
| 54  | MG   | 1A    | 3869 | 1/1   | 0.89 | 0.16 | 48,48,48,48                 | 0     |
| 54  | MG   | 1A    | 3721 | 1/1   | 0.89 | 0.13 | 28,28,28,28                 | 0     |
| 54  | MG   | 1A    | 3546 | 1/1   | 0.89 | 0.11 | 51,51,51,51                 | 0     |
| 54  | MG   | 1a    | 1634 | 1/1   | 0.89 | 0.18 | 60,60,60,60                 | 0     |
| 54  | MG   | 2A    | 3286 | 1/1   | 0.89 | 0.19 | 48,48,48,48                 | 0     |
| 54  | MG   | 2A    | 3577 | 1/1   | 0.89 | 0.12 | 56,56,56,56                 | 0     |
| 54  | MG   | 2A    | 3584 | 1/1   | 0.89 | 0.11 | 63,63,63,63                 | 0     |
| 54  | MG   | 1a    | 1771 | 1/1   | 0.89 | 0.16 | 62,62,62,62                 | 0     |
| 54  | MG   | 1a    | 1637 | 1/1   | 0.89 | 0.32 | 64,64,64,64                 | 0     |
| 54  | MG   | 1A    | 3303 | 1/1   | 0.89 | 0.10 | 31,31,31,31                 | 0     |
| 54  | MG   | 1a    | 1777 | 1/1   | 0.89 | 0.12 | 49,49,49,49                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 2A    | 3014 | 1/1   | 0.89 | 0.15 | 41,41,41,41                 | 0     |
| 54  | MG   | 1B    | 221  | 1/1   | 0.89 | 0.16 | 52,52,52,52                 | 0     |
| 54  | MG   | 2A    | 3608 | 1/1   | 0.89 | 0.13 | 52,52,52,52                 | 0     |
| 54  | MG   | 2a    | 3069 | 1/1   | 0.89 | 0.13 | 62,62,62,62                 | 0     |
| 54  | MG   | 1A    | 3883 | 1/1   | 0.89 | 0.19 | 34,34,34,34                 | 0     |
| 54  | MG   | 2A    | 3613 | 1/1   | 0.89 | 0.09 | 80,80,80,80                 | 0     |
| 54  | MG   | 1A    | 3551 | 1/1   | 0.89 | 0.09 | 44,44,44,44                 | 0     |
| 54  | MG   | 2a    | 3076 | 1/1   | 0.89 | 0.16 | 58,58,58,58                 | 0     |
| 54  | MG   | 2a    | 3077 | 1/1   | 0.89 | 0.16 | 63,63,63,63                 | 0     |
| 54  | MG   | 1A    | 3743 | 1/1   | 0.89 | 0.10 | 21,21,21,21                 | 0     |
| 54  | MG   | 2A    | 3322 | 1/1   | 0.89 | 0.08 | 43,43,43,43                 | 0     |
| 54  | MG   | 1A    | 3744 | 1/1   | 0.89 | 0.18 | 39,39,39,39                 | 0     |
| 54  | MG   | 1a    | 1790 | 1/1   | 0.89 | 0.15 | 64,64,64,64                 | 0     |
| 54  | MG   | 2A    | 3648 | 1/1   | 0.89 | 0.11 | 89,89,89,89                 | 0     |
| 54  | MG   | 1A    | 3749 | 1/1   | 0.89 | 0.07 | 42,42,42,42                 | 0     |
| 54  | MG   | 1A    | 3626 | 1/1   | 0.89 | 0.07 | 28,28,28,28                 | 0     |
| 54  | MG   | 1A    | 3049 | 1/1   | 0.89 | 0.22 | 31,31,31,31                 | 0     |
| 54  | MG   | 1A    | 3095 | 1/1   | 0.89 | 0.10 | 53,53,53,53                 | 0     |
| 54  | MG   | 1A    | 3316 | 1/1   | 0.89 | 0.14 | 33,33,33,33                 | 0     |
| 54  | MG   | 2a    | 3104 | 1/1   | 0.89 | 0.14 | 62,62,62,62                 | 0     |
| 54  | MG   | 2a    | 3108 | 1/1   | 0.89 | 0.22 | 52,52,52,52                 | 0     |
| 54  | MG   | 2A    | 3351 | 1/1   | 0.89 | 0.11 | 67,67,67,67                 | 0     |
| 54  | MG   | 2A    | 3355 | 1/1   | 0.89 | 0.15 | 46,46,46,46                 | 0     |
| 54  | MG   | 2A    | 3054 | 1/1   | 0.89 | 0.13 | 39,39,39,39                 | 0     |
| 54  | MG   | 1A    | 3460 | 1/1   | 0.89 | 0.09 | 43,43,43,43                 | 0     |
| 54  | MG   | 1A    | 3775 | 1/1   | 0.89 | 0.22 | 26,26,26,26                 | 0     |
| 54  | MG   | 2A    | 3708 | 1/1   | 0.89 | 0.14 | 59,59,59,59                 | 0     |
| 54  | MG   | 1a    | 1659 | 1/1   | 0.89 | 0.18 | 72,72,72,72                 | 0     |
| 54  | MG   | 2A    | 3711 | 1/1   | 0.89 | 0.34 | 47,47,47,47                 | 0     |
| 54  | MG   | 1A    | 3565 | 1/1   | 0.89 | 0.10 | 32,32,32,32                 | 0     |
| 54  | MG   | 2a    | 3145 | 1/1   | 0.89 | 0.12 | 78,78,78,78                 | 0     |
| 54  | MG   | 1a    | 1661 | 1/1   | 0.89 | 0.17 | 76,76,76,76                 | 0     |
| 54  | MG   | 1A    | 3280 | 1/1   | 0.89 | 0.09 | 35,35,35,35                 | 0     |
| 54  | MG   | 2A    | 3075 | 1/1   | 0.89 | 0.08 | 49,49,49,49                 | 0     |
| 54  | MG   | 2A    | 3076 | 1/1   | 0.89 | 0.13 | 55,55,55,55                 | 0     |
| 54  | MG   | 1a    | 1826 | 1/1   | 0.89 | 0.19 | 60,60,60,60                 | 0     |
| 54  | MG   | 2a    | 3158 | 1/1   | 0.89 | 0.14 | 68,68,68,68                 | 0     |
| 54  | MG   | 1A    | 3972 | 1/1   | 0.89 | 0.07 | 44,44,44,44                 | 0     |
| 54  | MG   | 1A    | 3781 | 1/1   | 0.89 | 0.18 | 51,51,51,51                 | 0     |
| 54  | MG   | 1A    | 3480 | 1/1   | 0.89 | 0.11 | 18,18,18,18                 | 0     |
| 54  | MG   | 1A    | 3420 | 1/1   | 0.89 | 0.08 | 22,22,22,22                 | 0     |
| 54  | MG   | 1A    | 3793 | 1/1   | 0.89 | 0.20 | 50,50,50,50                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 2A    | 3406 | 1/1   | 0.89 | 0.17 | 56,56,56,56                 | 0     |
| 54  | MG   | 1O    | 202  | 1/1   | 0.89 | 0.12 | 52,52,52,52                 | 0     |
| 54  | MG   | 1A    | 3421 | 1/1   | 0.89 | 0.06 | 16,16,16,16                 | 0     |
| 54  | MG   | 1A    | 3985 | 1/1   | 0.89 | 0.14 | 30,30,30,30                 | 0     |
| 54  | MG   | 1R    | 201  | 1/1   | 0.89 | 0.30 | 44,44,44,44                 | 0     |
| 54  | MG   | 1a    | 1693 | 1/1   | 0.89 | 0.12 | 45,45,45,45                 | 0     |
| 54  | MG   | 1A    | 3986 | 1/1   | 0.89 | 0.13 | 36,36,36,36                 | 0     |
| 54  | MG   | 1A    | 3497 | 1/1   | 0.89 | 0.08 | 38,38,38,38                 | 0     |
| 54  | MG   | 1a    | 1859 | 1/1   | 0.89 | 0.18 | 55,55,55,55                 | 0     |
| 54  | MG   | 2A    | 3149 | 1/1   | 0.89 | 0.17 | 45,45,45,45                 | 0     |
| 54  | MG   | 1A    | 3504 | 1/1   | 0.89 | 0.13 | 18,18,18,18                 | 0     |
| 54  | MG   | 1A    | 3101 | 1/1   | 0.89 | 0.22 | 20,20,20,20                 | 0     |
| 54  | MG   | 2A    | 3159 | 1/1   | 0.89 | 0.20 | 72,72,72,72                 | 0     |
| 54  | MG   | 1a    | 1715 | 1/1   | 0.89 | 0.14 | 81,81,81,81                 | 0     |
| 54  | MG   | 1A    | 3816 | 1/1   | 0.89 | 0.10 | 55,55,55,55                 | 0     |
| 54  | MG   | 1a    | 1717 | 1/1   | 0.89 | 0.14 | 49,49,49,49                 | 0     |
| 54  | MG   | 1A    | 3996 | 1/1   | 0.89 | 0.26 | 34,34,34,34                 | 0     |
| 54  | MG   | 1W    | 202  | 1/1   | 0.89 | 0.18 | 32,32,32,32                 | 0     |
| 54  | MG   | 1A    | 3820 | 1/1   | 0.89 | 0.08 | 17,17,17,17                 | 0     |
| 54  | MG   | 1A    | 3511 | 1/1   | 0.89 | 0.10 | 42,42,42,42                 | 0     |
| 54  | MG   | 1A    | 3516 | 1/1   | 0.89 | 0.14 | 54,54,54,54                 | 0     |
| 54  | MG   | 1A    | 3686 | 1/1   | 0.89 | 0.12 | 55,55,55,55                 | 0     |
| 54  | MG   | 1A    | 3699 | 1/1   | 0.90 | 0.09 | 44,44,44,44                 | 0     |
| 54  | MG   | 2A    | 3146 | 1/1   | 0.90 | 0.23 | 48,48,48,48                 | 0     |
| 54  | MG   | 2B    | 206  | 1/1   | 0.90 | 0.28 | 69,69,69,69                 | 0     |
| 54  | MG   | 1A    | 3808 | 1/1   | 0.90 | 0.10 | 53,53,53,53                 | 0     |
| 54  | MG   | 1a    | 1743 | 1/1   | 0.90 | 0.18 | 57,57,57,57                 | 0     |
| 54  | MG   | 2B    | 214  | 1/1   | 0.90 | 0.09 | 75,75,75,75                 | 0     |
| 54  | MG   | 2B    | 216  | 1/1   | 0.90 | 0.07 | 75,75,75,75                 | 0     |
| 54  | MG   | 2A    | 3418 | 1/1   | 0.90 | 0.10 | 61,61,61,61                 | 0     |
| 54  | MG   | 1a    | 1623 | 1/1   | 0.90 | 0.10 | 65,65,65,65                 | 0     |
| 54  | MG   | 1a    | 1745 | 1/1   | 0.90 | 0.16 | 52,52,52,52                 | 0     |
| 54  | MG   | 1A    | 3952 | 1/1   | 0.90 | 0.11 | 71,71,71,71                 | 0     |
| 54  | MG   | 2A    | 3428 | 1/1   | 0.90 | 0.11 | 51,51,51,51                 | 0     |
| 54  | MG   | 2A    | 3435 | 1/1   | 0.90 | 0.09 | 46,46,46,46                 | 0     |
| 54  | MG   | 1A    | 3963 | 1/1   | 0.90 | 0.09 | 23,23,23,23                 | 0     |
| 54  | MG   | 2E    | 304  | 1/1   | 0.90 | 0.12 | 33,33,33,33                 | 0     |
| 54  | MG   | 2E    | 305  | 1/1   | 0.90 | 0.14 | 74,74,74,74                 | 0     |
| 54  | MG   | 1A    | 3559 | 1/1   | 0.90 | 0.15 | 31,31,31,31                 | 0     |
| 54  | MG   | 2A    | 3440 | 1/1   | 0.90 | 0.12 | 58,58,58,58                 | 0     |
| 54  | MG   | 1A    | 3167 | 1/1   | 0.90 | 0.12 | 44,44,44,44                 | 0     |
| 54  | MG   | 2A    | 3170 | 1/1   | 0.90 | 0.13 | 45,45,45,45                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 1A    | 3300 | 1/1   | 0.90 | 0.15 | 65,65,65,65                 | 0     |
| 54  | MG   | 1A    | 3822 | 1/1   | 0.90 | 0.19 | 35,35,35,35                 | 0     |
| 54  | MG   | 1a    | 1754 | 1/1   | 0.90 | 0.17 | 69,69,69,69                 | 0     |
| 54  | MG   | 1A    | 3454 | 1/1   | 0.90 | 0.15 | 51,51,51,51                 | 0     |
| 54  | MG   | 1F    | 312  | 1/1   | 0.90 | 0.30 | 34,34,34,34                 | 0     |
| 54  | MG   | 2A    | 3456 | 1/1   | 0.90 | 0.08 | 56,56,56,56                 | 0     |
| 54  | MG   | 1A    | 3979 | 1/1   | 0.90 | 0.08 | 65,65,65,65                 | 0     |
| 54  | MG   | 1A    | 3327 | 1/1   | 0.90 | 0.13 | 8,8,8,8                     | 0     |
| 54  | MG   | 1A    | 3201 | 1/1   | 0.90 | 0.21 | 45,45,45,45                 | 0     |
| 54  | MG   | 1a    | 1765 | 1/1   | 0.90 | 0.09 | 56,56,56,56                 | 0     |
| 54  | MG   | 1A    | 3838 | 1/1   | 0.90 | 0.14 | 58,58,58,58                 | 0     |
| 54  | MG   | 1A    | 3225 | 1/1   | 0.90 | 0.24 | 27,27,27,27                 | 0     |
| 54  | MG   | 2A    | 3478 | 1/1   | 0.90 | 0.09 | 55,55,55,55                 | 0     |
| 54  | MG   | 2A    | 3203 | 1/1   | 0.90 | 0.22 | 64,64,64,64                 | 0     |
| 54  | MG   | 2A    | 3489 | 1/1   | 0.90 | 0.12 | 67,67,67,67                 | 0     |
| 54  | MG   | 2A    | 3204 | 1/1   | 0.90 | 0.18 | 65,65,65,65                 | 0     |
| 54  | MG   | 2a    | 3011 | 1/1   | 0.90 | 0.10 | 65,65,65,65                 | 0     |
| 54  | MG   | 2A    | 3205 | 1/1   | 0.90 | 0.07 | 54,54,54,54                 | 0     |
| 54  | MG   | 2A    | 3207 | 1/1   | 0.90 | 0.09 | 43,43,43,43                 | 0     |
| 54  | MG   | 2a    | 3017 | 1/1   | 0.90 | 0.10 | 45,45,45,45                 | 0     |
| 54  | MG   | 2A    | 3209 | 1/1   | 0.90 | 0.30 | 55,55,55,55                 | 0     |
| 54  | MG   | 1A    | 3719 | 1/1   | 0.90 | 0.08 | 25,25,25,25                 | 0     |
| 54  | MG   | 1A    | 3637 | 1/1   | 0.90 | 0.25 | 23,23,23,23                 | 0     |
| 54  | MG   | 1A    | 3419 | 1/1   | 0.90 | 0.07 | 20,20,20,20                 | 0     |
| 54  | MG   | 2A    | 3221 | 1/1   | 0.90 | 0.09 | 56,56,56,56                 | 0     |
| 54  | MG   | 1l    | 201  | 1/1   | 0.90 | 0.07 | 53,53,53,53                 | 0     |
| 54  | MG   | 1m    | 201  | 1/1   | 0.90 | 0.07 | 71,71,71,71                 | 0     |
| 54  | MG   | 2A    | 3233 | 1/1   | 0.90 | 0.09 | 47,47,47,47                 | 0     |
| 54  | MG   | 1a    | 1774 | 1/1   | 0.90 | 0.10 | 64,64,64,64                 | 0     |
| 54  | MG   | 2A    | 3520 | 1/1   | 0.90 | 0.10 | 33,33,33,33                 | 0     |
| 54  | MG   | 2a    | 3039 | 1/1   | 0.90 | 0.19 | 64,64,64,64                 | 0     |
| 54  | MG   | 1o    | 101  | 1/1   | 0.90 | 0.09 | 38,38,38,38                 | 0     |
| 54  | MG   | 1A    | 3531 | 1/1   | 0.90 | 0.08 | 9,9,9,9                     | 0     |
| 54  | MG   | 1A    | 3344 | 1/1   | 0.90 | 0.11 | 57,57,57,57                 | 0     |
| 54  | MG   | 2A    | 3528 | 1/1   | 0.90 | 0.10 | 83,83,83,83                 | 0     |
| 54  | MG   | 1A    | 3534 | 1/1   | 0.90 | 0.09 | 26,26,26,26                 | 0     |
| 54  | MG   | 1A    | 4002 | 1/1   | 0.90 | 0.24 | 44,44,44,44                 | 0     |
| 54  | MG   | 1A    | 3352 | 1/1   | 0.90 | 0.09 | 50,50,50,50                 | 0     |
| 54  | MG   | 2a    | 3058 | 1/1   | 0.90 | 0.32 | 65,65,65,65                 | 0     |
| 54  | MG   | 2A    | 3258 | 1/1   | 0.90 | 0.16 | 52,52,52,52                 | 0     |
| 54  | MG   | 2A    | 3550 | 1/1   | 0.90 | 0.13 | 28,28,28,28                 | 0     |
| 54  | MG   | 1a    | 1662 | 1/1   | 0.90 | 0.11 | 55,55,55,55                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 54  | MG   | 1a    | 1664 | 1/1   | 0.90 | 0.25 | 57,57,57,57                | 0     |
| 54  | MG   | 1a    | 1668 | 1/1   | 0.90 | 0.18 | 66,66,66,66                | 0     |
| 54  | MG   | 2A    | 3271 | 1/1   | 0.90 | 0.27 | 53,53,53,53                | 0     |
| 54  | MG   | 1A    | 3861 | 1/1   | 0.90 | 0.14 | 59,59,59,59                | 0     |
| 54  | MG   | 1A    | 3472 | 1/1   | 0.90 | 0.09 | 18,18,18,18                | 0     |
| 54  | MG   | 1A    | 3478 | 1/1   | 0.90 | 0.10 | 14,14,14,14                | 0     |
| 54  | MG   | 1A    | 3669 | 1/1   | 0.90 | 0.09 | 59,59,59,59                | 0     |
| 54  | MG   | 2A    | 3586 | 1/1   | 0.90 | 0.08 | 35,35,35,35                | 0     |
| 54  | MG   | 2A    | 3024 | 1/1   | 0.90 | 0.08 | 43,43,43,43                | 0     |
| 54  | MG   | 1A    | 3766 | 1/1   | 0.90 | 0.09 | 43,43,43,43                | 0     |
| 54  | MG   | 1a    | 1808 | 1/1   | 0.90 | 0.27 | 60,60,60,60                | 0     |
| 54  | MG   | 1A    | 3548 | 1/1   | 0.90 | 0.08 | 32,32,32,32                | 0     |
| 54  | MG   | 2a    | 3089 | 1/1   | 0.90 | 0.14 | 54,54,54,54                | 0     |
| 54  | MG   | 2a    | 3090 | 1/1   | 0.90 | 0.11 | 44,44,44,44                | 0     |
| 54  | MG   | 2a    | 3091 | 1/1   | 0.90 | 0.13 | 71,71,71,71                | 0     |
| 54  | MG   | 2A    | 3595 | 1/1   | 0.90 | 0.12 | 26,26,26,26                | 0     |
| 54  | MG   | 1X    | 101  | 1/1   | 0.90 | 0.11 | 56,56,56,56                | 0     |
| 54  | MG   | 1a    | 1816 | 1/1   | 0.90 | 0.25 | 66,66,66,66                | 0     |
| 54  | MG   | 1A    | 3672 | 1/1   | 0.90 | 0.07 | 57,57,57,57                | 0     |
| 54  | MG   | 1a    | 1821 | 1/1   | 0.90 | 0.13 | 59,59,59,59                | 0     |
| 54  | MG   | 2A    | 3611 | 1/1   | 0.90 | 0.09 | 52,52,52,52                | 0     |
| 54  | MG   | 1A    | 3673 | 1/1   | 0.90 | 0.13 | 56,56,56,56                | 0     |
| 54  | MG   | 2A    | 3615 | 1/1   | 0.90 | 0.15 | 45,45,45,45                | 0     |
| 54  | MG   | 11    | 103  | 1/1   | 0.90 | 0.08 | 35,35,35,35                | 0     |
| 54  | MG   | 1A    | 3676 | 1/1   | 0.90 | 0.10 | 31,31,31,31                | 0     |
| 54  | MG   | 1a    | 1700 | 1/1   | 0.90 | 0.11 | 74,74,74,74                | 0     |
| 54  | MG   | 1A    | 3204 | 1/1   | 0.90 | 0.07 | 33,33,33,33                | 0     |
| 54  | MG   | 2A    | 3330 | 1/1   | 0.90 | 0.08 | 38,38,38,38                | 0     |
| 54  | MG   | 2A    | 3645 | 1/1   | 0.90 | 0.14 | 52,52,52,52                | 0     |
| 54  | MG   | 2a    | 3121 | 1/1   | 0.90 | 0.10 | 53,53,53,53                | 0     |
| 54  | MG   | 2a    | 3122 | 1/1   | 0.90 | 0.14 | 57,57,57,57                | 0     |
| 54  | MG   | 2A    | 3070 | 1/1   | 0.90 | 0.27 | 41,41,41,41                | 0     |
| 54  | MG   | 1A    | 3898 | 1/1   | 0.90 | 0.10 | 13,13,13,13                | 0     |
| 54  | MG   | 1A    | 3485 | 1/1   | 0.90 | 0.09 | 16,16,16,16                | 0     |
| 54  | MG   | 1A    | 3681 | 1/1   | 0.90 | 0.11 | 66,66,66,66                | 0     |
| 54  | MG   | 1A    | 3609 | 1/1   | 0.90 | 0.29 | 44,44,44,44                | 0     |
| 54  | MG   | 1a    | 1605 | 1/1   | 0.90 | 0.36 | 68,68,68,68                | 0     |
| 54  | MG   | 2A    | 3689 | 1/1   | 0.90 | 0.15 | 65,65,65,65                | 0     |
| 54  | MG   | 2a    | 3153 | 1/1   | 0.90 | 0.14 | 53,53,53,53                | 0     |
| 54  | MG   | 1A    | 3788 | 1/1   | 0.90 | 0.14 | 63,63,63,63                | 0     |
| 54  | MG   | 2A    | 3695 | 1/1   | 0.90 | 0.14 | 65,65,65,65                | 0     |
| 54  | MG   | 2A    | 3357 | 1/1   | 0.90 | 0.13 | 56,56,56,56                | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 54  | MG   | 1a    | 1720 | 1/1   | 0.90 | 0.07 | 56,56,56,56                | 0     |
| 54  | MG   | 1A    | 3920 | 1/1   | 0.90 | 0.14 | 47,47,47,47                | 0     |
| 54  | MG   | 2a    | 3163 | 1/1   | 0.90 | 0.09 | 81,81,81,81                | 0     |
| 54  | MG   | 2a    | 3167 | 1/1   | 0.90 | 0.15 | 49,49,49,49                | 0     |
| 54  | MG   | 2A    | 3363 | 1/1   | 0.90 | 0.10 | 27,27,27,27                | 0     |
| 54  | MG   | 2A    | 3091 | 1/1   | 0.90 | 0.18 | 51,51,51,51                | 0     |
| 54  | MG   | 1a    | 1852 | 1/1   | 0.90 | 0.41 | 73,73,73,73                | 0     |
| 54  | MG   | 2A    | 3093 | 1/1   | 0.90 | 0.12 | 52,52,52,52                | 0     |
| 54  | MG   | 2A    | 3099 | 1/1   | 0.90 | 0.22 | 38,38,38,38                | 0     |
| 54  | MG   | 1a    | 1608 | 1/1   | 0.90 | 0.08 | 77,77,77,77                | 0     |
| 54  | MG   | 2A    | 3720 | 1/1   | 0.90 | 0.08 | 46,46,46,46                | 0     |
| 54  | MG   | 1A    | 3610 | 1/1   | 0.90 | 0.12 | 24,24,24,24                | 0     |
| 54  | MG   | 2A    | 3110 | 1/1   | 0.90 | 0.11 | 29,29,29,29                | 0     |
| 54  | MG   | 2A    | 3113 | 1/1   | 0.90 | 0.10 | 50,50,50,50                | 0     |
| 54  | MG   | 2A    | 3388 | 1/1   | 0.90 | 0.13 | 64,64,64,64                | 0     |
| 54  | MG   | 2A    | 3733 | 1/1   | 0.90 | 0.12 | 62,62,62,62                | 0     |
| 54  | MG   | 2A    | 3734 | 1/1   | 0.90 | 0.21 | 64,64,64,64                | 0     |
| 54  | MG   | 1A    | 3368 | 1/1   | 0.90 | 0.10 | 39,39,39,39                | 0     |
| 54  | MG   | 2a    | 3193 | 1/1   | 0.90 | 0.10 | 39,39,39,39                | 0     |
| 54  | MG   | 2A    | 3393 | 1/1   | 0.90 | 0.11 | 42,42,42,42                | 0     |
| 54  | MG   | 1A    | 3695 | 1/1   | 0.90 | 0.28 | 45,45,45,45                | 0     |
| 54  | MG   | 2A    | 3741 | 1/1   | 0.90 | 0.09 | 50,50,50,50                | 0     |
| 54  | MG   | 2A    | 3399 | 1/1   | 0.90 | 0.16 | 34,34,34,34                | 0     |
| 54  | MG   | 2A    | 3119 | 1/1   | 0.90 | 0.15 | 40,40,40,40                | 0     |
| 54  | MG   | 2A    | 3122 | 1/1   | 0.90 | 0.18 | 64,64,64,64                | 0     |
| 54  | MG   | 2A    | 3404 | 1/1   | 0.90 | 0.14 | 48,48,48,48                | 0     |
| 54  | MG   | 1a    | 1862 | 1/1   | 0.90 | 0.09 | 82,82,82,82                | 0     |
| 54  | MG   | 1a    | 1733 | 1/1   | 0.90 | 0.18 | 88,88,88,88                | 0     |
| 54  | MG   | 1B    | 222  | 1/1   | 0.90 | 0.12 | 57,57,57,57                | 0     |
| 54  | MG   | 2B    | 201  | 1/1   | 0.90 | 0.08 | 68,68,68,68                | 0     |
| 54  | MG   | 1A    | 3212 | 1/1   | 0.90 | 0.20 | 28,28,28,28                | 0     |
| 54  | MG   | 1a    | 1738 | 1/1   | 0.91 | 0.09 | 62,62,62,62                | 0     |
| 54  | MG   | 2A    | 3180 | 1/1   | 0.91 | 0.16 | 58,58,58,58                | 0     |
| 54  | MG   | 1A    | 3549 | 1/1   | 0.91 | 0.08 | 42,42,42,42                | 0     |
| 54  | MG   | 1A    | 3911 | 1/1   | 0.91 | 0.18 | 36,36,36,36                | 0     |
| 54  | MG   | 2D    | 306  | 1/1   | 0.91 | 0.11 | 37,37,37,37                | 0     |
| 54  | MG   | 1A    | 3779 | 1/1   | 0.91 | 0.11 | 29,29,29,29                | 0     |
| 54  | MG   | 2D    | 309  | 1/1   | 0.91 | 0.08 | 30,30,30,30                | 0     |
| 54  | MG   | 2A    | 3186 | 1/1   | 0.91 | 0.13 | 45,45,45,45                | 0     |
| 54  | MG   | 2A    | 3187 | 1/1   | 0.91 | 0.14 | 45,45,45,45                | 0     |
| 54  | MG   | 2A    | 3188 | 1/1   | 0.91 | 0.20 | 56,56,56,56                | 0     |
| 54  | MG   | 2A    | 3190 | 1/1   | 0.91 | 0.10 | 48,48,48,48                | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 1B    | 208  | 1/1   | 0.91 | 0.16 | 44,44,44,44                 | 0     |
| 54  | MG   | 1A    | 3425 | 1/1   | 0.91 | 0.08 | 19,19,19,19                 | 0     |
| 54  | MG   | 2A    | 3470 | 1/1   | 0.91 | 0.11 | 52,52,52,52                 | 0     |
| 54  | MG   | 1B    | 210  | 1/1   | 0.91 | 0.10 | 52,52,52,52                 | 0     |
| 54  | MG   | 2P    | 201  | 1/1   | 0.91 | 0.09 | 61,61,61,61                 | 0     |
| 54  | MG   | 2A    | 3476 | 1/1   | 0.91 | 0.07 | 47,47,47,47                 | 0     |
| 54  | MG   | 1B    | 211  | 1/1   | 0.91 | 0.11 | 49,49,49,49                 | 0     |
| 54  | MG   | 1A    | 3180 | 1/1   | 0.91 | 0.25 | 36,36,36,36                 | 0     |
| 54  | MG   | 2T    | 201  | 1/1   | 0.91 | 0.13 | 60,60,60,60                 | 0     |
| 54  | MG   | 1A    | 3428 | 1/1   | 0.91 | 0.11 | 39,39,39,39                 | 0     |
| 54  | MG   | 2W    | 201  | 1/1   | 0.91 | 0.36 | 45,45,45,45                 | 0     |
| 54  | MG   | 1a    | 1625 | 1/1   | 0.91 | 0.12 | 46,46,46,46                 | 0     |
| 54  | MG   | 2Y    | 201  | 1/1   | 0.91 | 0.13 | 51,51,51,51                 | 0     |
| 54  | MG   | 2A    | 3494 | 1/1   | 0.91 | 0.08 | 40,40,40,40                 | 0     |
| 54  | MG   | 1g    | 201  | 1/1   | 0.91 | 0.20 | 57,57,57,57                 | 0     |
| 54  | MG   | 1B    | 218  | 1/1   | 0.91 | 0.07 | 50,50,50,50                 | 0     |
| 54  | MG   | 2a    | 3001 | 1/1   | 0.91 | 0.09 | 46,46,46,46                 | 0     |
| 54  | MG   | 1a    | 1627 | 1/1   | 0.91 | 0.17 | 45,45,45,45                 | 0     |
| 54  | MG   | 2a    | 3003 | 1/1   | 0.91 | 0.17 | 50,50,50,50                 | 0     |
| 54  | MG   | 2A    | 3212 | 1/1   | 0.91 | 0.16 | 61,61,61,61                 | 0     |
| 54  | MG   | 2A    | 3214 | 1/1   | 0.91 | 0.15 | 54,54,54,54                 | 0     |
| 54  | MG   | 1A    | 3922 | 1/1   | 0.91 | 0.34 | 55,55,55,55                 | 0     |
| 54  | MG   | 2A    | 3511 | 1/1   | 0.91 | 0.12 | 56,56,56,56                 | 0     |
| 54  | MG   | 1a    | 1757 | 1/1   | 0.91 | 0.11 | 73,73,73,73                 | 0     |
| 54  | MG   | 1a    | 1630 | 1/1   | 0.91 | 0.15 | 51,51,51,51                 | 0     |
| 54  | MG   | 1A    | 3930 | 1/1   | 0.91 | 0.11 | 35,35,35,35                 | 0     |
| 54  | MG   | 1A    | 3786 | 1/1   | 0.91 | 0.15 | 60,60,60,60                 | 0     |
| 54  | MG   | 1A    | 3151 | 1/1   | 0.91 | 0.14 | 38,38,38,38                 | 0     |
| 54  | MG   | 2A    | 3235 | 1/1   | 0.91 | 0.11 | 34,34,34,34                 | 0     |
| 54  | MG   | 1A    | 3936 | 1/1   | 0.91 | 0.08 | 23,23,23,23                 | 0     |
| 54  | MG   | 1A    | 3937 | 1/1   | 0.91 | 0.12 | 41,41,41,41                 | 0     |
| 54  | MG   | 1A    | 3688 | 1/1   | 0.91 | 0.32 | 41,41,41,41                 | 0     |
| 54  | MG   | 1a    | 1768 | 1/1   | 0.91 | 0.08 | 60,60,60,60                 | 0     |
| 54  | MG   | 1y    | 3103 | 1/1   | 0.91 | 0.10 | 69,69,69,69                 | 0     |
| 54  | MG   | 1a    | 1642 | 1/1   | 0.91 | 0.20 | 46,46,46,46                 | 0     |
| 54  | MG   | 2A    | 3001 | 1/1   | 0.91 | 0.31 | 59,59,59,59                 | 0     |
| 54  | MG   | 1a    | 1643 | 1/1   | 0.91 | 0.17 | 46,46,46,46                 | 0     |
| 54  | MG   | 2a    | 3036 | 1/1   | 0.91 | 0.14 | 58,58,58,58                 | 0     |
| 54  | MG   | 2A    | 3548 | 1/1   | 0.91 | 0.07 | 73,73,73,73                 | 0     |
| 54  | MG   | 1D    | 319  | 1/1   | 0.91 | 0.11 | 58,58,58,58                 | 0     |
| 54  | MG   | 2A    | 3263 | 1/1   | 0.91 | 0.19 | 45,45,45,45                 | 0     |
| 54  | MG   | 1A    | 3941 | 1/1   | 0.91 | 0.15 | 49,49,49,49                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 2A    | 3015 | 1/1   | 0.91 | 0.32 | 60,60,60,60                 | 0     |
| 54  | MG   | 2A    | 3561 | 1/1   | 0.91 | 0.10 | 44,44,44,44                 | 0     |
| 54  | MG   | 2A    | 3563 | 1/1   | 0.91 | 0.11 | 66,66,66,66                 | 0     |
| 54  | MG   | 1A    | 3558 | 1/1   | 0.91 | 0.11 | 43,43,43,43                 | 0     |
| 54  | MG   | 1A    | 3061 | 1/1   | 0.91 | 0.22 | 54,54,54,54                 | 0     |
| 54  | MG   | 2a    | 3050 | 1/1   | 0.91 | 0.25 | 51,51,51,51                 | 0     |
| 54  | MG   | 1A    | 3696 | 1/1   | 0.91 | 0.10 | 40,40,40,40                 | 0     |
| 54  | MG   | 2A    | 3575 | 1/1   | 0.91 | 0.08 | 42,42,42,42                 | 0     |
| 54  | MG   | 2A    | 3276 | 1/1   | 0.91 | 0.11 | 42,42,42,42                 | 0     |
| 54  | MG   | 1A    | 3801 | 1/1   | 0.91 | 0.11 | 59,59,59,59                 | 0     |
| 54  | MG   | 2A    | 3026 | 1/1   | 0.91 | 0.12 | 49,49,49,49                 | 0     |
| 54  | MG   | 2A    | 3030 | 1/1   | 0.91 | 0.24 | 48,48,48,48                 | 0     |
| 54  | MG   | 1a    | 1780 | 1/1   | 0.91 | 0.12 | 72,72,72,72                 | 0     |
| 54  | MG   | 1F    | 303  | 1/1   | 0.91 | 0.22 | 27,27,27,27                 | 0     |
| 54  | MG   | 1A    | 3623 | 1/1   | 0.91 | 0.07 | 19,19,19,19                 | 0     |
| 54  | MG   | 1A    | 3157 | 1/1   | 0.91 | 0.25 | 25,25,25,25                 | 0     |
| 54  | MG   | 2a    | 3072 | 1/1   | 0.91 | 0.12 | 56,56,56,56                 | 0     |
| 54  | MG   | 2a    | 3073 | 1/1   | 0.91 | 0.28 | 51,51,51,51                 | 0     |
| 54  | MG   | 2A    | 3599 | 1/1   | 0.91 | 0.12 | 34,34,34,34                 | 0     |
| 54  | MG   | 1a    | 1789 | 1/1   | 0.91 | 0.19 | 59,59,59,59                 | 0     |
| 54  | MG   | 1A    | 3564 | 1/1   | 0.91 | 0.20 | 48,48,48,48                 | 0     |
| 54  | MG   | 2A    | 3607 | 1/1   | 0.91 | 0.15 | 35,35,35,35                 | 0     |
| 54  | MG   | 1a    | 1792 | 1/1   | 0.91 | 0.10 | 68,68,68,68                 | 0     |
| 54  | MG   | 1A    | 3372 | 1/1   | 0.91 | 0.14 | 40,40,40,40                 | 0     |
| 54  | MG   | 1A    | 3567 | 1/1   | 0.91 | 0.07 | 40,40,40,40                 | 0     |
| 54  | MG   | 1A    | 3568 | 1/1   | 0.91 | 0.14 | 13,13,13,13                 | 0     |
| 54  | MG   | 2A    | 3614 | 1/1   | 0.91 | 0.13 | 48,48,48,48                 | 0     |
| 54  | MG   | 1A    | 3978 | 1/1   | 0.91 | 0.08 | 36,36,36,36                 | 0     |
| 54  | MG   | 2A    | 3327 | 1/1   | 0.91 | 0.13 | 38,38,38,38                 | 0     |
| 54  | MG   | 2A    | 3619 | 1/1   | 0.91 | 0.11 | 75,75,75,75                 | 0     |
| 54  | MG   | 1a    | 1663 | 1/1   | 0.91 | 0.16 | 64,64,64,64                 | 0     |
| 54  | MG   | 2A    | 3068 | 1/1   | 0.91 | 0.07 | 31,31,31,31                 | 0     |
| 54  | MG   | 1H    | 201  | 1/1   | 0.91 | 0.12 | 57,57,57,57                 | 0     |
| 54  | MG   | 1a    | 1667 | 1/1   | 0.91 | 0.11 | 58,58,58,58                 | 0     |
| 54  | MG   | 1A    | 3275 | 1/1   | 0.91 | 0.45 | 42,42,42,42                 | 0     |
| 54  | MG   | 1A    | 3636 | 1/1   | 0.91 | 0.09 | 41,41,41,41                 | 0     |
| 54  | MG   | 1A    | 3982 | 1/1   | 0.91 | 0.08 | 46,46,46,46                 | 0     |
| 54  | MG   | 1a    | 1820 | 1/1   | 0.91 | 0.10 | 75,75,75,75                 | 0     |
| 54  | MG   | 2A    | 3666 | 1/1   | 0.91 | 0.11 | 34,34,34,34                 | 0     |
| 54  | MG   | 2A    | 3677 | 1/1   | 0.91 | 0.11 | 74,74,74,74                 | 0     |
| 54  | MG   | 1A    | 3276 | 1/1   | 0.91 | 0.11 | 47,47,47,47                 | 0     |
| 54  | MG   | 2A    | 3086 | 1/1   | 0.91 | 0.19 | 67,67,67,67                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 1a    | 1675 | 1/1   | 0.91 | 0.10 | 45,45,45,45                 | 0     |
| 54  | MG   | 1A    | 3315 | 1/1   | 0.91 | 0.11 | 32,32,32,32                 | 0     |
| 54  | MG   | 2a    | 3123 | 1/1   | 0.91 | 0.08 | 71,71,71,71                 | 0     |
| 54  | MG   | 2A    | 3690 | 1/1   | 0.91 | 0.09 | 55,55,55,55                 | 0     |
| 54  | MG   | 1A    | 3525 | 1/1   | 0.91 | 0.11 | 46,46,46,46                 | 0     |
| 54  | MG   | 1A    | 3722 | 1/1   | 0.91 | 0.18 | 64,64,64,64                 | 0     |
| 54  | MG   | 1A    | 3649 | 1/1   | 0.91 | 0.09 | 32,32,32,32                 | 0     |
| 54  | MG   | 2A    | 3094 | 1/1   | 0.91 | 0.11 | 56,56,56,56                 | 0     |
| 54  | MG   | 2A    | 3097 | 1/1   | 0.91 | 0.15 | 44,44,44,44                 | 0     |
| 54  | MG   | 2a    | 3147 | 1/1   | 0.91 | 0.09 | 81,81,81,81                 | 0     |
| 54  | MG   | 2A    | 3704 | 1/1   | 0.91 | 0.14 | 77,77,77,77                 | 0     |
| 54  | MG   | 1a    | 1685 | 1/1   | 0.91 | 0.15 | 47,47,47,47                 | 0     |
| 54  | MG   | 1a    | 1832 | 1/1   | 0.91 | 0.09 | 67,67,67,67                 | 0     |
| 54  | MG   | 1A    | 3844 | 1/1   | 0.91 | 0.17 | 51,51,51,51                 | 0     |
| 54  | MG   | 1a    | 1688 | 1/1   | 0.91 | 0.19 | 57,57,57,57                 | 0     |
| 54  | MG   | 1A    | 3729 | 1/1   | 0.91 | 0.10 | 42,42,42,42                 | 0     |
| 54  | MG   | 1A    | 3730 | 1/1   | 0.91 | 0.09 | 29,29,29,29                 | 0     |
| 54  | MG   | 1a    | 1692 | 1/1   | 0.91 | 0.20 | 48,48,48,48                 | 0     |
| 54  | MG   | 2a    | 3166 | 1/1   | 0.91 | 0.17 | 63,63,63,63                 | 0     |
| 54  | MG   | 1A    | 3652 | 1/1   | 0.91 | 0.11 | 47,47,47,47                 | 0     |
| 54  | MG   | 2A    | 3120 | 1/1   | 0.91 | 0.16 | 52,52,52,52                 | 0     |
| 54  | MG   | 2a    | 3175 | 1/1   | 0.91 | 0.07 | 57,57,57,57                 | 0     |
| 54  | MG   | 1a    | 1695 | 1/1   | 0.91 | 0.13 | 38,38,38,38                 | 0     |
| 54  | MG   | 1A    | 3530 | 1/1   | 0.91 | 0.07 | 35,35,35,35                 | 0     |
| 54  | MG   | 2a    | 3179 | 1/1   | 0.91 | 0.14 | 62,62,62,62                 | 0     |
| 54  | MG   | 2A    | 3129 | 1/1   | 0.91 | 0.15 | 59,59,59,59                 | 0     |
| 54  | MG   | 1A    | 3655 | 1/1   | 0.91 | 0.13 | 16,16,16,16                 | 0     |
| 54  | MG   | 1A    | 3277 | 1/1   | 0.91 | 0.23 | 43,43,43,43                 | 0     |
| 54  | MG   | 1A    | 3091 | 1/1   | 0.91 | 0.11 | 41,41,41,41                 | 0     |
| 54  | MG   | 1A    | 3590 | 1/1   | 0.91 | 0.11 | 48,48,48,48                 | 0     |
| 54  | MG   | 1A    | 4015 | 1/1   | 0.91 | 0.07 | 61,61,61,61                 | 0     |
| 54  | MG   | 2A    | 3147 | 1/1   | 0.91 | 0.08 | 38,38,38,38                 | 0     |
| 54  | MG   | 2A    | 3744 | 1/1   | 0.91 | 0.13 | 38,38,38,38                 | 0     |
| 54  | MG   | 1A    | 3164 | 1/1   | 0.91 | 0.07 | 34,34,34,34                 | 0     |
| 54  | MG   | 1A    | 3765 | 1/1   | 0.91 | 0.08 | 30,30,30,30                 | 0     |
| 54  | MG   | 17    | 105  | 1/1   | 0.91 | 0.07 | 36,36,36,36                 | 0     |
| 54  | MG   | 1A    | 3416 | 1/1   | 0.91 | 0.09 | 19,19,19,19                 | 0     |
| 54  | MG   | 1A    | 3121 | 1/1   | 0.91 | 0.23 | 38,38,38,38                 | 0     |
| 54  | MG   | 1a    | 1725 | 1/1   | 0.91 | 0.20 | 69,69,69,69                 | 0     |
| 54  | MG   | 19    | 102  | 1/1   | 0.91 | 0.11 | 49,49,49,49                 | 0     |
| 54  | MG   | 2A    | 3433 | 1/1   | 0.91 | 0.14 | 52,52,52,52                 | 0     |
| 54  | MG   | 1A    | 3244 | 1/1   | 0.91 | 0.17 | 35,35,35,35                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 2A    | 3169 | 1/1   | 0.91 | 0.09 | 45,45,45,45                 | 0     |
| 54  | MG   | 1A    | 3032 | 1/1   | 0.91 | 0.17 | 46,46,46,46                 | 0     |
| 54  | MG   | 1A    | 3774 | 1/1   | 0.91 | 0.08 | 50,50,50,50                 | 0     |
| 54  | MG   | 2A    | 3442 | 1/1   | 0.91 | 0.09 | 25,25,25,25                 | 0     |
| 54  | MG   | 1A    | 4039 | 1/1   | 0.91 | 0.09 | 41,41,41,41                 | 0     |
| 54  | MG   | 2A    | 3445 | 1/1   | 0.91 | 0.16 | 53,53,53,53                 | 0     |
| 54  | MG   | 1A    | 3597 | 1/1   | 0.91 | 0.12 | 29,29,29,29                 | 0     |
| 58  | ZN   | 24    | 501  | 1/1   | 0.91 | 0.20 | 158,158,158,158             | 0     |
| 54  | MG   | 1a    | 1614 | 1/1   | 0.92 | 0.11 | 18,18,18,18                 | 0     |
| 54  | MG   | 1a    | 1730 | 1/1   | 0.92 | 0.14 | 55,55,55,55                 | 0     |
| 54  | MG   | 1A    | 3575 | 1/1   | 0.92 | 0.12 | 59,59,59,59                 | 0     |
| 54  | MG   | 1A    | 3285 | 1/1   | 0.92 | 0.16 | 28,28,28,28                 | 0     |
| 54  | MG   | 1a    | 1620 | 1/1   | 0.92 | 0.10 | 49,49,49,49                 | 0     |
| 54  | MG   | 2W    | 202  | 1/1   | 0.92 | 0.23 | 47,47,47,47                 | 0     |
| 54  | MG   | 2A    | 3295 | 1/1   | 0.92 | 0.10 | 56,56,56,56                 | 0     |
| 54  | MG   | 2A    | 3301 | 1/1   | 0.92 | 0.09 | 24,24,24,24                 | 0     |
| 54  | MG   | 1a    | 1860 | 1/1   | 0.92 | 0.10 | 58,58,58,58                 | 0     |
| 54  | MG   | 2A    | 3305 | 1/1   | 0.92 | 0.15 | 36,36,36,36                 | 0     |
| 54  | MG   | 27    | 101  | 1/1   | 0.92 | 0.23 | 40,40,40,40                 | 0     |
| 54  | MG   | 2A    | 3556 | 1/1   | 0.92 | 0.10 | 41,41,41,41                 | 0     |
| 54  | MG   | 1A    | 3486 | 1/1   | 0.92 | 0.11 | 30,30,30,30                 | 0     |
| 54  | MG   | 1A    | 3176 | 1/1   | 0.92 | 0.16 | 32,32,32,32                 | 0     |
| 54  | MG   | 2A    | 3314 | 1/1   | 0.92 | 0.09 | 27,27,27,27                 | 0     |
| 54  | MG   | 2A    | 3105 | 1/1   | 0.92 | 0.10 | 44,44,44,44                 | 0     |
| 54  | MG   | 1A    | 3585 | 1/1   | 0.92 | 0.11 | 42,42,42,42                 | 0     |
| 54  | MG   | 1A    | 3295 | 1/1   | 0.92 | 0.19 | 24,24,24,24                 | 0     |
| 54  | MG   | 1A    | 3387 | 1/1   | 0.92 | 0.08 | 14,14,14,14                 | 0     |
| 54  | MG   | 2A    | 3112 | 1/1   | 0.92 | 0.16 | 53,53,53,53                 | 0     |
| 54  | MG   | 1B    | 227  | 1/1   | 0.92 | 0.05 | 51,51,51,51                 | 0     |
| 54  | MG   | 1A    | 3683 | 1/1   | 0.92 | 0.10 | 46,46,46,46                 | 0     |
| 54  | MG   | 1A    | 3177 | 1/1   | 0.92 | 0.12 | 23,23,23,23                 | 0     |
| 54  | MG   | 1D    | 318  | 1/1   | 0.92 | 0.12 | 59,59,59,59                 | 0     |
| 54  | MG   | 1A    | 3410 | 1/1   | 0.92 | 0.12 | 14,14,14,14                 | 0     |
| 54  | MG   | 2A    | 3348 | 1/1   | 0.92 | 0.14 | 37,37,37,37                 | 0     |
| 54  | MG   | 1A    | 3954 | 1/1   | 0.92 | 0.10 | 62,62,62,62                 | 0     |
| 54  | MG   | 1A    | 3955 | 1/1   | 0.92 | 0.14 | 53,53,53,53                 | 0     |
| 54  | MG   | 1A    | 3510 | 1/1   | 0.92 | 0.08 | 38,38,38,38                 | 0     |
| 54  | MG   | 2a    | 3028 | 1/1   | 0.92 | 0.10 | 43,43,43,43                 | 0     |
| 54  | MG   | 2A    | 3130 | 1/1   | 0.92 | 0.12 | 46,46,46,46                 | 0     |
| 54  | MG   | 2A    | 3603 | 1/1   | 0.92 | 0.10 | 68,68,68,68                 | 0     |
| 54  | MG   | 1A    | 3691 | 1/1   | 0.92 | 0.20 | 47,47,47,47                 | 0     |
| 54  | MG   | 1A    | 3138 | 1/1   | 0.92 | 0.19 | 38,38,38,38                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 1A    | 3414 | 1/1   | 0.92 | 0.11 | 54,54,54,54                 | 0     |
| 54  | MG   | 1a    | 1758 | 1/1   | 0.92 | 0.12 | 68,68,68,68                 | 0     |
| 54  | MG   | 1A    | 3815 | 1/1   | 0.92 | 0.18 | 19,19,19,19                 | 0     |
| 54  | MG   | 2A    | 3366 | 1/1   | 0.92 | 0.10 | 43,43,43,43                 | 0     |
| 54  | MG   | 1A    | 3036 | 1/1   | 0.92 | 0.16 | 37,37,37,37                 | 0     |
| 54  | MG   | 2a    | 3041 | 1/1   | 0.92 | 0.28 | 61,61,61,61                 | 0     |
| 54  | MG   | 1A    | 3606 | 1/1   | 0.92 | 0.23 | 29,29,29,29                 | 0     |
| 54  | MG   | 1A    | 3417 | 1/1   | 0.92 | 0.10 | 31,31,31,31                 | 0     |
| 54  | MG   | 2A    | 3155 | 1/1   | 0.92 | 0.14 | 41,41,41,41                 | 0     |
| 54  | MG   | 1A    | 3824 | 1/1   | 0.92 | 0.10 | 36,36,36,36                 | 0     |
| 54  | MG   | 2A    | 3624 | 1/1   | 0.92 | 0.11 | 48,48,48,48                 | 0     |
| 54  | MG   | 1F    | 318  | 1/1   | 0.92 | 0.08 | 49,49,49,49                 | 0     |
| 54  | MG   | 2a    | 3051 | 1/1   | 0.92 | 0.28 | 46,46,46,46                 | 0     |
| 54  | MG   | 2A    | 3629 | 1/1   | 0.92 | 0.08 | 74,74,74,74                 | 0     |
| 54  | MG   | 2A    | 3385 | 1/1   | 0.92 | 0.09 | 39,39,39,39                 | 0     |
| 54  | MG   | 1A    | 3308 | 1/1   | 0.92 | 0.18 | 36,36,36,36                 | 0     |
| 54  | MG   | 1A    | 3003 | 1/1   | 0.92 | 0.07 | 22,22,22,22                 | 0     |
| 54  | MG   | 2a    | 3062 | 1/1   | 0.92 | 0.23 | 60,60,60,60                 | 0     |
| 54  | MG   | 2A    | 3646 | 1/1   | 0.92 | 0.07 | 46,46,46,46                 | 0     |
| 54  | MG   | 1A    | 3257 | 1/1   | 0.92 | 0.14 | 27,27,27,27                 | 0     |
| 54  | MG   | 1a    | 1770 | 1/1   | 0.92 | 0.09 | 70,70,70,70                 | 0     |
| 54  | MG   | 2A    | 3167 | 1/1   | 0.92 | 0.12 | 49,49,49,49                 | 0     |
| 54  | MG   | 2A    | 3664 | 1/1   | 0.92 | 0.09 | 58,58,58,58                 | 0     |
| 54  | MG   | 1A    | 3708 | 1/1   | 0.92 | 0.08 | 70,70,70,70                 | 0     |
| 54  | MG   | 2A    | 3671 | 1/1   | 0.92 | 0.09 | 68,68,68,68                 | 0     |
| 54  | MG   | 2A    | 3675 | 1/1   | 0.92 | 0.14 | 69,69,69,69                 | 0     |
| 54  | MG   | 1A    | 3042 | 1/1   | 0.92 | 0.23 | 24,24,24,24                 | 0     |
| 54  | MG   | 1A    | 3988 | 1/1   | 0.92 | 0.18 | 34,34,34,34                 | 0     |
| 54  | MG   | 2A    | 3682 | 1/1   | 0.92 | 0.13 | 55,55,55,55                 | 0     |
| 54  | MG   | 1A    | 3616 | 1/1   | 0.92 | 0.14 | 22,22,22,22                 | 0     |
| 54  | MG   | 2A    | 3684 | 1/1   | 0.92 | 0.12 | 60,60,60,60                 | 0     |
| 54  | MG   | 2a    | 3080 | 1/1   | 0.92 | 0.34 | 46,46,46,46                 | 0     |
| 54  | MG   | 1A    | 3019 | 1/1   | 0.92 | 0.18 | 33,33,33,33                 | 0     |
| 54  | MG   | 1A    | 3194 | 1/1   | 0.92 | 0.13 | 39,39,39,39                 | 0     |
| 54  | MG   | 2a    | 3083 | 1/1   | 0.92 | 0.28 | 48,48,48,48                 | 0     |
| 54  | MG   | 2a    | 3085 | 1/1   | 0.92 | 0.19 | 54,54,54,54                 | 0     |
| 54  | MG   | 2A    | 3408 | 1/1   | 0.92 | 0.10 | 50,50,50,50                 | 0     |
| 54  | MG   | 2A    | 3179 | 1/1   | 0.92 | 0.16 | 47,47,47,47                 | 0     |
| 54  | MG   | 1Q    | 201  | 1/1   | 0.92 | 0.11 | 32,32,32,32                 | 0     |
| 54  | MG   | 2A    | 3697 | 1/1   | 0.92 | 0.08 | 46,46,46,46                 | 0     |
| 54  | MG   | 2a    | 3097 | 1/1   | 0.92 | 0.17 | 52,52,52,52                 | 0     |
| 54  | MG   | 1A    | 3271 | 1/1   | 0.92 | 0.34 | 42,42,42,42                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 2A    | 3413 | 1/1   | 0.92 | 0.10 | 37,37,37,37                 | 0     |
| 54  | MG   | 1A    | 3028 | 1/1   | 0.92 | 0.11 | 29,29,29,29                 | 0     |
| 54  | MG   | 1A    | 3438 | 1/1   | 0.92 | 0.15 | 52,52,52,52                 | 0     |
| 54  | MG   | 1a    | 1785 | 1/1   | 0.92 | 0.10 | 58,58,58,58                 | 0     |
| 54  | MG   | 2A    | 3706 | 1/1   | 0.92 | 0.06 | 51,51,51,51                 | 0     |
| 54  | MG   | 1A    | 3196 | 1/1   | 0.92 | 0.18 | 56,56,56,56                 | 0     |
| 54  | MG   | 1a    | 1674 | 1/1   | 0.92 | 0.10 | 43,43,43,43                 | 0     |
| 54  | MG   | 1A    | 3445 | 1/1   | 0.92 | 0.11 | 31,31,31,31                 | 0     |
| 54  | MG   | 2A    | 3714 | 1/1   | 0.92 | 0.11 | 37,37,37,37                 | 0     |
| 54  | MG   | 2A    | 3009 | 1/1   | 0.92 | 0.11 | 57,57,57,57                 | 0     |
| 54  | MG   | 1A    | 3197 | 1/1   | 0.92 | 0.07 | 30,30,30,30                 | 0     |
| 54  | MG   | 1U    | 206  | 1/1   | 0.92 | 0.15 | 34,34,34,34                 | 0     |
| 54  | MG   | 2A    | 3436 | 1/1   | 0.92 | 0.23 | 45,45,45,45                 | 0     |
| 54  | MG   | 1A    | 3110 | 1/1   | 0.92 | 0.18 | 35,35,35,35                 | 0     |
| 54  | MG   | 2A    | 3200 | 1/1   | 0.92 | 0.17 | 42,42,42,42                 | 0     |
| 54  | MG   | 1A    | 3350 | 1/1   | 0.92 | 0.12 | 18,18,18,18                 | 0     |
| 54  | MG   | 2A    | 3731 | 1/1   | 0.92 | 0.23 | 61,61,61,61                 | 0     |
| 54  | MG   | 1A    | 4017 | 1/1   | 0.92 | 0.08 | 33,33,33,33                 | 0     |
| 54  | MG   | 2A    | 3020 | 1/1   | 0.92 | 0.08 | 39,39,39,39                 | 0     |
| 54  | MG   | 1A    | 3639 | 1/1   | 0.92 | 0.08 | 23,23,23,23                 | 0     |
| 54  | MG   | 1a    | 1807 | 1/1   | 0.92 | 0.09 | 73,73,73,73                 | 0     |
| 54  | MG   | 2A    | 3210 | 1/1   | 0.92 | 0.08 | 51,51,51,51                 | 0     |
| 54  | MG   | 2a    | 3150 | 1/1   | 0.92 | 0.11 | 44,44,44,44                 | 0     |
| 54  | MG   | 2a    | 3151 | 1/1   | 0.92 | 0.10 | 80,80,80,80                 | 0     |
| 54  | MG   | 1A    | 3075 | 1/1   | 0.92 | 0.13 | 50,50,50,50                 | 0     |
| 54  | MG   | 2A    | 3029 | 1/1   | 0.92 | 0.17 | 54,54,54,54                 | 0     |
| 54  | MG   | 1A    | 3746 | 1/1   | 0.92 | 0.12 | 38,38,38,38                 | 0     |
| 54  | MG   | 1l    | 105  | 1/1   | 0.92 | 0.07 | 35,35,35,35                 | 0     |
| 54  | MG   | 2A    | 3219 | 1/1   | 0.92 | 0.21 | 51,51,51,51                 | 0     |
| 54  | MG   | 2A    | 3748 | 1/1   | 0.92 | 0.18 | 53,53,53,53                 | 0     |
| 54  | MG   | 2A    | 3751 | 1/1   | 0.92 | 0.15 | 54,54,54,54                 | 0     |
| 54  | MG   | 1A    | 4024 | 1/1   | 0.92 | 0.08 | 58,58,58,58                 | 0     |
| 54  | MG   | 1A    | 3877 | 1/1   | 0.92 | 0.07 | 19,19,19,19                 | 0     |
| 54  | MG   | 1A    | 3361 | 1/1   | 0.92 | 0.08 | 24,24,24,24                 | 0     |
| 54  | MG   | 2A    | 3227 | 1/1   | 0.92 | 0.14 | 50,50,50,50                 | 0     |
| 54  | MG   | 1a    | 1696 | 1/1   | 0.92 | 0.14 | 62,62,62,62                 | 0     |
| 54  | MG   | 2A    | 3465 | 1/1   | 0.92 | 0.15 | 23,23,23,23                 | 0     |
| 54  | MG   | 1A    | 3364 | 1/1   | 0.92 | 0.10 | 50,50,50,50                 | 0     |
| 54  | MG   | 1A    | 3758 | 1/1   | 0.92 | 0.08 | 53,53,53,53                 | 0     |
| 54  | MG   | 1A    | 3760 | 1/1   | 0.92 | 0.13 | 57,57,57,57                 | 0     |
| 54  | MG   | 2A    | 3237 | 1/1   | 0.92 | 0.16 | 49,49,49,49                 | 0     |
| 54  | MG   | 2A    | 3480 | 1/1   | 0.92 | 0.10 | 45,45,45,45                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 2B    | 213  | 1/1   | 0.92 | 0.07 | 54,54,54,54                 | 0     |
| 54  | MG   | 2A    | 3052 | 1/1   | 0.92 | 0.36 | 56,56,56,56                 | 0     |
| 54  | MG   | 1A    | 3002 | 1/1   | 0.92 | 0.17 | 43,43,43,43                 | 0     |
| 54  | MG   | 1A    | 3081 | 1/1   | 0.92 | 0.23 | 23,23,23,23                 | 0     |
| 54  | MG   | 1a    | 1830 | 1/1   | 0.92 | 0.09 | 53,53,53,53                 | 0     |
| 54  | MG   | 2D    | 302  | 1/1   | 0.92 | 0.16 | 54,54,54,54                 | 0     |
| 54  | MG   | 1a    | 1710 | 1/1   | 0.92 | 0.11 | 69,69,69,69                 | 0     |
| 54  | MG   | 2A    | 3062 | 1/1   | 0.92 | 0.13 | 43,43,43,43                 | 0     |
| 54  | MG   | 1A    | 3465 | 1/1   | 0.92 | 0.13 | 33,33,33,33                 | 0     |
| 54  | MG   | 2A    | 3069 | 1/1   | 0.92 | 0.22 | 57,57,57,57                 | 0     |
| 54  | MG   | 1B    | 206  | 1/1   | 0.92 | 0.23 | 54,54,54,54                 | 0     |
| 54  | MG   | 2p    | 101  | 1/1   | 0.92 | 0.22 | 44,44,44,44                 | 0     |
| 54  | MG   | 2A    | 3508 | 1/1   | 0.92 | 0.12 | 59,59,59,59                 | 0     |
| 54  | MG   | 1A    | 3467 | 1/1   | 0.92 | 0.07 | 15,15,15,15                 | 0     |
| 54  | MG   | 1a    | 1838 | 1/1   | 0.92 | 0.09 | 63,63,63,63                 | 0     |
| 54  | MG   | 2y    | 201  | 1/1   | 0.92 | 0.12 | 54,54,54,54                 | 0     |
| 54  | MG   | 1A    | 3470 | 1/1   | 0.92 | 0.12 | 28,28,28,28                 | 0     |
| 54  | MG   | 1A    | 3136 | 1/1   | 0.92 | 0.11 | 35,35,35,35                 | 0     |
| 54  | MG   | 1A    | 3660 | 1/1   | 0.92 | 0.07 | 39,39,39,39                 | 0     |
| 54  | MG   | 2A    | 3079 | 1/1   | 0.92 | 0.28 | 58,58,58,58                 | 0     |
| 54  | MG   | 2A    | 3279 | 1/1   | 0.92 | 0.07 | 31,31,31,31                 | 0     |
| 54  | MG   | 1A    | 3376 | 1/1   | 0.92 | 0.10 | 46,46,46,46                 | 0     |
| 54  | MG   | 2A    | 3083 | 1/1   | 0.92 | 0.13 | 63,63,63,63                 | 0     |
| 54  | MG   | 1A    | 3173 | 1/1   | 0.92 | 0.08 | 20,20,20,20                 | 0     |
| 54  | MG   | 1A    | 3089 | 1/1   | 0.93 | 0.23 | 30,30,30,30                 | 0     |
| 54  | MG   | 1a    | 1640 | 1/1   | 0.93 | 0.08 | 62,62,62,62                 | 0     |
| 54  | MG   | 1a    | 1815 | 1/1   | 0.93 | 0.10 | 57,57,57,57                 | 0     |
| 54  | MG   | 1A    | 3260 | 1/1   | 0.93 | 0.20 | 47,47,47,47                 | 0     |
| 54  | MG   | 1A    | 4029 | 1/1   | 0.93 | 0.09 | 46,46,46,46                 | 0     |
| 54  | MG   | 1A    | 3261 | 1/1   | 0.93 | 0.16 | 37,37,37,37                 | 0     |
| 54  | MG   | 1A    | 4032 | 1/1   | 0.93 | 0.10 | 37,37,37,37                 | 0     |
| 54  | MG   | 2A    | 3114 | 1/1   | 0.93 | 0.14 | 41,41,41,41                 | 0     |
| 54  | MG   | 2A    | 3116 | 1/1   | 0.93 | 0.13 | 43,43,43,43                 | 0     |
| 54  | MG   | 1A    | 3690 | 1/1   | 0.93 | 0.13 | 46,46,46,46                 | 0     |
| 54  | MG   | 1A    | 3182 | 1/1   | 0.93 | 0.09 | 41,41,41,41                 | 0     |
| 54  | MG   | 1a    | 1651 | 1/1   | 0.93 | 0.14 | 44,44,44,44                 | 0     |
| 54  | MG   | 1A    | 4040 | 1/1   | 0.93 | 0.07 | 60,60,60,60                 | 0     |
| 54  | MG   | 1a    | 1827 | 1/1   | 0.93 | 0.14 | 55,55,55,55                 | 0     |
| 54  | MG   | 2A    | 3416 | 1/1   | 0.93 | 0.08 | 35,35,35,35                 | 0     |
| 54  | MG   | 2A    | 3123 | 1/1   | 0.93 | 0.21 | 45,45,45,45                 | 0     |
| 54  | MG   | 1A    | 3354 | 1/1   | 0.93 | 0.07 | 35,35,35,35                 | 0     |
| 54  | MG   | 1A    | 3842 | 1/1   | 0.93 | 0.10 | 27,27,27,27                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 2B    | 205  | 1/1   | 0.93 | 0.23 | 53,53,53,53                 | 0     |
| 54  | MG   | 1A    | 4047 | 1/1   | 0.93 | 0.10 | 46,46,46,46                 | 0     |
| 54  | MG   | 1A    | 3693 | 1/1   | 0.93 | 0.21 | 32,32,32,32                 | 0     |
| 54  | MG   | 2B    | 211  | 1/1   | 0.93 | 0.12 | 59,59,59,59                 | 0     |
| 54  | MG   | 1A    | 3589 | 1/1   | 0.93 | 0.08 | 43,43,43,43                 | 0     |
| 54  | MG   | 2A    | 3429 | 1/1   | 0.93 | 0.09 | 60,60,60,60                 | 0     |
| 54  | MG   | 2A    | 3430 | 1/1   | 0.93 | 0.07 | 51,51,51,51                 | 0     |
| 54  | MG   | 1A    | 3356 | 1/1   | 0.93 | 0.07 | 37,37,37,37                 | 0     |
| 54  | MG   | 2A    | 3434 | 1/1   | 0.93 | 0.08 | 53,53,53,53                 | 0     |
| 54  | MG   | 1a    | 1837 | 1/1   | 0.93 | 0.08 | 40,40,40,40                 | 0     |
| 54  | MG   | 1A    | 3360 | 1/1   | 0.93 | 0.06 | 28,28,28,28                 | 0     |
| 54  | MG   | 1A    | 3851 | 1/1   | 0.93 | 0.09 | 31,31,31,31                 | 0     |
| 54  | MG   | 1A    | 3021 | 1/1   | 0.93 | 0.08 | 38,38,38,38                 | 0     |
| 54  | MG   | 1a    | 1847 | 1/1   | 0.93 | 0.12 | 75,75,75,75                 | 0     |
| 54  | MG   | 2A    | 3441 | 1/1   | 0.93 | 0.08 | 61,61,61,61                 | 0     |
| 54  | MG   | 1A    | 3094 | 1/1   | 0.93 | 0.08 | 45,45,45,45                 | 0     |
| 54  | MG   | 1A    | 3189 | 1/1   | 0.93 | 0.09 | 39,39,39,39                 | 0     |
| 54  | MG   | 1A    | 3366 | 1/1   | 0.93 | 0.14 | 37,37,37,37                 | 0     |
| 54  | MG   | 2E    | 303  | 1/1   | 0.93 | 0.21 | 47,47,47,47                 | 0     |
| 54  | MG   | 1A    | 3068 | 1/1   | 0.93 | 0.08 | 35,35,35,35                 | 0     |
| 54  | MG   | 1a    | 1853 | 1/1   | 0.93 | 0.08 | 50,50,50,50                 | 0     |
| 54  | MG   | 1A    | 3709 | 1/1   | 0.93 | 0.25 | 24,24,24,24                 | 0     |
| 54  | MG   | 2A    | 3163 | 1/1   | 0.93 | 0.09 | 48,48,48,48                 | 0     |
| 54  | MG   | 1A    | 3865 | 1/1   | 0.93 | 0.10 | 22,22,22,22                 | 0     |
| 54  | MG   | 1A    | 3097 | 1/1   | 0.93 | 0.17 | 36,36,36,36                 | 0     |
| 54  | MG   | 1A    | 3601 | 1/1   | 0.93 | 0.22 | 23,23,23,23                 | 0     |
| 54  | MG   | 1A    | 3604 | 1/1   | 0.93 | 0.26 | 26,26,26,26                 | 0     |
| 54  | MG   | 1A    | 3875 | 1/1   | 0.93 | 0.07 | 18,18,18,18                 | 0     |
| 54  | MG   | 1A    | 3375 | 1/1   | 0.93 | 0.22 | 43,43,43,43                 | 0     |
| 54  | MG   | 1A    | 3192 | 1/1   | 0.93 | 0.20 | 44,44,44,44                 | 0     |
| 54  | MG   | 1D    | 315  | 1/1   | 0.93 | 0.21 | 29,29,29,29                 | 0     |
| 54  | MG   | 1A    | 3720 | 1/1   | 0.93 | 0.09 | 53,53,53,53                 | 0     |
| 54  | MG   | 2V    | 201  | 1/1   | 0.93 | 0.45 | 45,45,45,45                 | 0     |
| 54  | MG   | 2A    | 3469 | 1/1   | 0.93 | 0.07 | 40,40,40,40                 | 0     |
| 54  | MG   | 1A    | 3150 | 1/1   | 0.93 | 0.12 | 36,36,36,36                 | 0     |
| 54  | MG   | 2A    | 3472 | 1/1   | 0.93 | 0.07 | 27,27,27,27                 | 0     |
| 54  | MG   | 1A    | 3505 | 1/1   | 0.93 | 0.08 | 12,12,12,12                 | 0     |
| 54  | MG   | 20    | 101  | 1/1   | 0.93 | 0.12 | 57,57,57,57                 | 0     |
| 54  | MG   | 2A    | 3474 | 1/1   | 0.93 | 0.09 | 38,38,38,38                 | 0     |
| 54  | MG   | 25    | 101  | 1/1   | 0.93 | 0.30 | 44,44,44,44                 | 0     |
| 54  | MG   | 1E    | 301  | 1/1   | 0.93 | 0.12 | 20,20,20,20                 | 0     |
| 54  | MG   | 1A    | 3379 | 1/1   | 0.93 | 0.07 | 24,24,24,24                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 1A    | 3903 | 1/1   | 0.93 | 0.07 | 18,18,18,18                 | 0     |
| 54  | MG   | 1A    | 3728 | 1/1   | 0.93 | 0.12 | 41,41,41,41                 | 0     |
| 54  | MG   | 2A    | 3482 | 1/1   | 0.93 | 0.08 | 42,42,42,42                 | 0     |
| 54  | MG   | 2A    | 3485 | 1/1   | 0.93 | 0.14 | 40,40,40,40                 | 0     |
| 54  | MG   | 1a    | 1875 | 1/1   | 0.93 | 0.11 | 42,42,42,42                 | 0     |
| 54  | MG   | 2A    | 3490 | 1/1   | 0.93 | 0.10 | 53,53,53,53                 | 0     |
| 54  | MG   | 1A    | 3033 | 1/1   | 0.93 | 0.07 | 32,32,32,32                 | 0     |
| 54  | MG   | 2A    | 3492 | 1/1   | 0.93 | 0.18 | 46,46,46,46                 | 0     |
| 54  | MG   | 1a    | 1877 | 1/1   | 0.93 | 0.16 | 53,53,53,53                 | 0     |
| 54  | MG   | 2a    | 3009 | 1/1   | 0.93 | 0.07 | 70,70,70,70                 | 0     |
| 54  | MG   | 1A    | 3153 | 1/1   | 0.93 | 0.31 | 39,39,39,39                 | 0     |
| 54  | MG   | 2A    | 3196 | 1/1   | 0.93 | 0.20 | 57,57,57,57                 | 0     |
| 54  | MG   | 1A    | 3915 | 1/1   | 0.93 | 0.13 | 34,34,34,34                 | 0     |
| 54  | MG   | 1A    | 3735 | 1/1   | 0.93 | 0.09 | 34,34,34,34                 | 0     |
| 54  | MG   | 1a    | 1881 | 1/1   | 0.93 | 0.11 | 44,44,44,44                 | 0     |
| 54  | MG   | 1A    | 3104 | 1/1   | 0.93 | 0.17 | 44,44,44,44                 | 0     |
| 54  | MG   | 2A    | 3509 | 1/1   | 0.93 | 0.07 | 37,37,37,37                 | 0     |
| 54  | MG   | 2a    | 3022 | 1/1   | 0.93 | 0.13 | 37,37,37,37                 | 0     |
| 54  | MG   | 2a    | 3023 | 1/1   | 0.93 | 0.21 | 44,44,44,44                 | 0     |
| 54  | MG   | 2a    | 3025 | 1/1   | 0.93 | 0.23 | 50,50,50,50                 | 0     |
| 54  | MG   | 1A    | 3014 | 1/1   | 0.93 | 0.16 | 33,33,33,33                 | 0     |
| 54  | MG   | 1A    | 3624 | 1/1   | 0.93 | 0.13 | 17,17,17,17                 | 0     |
| 54  | MG   | 1A    | 3926 | 1/1   | 0.93 | 0.12 | 35,35,35,35                 | 0     |
| 54  | MG   | 2A    | 3208 | 1/1   | 0.93 | 0.10 | 43,43,43,43                 | 0     |
| 54  | MG   | 2A    | 3514 | 1/1   | 0.93 | 0.11 | 36,36,36,36                 | 0     |
| 54  | MG   | 1d    | 304  | 1/1   | 0.93 | 0.11 | 45,45,45,45                 | 0     |
| 54  | MG   | 1A    | 3928 | 1/1   | 0.93 | 0.12 | 47,47,47,47                 | 0     |
| 54  | MG   | 1A    | 3078 | 1/1   | 0.93 | 0.27 | 25,25,25,25                 | 0     |
| 54  | MG   | 2A    | 3519 | 1/1   | 0.93 | 0.09 | 48,48,48,48                 | 0     |
| 54  | MG   | 1A    | 3111 | 1/1   | 0.93 | 0.10 | 22,22,22,22                 | 0     |
| 54  | MG   | 1A    | 3747 | 1/1   | 0.93 | 0.07 | 26,26,26,26                 | 0     |
| 54  | MG   | 1A    | 3627 | 1/1   | 0.93 | 0.11 | 39,39,39,39                 | 0     |
| 54  | MG   | 1A    | 3529 | 1/1   | 0.93 | 0.10 | 46,46,46,46                 | 0     |
| 54  | MG   | 2a    | 3042 | 1/1   | 0.93 | 0.16 | 71,71,71,71                 | 0     |
| 54  | MG   | 1A    | 3755 | 1/1   | 0.93 | 0.06 | 35,35,35,35                 | 0     |
| 54  | MG   | 1A    | 3631 | 1/1   | 0.93 | 0.17 | 16,16,16,16                 | 0     |
| 54  | MG   | 2A    | 3535 | 1/1   | 0.93 | 0.22 | 44,44,44,44                 | 0     |
| 54  | MG   | 1P    | 204  | 1/1   | 0.93 | 0.14 | 30,30,30,30                 | 0     |
| 54  | MG   | 2A    | 3226 | 1/1   | 0.93 | 0.16 | 57,57,57,57                 | 0     |
| 54  | MG   | 2A    | 3546 | 1/1   | 0.93 | 0.07 | 57,57,57,57                 | 0     |
| 54  | MG   | 1a    | 1727 | 1/1   | 0.93 | 0.07 | 56,56,56,56                 | 0     |
| 54  | MG   | 2a    | 3052 | 1/1   | 0.93 | 0.17 | 60,60,60,60                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 2a    | 3055 | 1/1   | 0.93 | 0.09 | 58,58,58,58                 | 0     |
| 54  | MG   | 1A    | 3942 | 1/1   | 0.93 | 0.17 | 68,68,68,68                 | 0     |
| 54  | MG   | 1A    | 3943 | 1/1   | 0.93 | 0.11 | 19,19,19,19                 | 0     |
| 54  | MG   | 1Q    | 202  | 1/1   | 0.93 | 0.07 | 24,24,24,24                 | 0     |
| 54  | MG   | 1A    | 3411 | 1/1   | 0.93 | 0.07 | 11,11,11,11                 | 0     |
| 54  | MG   | 1A    | 3286 | 1/1   | 0.93 | 0.14 | 45,45,45,45                 | 0     |
| 54  | MG   | 1A    | 3112 | 1/1   | 0.93 | 0.10 | 29,29,29,29                 | 0     |
| 54  | MG   | 2A    | 3239 | 1/1   | 0.93 | 0.13 | 41,41,41,41                 | 0     |
| 54  | MG   | 1A    | 3208 | 1/1   | 0.93 | 0.16 | 33,33,33,33                 | 0     |
| 54  | MG   | 2A    | 3565 | 1/1   | 0.93 | 0.13 | 59,59,59,59                 | 0     |
| 54  | MG   | 2A    | 3568 | 1/1   | 0.93 | 0.08 | 52,52,52,52                 | 0     |
| 54  | MG   | 1A    | 3770 | 1/1   | 0.93 | 0.07 | 30,30,30,30                 | 0     |
| 54  | MG   | 1A    | 3298 | 1/1   | 0.93 | 0.09 | 60,60,60,60                 | 0     |
| 54  | MG   | 1U    | 205  | 1/1   | 0.93 | 0.22 | 43,43,43,43                 | 0     |
| 54  | MG   | 1A    | 3960 | 1/1   | 0.93 | 0.16 | 26,26,26,26                 | 0     |
| 54  | MG   | 2A    | 3002 | 1/1   | 0.93 | 0.18 | 52,52,52,52                 | 0     |
| 54  | MG   | 2A    | 3583 | 1/1   | 0.93 | 0.08 | 29,29,29,29                 | 0     |
| 54  | MG   | 1A    | 3638 | 1/1   | 0.93 | 0.08 | 46,46,46,46                 | 0     |
| 54  | MG   | 2A    | 3585 | 1/1   | 0.93 | 0.07 | 23,23,23,23                 | 0     |
| 54  | MG   | 2a    | 3079 | 1/1   | 0.93 | 0.18 | 60,60,60,60                 | 0     |
| 54  | MG   | 1a    | 1746 | 1/1   | 0.93 | 0.10 | 63,63,63,63                 | 0     |
| 54  | MG   | 2A    | 3011 | 1/1   | 0.93 | 0.05 | 50,50,50,50                 | 0     |
| 54  | MG   | 1A    | 3967 | 1/1   | 0.93 | 0.14 | 56,56,56,56                 | 0     |
| 54  | MG   | 1W    | 203  | 1/1   | 0.93 | 0.08 | 28,28,28,28                 | 0     |
| 54  | MG   | 1A    | 3539 | 1/1   | 0.93 | 0.19 | 32,32,32,32                 | 0     |
| 54  | MG   | 1A    | 3971 | 1/1   | 0.93 | 0.09 | 44,44,44,44                 | 0     |
| 54  | MG   | 10    | 107  | 1/1   | 0.93 | 0.07 | 53,53,53,53                 | 0     |
| 54  | MG   | 2A    | 3600 | 1/1   | 0.93 | 0.09 | 62,62,62,62                 | 0     |
| 54  | MG   | 2A    | 3277 | 1/1   | 0.93 | 0.10 | 51,51,51,51                 | 0     |
| 54  | MG   | 2a    | 3094 | 1/1   | 0.93 | 0.09 | 52,52,52,52                 | 0     |
| 54  | MG   | 2A    | 3018 | 1/1   | 0.93 | 0.23 | 36,36,36,36                 | 0     |
| 54  | MG   | 2A    | 3282 | 1/1   | 0.93 | 0.12 | 38,38,38,38                 | 0     |
| 54  | MG   | 1A    | 3543 | 1/1   | 0.93 | 0.07 | 26,26,26,26                 | 0     |
| 54  | MG   | 1A    | 3418 | 1/1   | 0.93 | 0.12 | 30,30,30,30                 | 0     |
| 54  | MG   | 1A    | 3168 | 1/1   | 0.93 | 0.05 | 32,32,32,32                 | 0     |
| 54  | MG   | 13    | 103  | 1/1   | 0.93 | 0.13 | 37,37,37,37                 | 0     |
| 54  | MG   | 1A    | 3080 | 1/1   | 0.93 | 0.16 | 43,43,43,43                 | 0     |
| 54  | MG   | 1A    | 3215 | 1/1   | 0.93 | 0.11 | 51,51,51,51                 | 0     |
| 54  | MG   | 2a    | 3107 | 1/1   | 0.93 | 0.13 | 63,63,63,63                 | 0     |
| 54  | MG   | 2A    | 3290 | 1/1   | 0.93 | 0.14 | 50,50,50,50                 | 0     |
| 54  | MG   | 2a    | 3109 | 1/1   | 0.93 | 0.19 | 58,58,58,58                 | 0     |
| 54  | MG   | 2A    | 3616 | 1/1   | 0.93 | 0.12 | 53,53,53,53                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 17    | 102  | 1/1   | 0.93 | 0.21 | 29,29,29,29                 | 0     |
| 54  | MG   | 1A    | 3654 | 1/1   | 0.93 | 0.12 | 37,37,37,37                 | 0     |
| 54  | MG   | 2A    | 3035 | 1/1   | 0.93 | 0.13 | 46,46,46,46                 | 0     |
| 54  | MG   | 1A    | 3782 | 1/1   | 0.93 | 0.08 | 24,24,24,24                 | 0     |
| 54  | MG   | 2A    | 3039 | 1/1   | 0.93 | 0.14 | 22,22,22,22                 | 0     |
| 54  | MG   | 1A    | 3304 | 1/1   | 0.93 | 0.12 | 27,27,27,27                 | 0     |
| 54  | MG   | 2A    | 3630 | 1/1   | 0.93 | 0.09 | 76,76,76,76                 | 0     |
| 54  | MG   | 1A    | 3054 | 1/1   | 0.93 | 0.12 | 15,15,15,15                 | 0     |
| 54  | MG   | 2a    | 3127 | 1/1   | 0.93 | 0.08 | 73,73,73,73                 | 0     |
| 54  | MG   | 2A    | 3639 | 1/1   | 0.93 | 0.09 | 95,95,95,95                 | 0     |
| 54  | MG   | 2A    | 3642 | 1/1   | 0.93 | 0.13 | 72,72,72,72                 | 0     |
| 54  | MG   | 1A    | 3787 | 1/1   | 0.93 | 0.09 | 83,83,83,83                 | 0     |
| 54  | MG   | 2a    | 3144 | 1/1   | 0.93 | 0.09 | 52,52,52,52                 | 0     |
| 54  | MG   | 1A    | 3174 | 1/1   | 0.93 | 0.09 | 54,54,54,54                 | 0     |
| 54  | MG   | 1A    | 3229 | 1/1   | 0.93 | 0.27 | 27,27,27,27                 | 0     |
| 54  | MG   | 1A    | 3313 | 1/1   | 0.93 | 0.08 | 54,54,54,54                 | 0     |
| 54  | MG   | 2a    | 3148 | 1/1   | 0.93 | 0.10 | 62,62,62,62                 | 0     |
| 54  | MG   | 2A    | 3650 | 1/1   | 0.93 | 0.10 | 36,36,36,36                 | 0     |
| 54  | MG   | 1A    | 3127 | 1/1   | 0.93 | 0.10 | 28,28,28,28                 | 0     |
| 54  | MG   | 1A    | 3992 | 1/1   | 0.93 | 0.24 | 63,63,63,63                 | 0     |
| 54  | MG   | 1A    | 3665 | 1/1   | 0.93 | 0.10 | 39,39,39,39                 | 0     |
| 54  | MG   | 2A    | 3059 | 1/1   | 0.93 | 0.12 | 34,34,34,34                 | 0     |
| 54  | MG   | 1A    | 3799 | 1/1   | 0.93 | 0.20 | 42,42,42,42                 | 0     |
| 54  | MG   | 2A    | 3333 | 1/1   | 0.93 | 0.10 | 56,56,56,56                 | 0     |
| 54  | MG   | 2A    | 3336 | 1/1   | 0.93 | 0.09 | 32,32,32,32                 | 0     |
| 54  | MG   | 1a    | 1776 | 1/1   | 0.93 | 0.12 | 61,61,61,61                 | 0     |
| 54  | MG   | 2A    | 3681 | 1/1   | 0.93 | 0.07 | 54,54,54,54                 | 0     |
| 54  | MG   | 2A    | 3065 | 1/1   | 0.93 | 0.20 | 49,49,49,49                 | 0     |
| 54  | MG   | 2A    | 3339 | 1/1   | 0.93 | 0.15 | 44,44,44,44                 | 0     |
| 54  | MG   | 1A    | 3995 | 1/1   | 0.93 | 0.09 | 83,83,83,83                 | 0     |
| 54  | MG   | 2a    | 3174 | 1/1   | 0.93 | 0.08 | 55,55,55,55                 | 0     |
| 54  | MG   | 1A    | 3238 | 1/1   | 0.93 | 0.10 | 56,56,56,56                 | 0     |
| 54  | MG   | 2A    | 3349 | 1/1   | 0.93 | 0.08 | 43,43,43,43                 | 0     |
| 54  | MG   | 1A    | 3441 | 1/1   | 0.93 | 0.08 | 29,29,29,29                 | 0     |
| 54  | MG   | 2a    | 3178 | 1/1   | 0.93 | 0.11 | 59,59,59,59                 | 0     |
| 54  | MG   | 1A    | 3805 | 1/1   | 0.93 | 0.23 | 61,61,61,61                 | 0     |
| 54  | MG   | 1A    | 3806 | 1/1   | 0.93 | 0.08 | 32,32,32,32                 | 0     |
| 54  | MG   | 1A    | 3807 | 1/1   | 0.93 | 0.07 | 32,32,32,32                 | 0     |
| 54  | MG   | 1A    | 3442 | 1/1   | 0.93 | 0.06 | 32,32,32,32                 | 0     |
| 54  | MG   | 1A    | 3241 | 1/1   | 0.93 | 0.33 | 65,65,65,65                 | 0     |
| 54  | MG   | 2A    | 3702 | 1/1   | 0.93 | 0.10 | 50,50,50,50                 | 0     |
| 54  | MG   | 2A    | 3078 | 1/1   | 0.93 | 0.21 | 55,55,55,55                 | 0     |

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| Mol | Type  | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|-------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG    | 1A    | 4014 | 1/1   | 0.93 | 0.14 | 46,46,46,46                 | 0     |
| 54  | MG    | 2A    | 3080 | 1/1   | 0.93 | 0.23 | 35,35,35,35                 | 0     |
| 54  | MG    | 1A    | 3055 | 1/1   | 0.93 | 0.16 | 39,39,39,39                 | 0     |
| 54  | MG    | 1A    | 3449 | 1/1   | 0.93 | 0.10 | 57,57,57,57                 | 0     |
| 54  | MG    | 2A    | 3369 | 1/1   | 0.93 | 0.08 | 45,45,45,45                 | 0     |
| 54  | MG    | 2A    | 3710 | 1/1   | 0.93 | 0.11 | 53,53,53,53                 | 0     |
| 54  | MG    | 2e    | 201  | 1/1   | 0.93 | 0.19 | 42,42,42,42                 | 0     |
| 54  | MG    | 2f    | 201  | 1/1   | 0.93 | 0.11 | 45,45,45,45                 | 0     |
| 54  | MG    | 2A    | 3370 | 1/1   | 0.93 | 0.15 | 36,36,36,36                 | 0     |
| 54  | MG    | 2A    | 3085 | 1/1   | 0.93 | 0.14 | 58,58,58,58                 | 0     |
| 54  | MG    | 2A    | 3715 | 1/1   | 0.93 | 0.11 | 39,39,39,39                 | 0     |
| 54  | MG    | 2A    | 3372 | 1/1   | 0.93 | 0.11 | 45,45,45,45                 | 0     |
| 54  | MG    | 1a    | 1628 | 1/1   | 0.93 | 0.20 | 51,51,51,51                 | 0     |
| 54  | MG    | 1A    | 3818 | 1/1   | 0.93 | 0.12 | 31,31,31,31                 | 0     |
| 54  | MG    | 1A    | 3179 | 1/1   | 0.93 | 0.18 | 42,42,42,42                 | 0     |
| 55  | A1CQ5 | 2A    | 3757 | 45/45 | 0.93 | 0.13 | 30,35,59,63                 | 0     |
| 54  | MG    | 1A    | 3331 | 1/1   | 0.93 | 0.11 | 33,33,33,33                 | 0     |
| 54  | MG    | 2A    | 3727 | 1/1   | 0.93 | 0.07 | 55,55,55,55                 | 0     |
| 54  | MG    | 1a    | 1801 | 1/1   | 0.93 | 0.09 | 39,39,39,39                 | 0     |
| 54  | MG    | 1A    | 4023 | 1/1   | 0.93 | 0.09 | 33,33,33,33                 | 0     |
| 54  | MG    | 2A    | 3389 | 1/1   | 0.93 | 0.17 | 48,48,48,48                 | 0     |
| 54  | MG    | 2A    | 3732 | 1/1   | 0.93 | 0.12 | 55,55,55,55                 | 0     |
| 54  | MG    | 1A    | 3252 | 1/1   | 0.93 | 0.06 | 32,32,32,32                 | 0     |
| 54  | MG    | 1A    | 4026 | 1/1   | 0.93 | 0.07 | 52,52,52,52                 | 0     |
| 54  | MG    | 2B    | 209  | 1/1   | 0.94 | 0.22 | 60,60,60,60                 | 0     |
| 54  | MG    | 1A    | 3226 | 1/1   | 0.94 | 0.30 | 19,19,19,19                 | 0     |
| 54  | MG    | 2A    | 3197 | 1/1   | 0.94 | 0.24 | 50,50,50,50                 | 0     |
| 54  | MG    | 1A    | 4025 | 1/1   | 0.94 | 0.08 | 56,56,56,56                 | 0     |
| 54  | MG    | 19    | 101  | 1/1   | 0.94 | 0.26 | 40,40,40,40                 | 0     |
| 54  | MG    | 1A    | 3897 | 1/1   | 0.94 | 0.21 | 24,24,24,24                 | 0     |
| 54  | MG    | 2A    | 3463 | 1/1   | 0.94 | 0.11 | 52,52,52,52                 | 0     |
| 54  | MG    | 2B    | 218  | 1/1   | 0.94 | 0.10 | 62,62,62,62                 | 0     |
| 54  | MG    | 1A    | 3682 | 1/1   | 0.94 | 0.06 | 22,22,22,22                 | 0     |
| 54  | MG    | 1A    | 3902 | 1/1   | 0.94 | 0.10 | 24,24,24,24                 | 0     |
| 54  | MG    | 1A    | 3228 | 1/1   | 0.94 | 0.24 | 30,30,30,30                 | 0     |
| 54  | MG    | 2A    | 3206 | 1/1   | 0.94 | 0.10 | 40,40,40,40                 | 0     |
| 54  | MG    | 2A    | 3471 | 1/1   | 0.94 | 0.08 | 47,47,47,47                 | 0     |
| 54  | MG    | 1A    | 3535 | 1/1   | 0.94 | 0.06 | 19,19,19,19                 | 0     |
| 54  | MG    | 2D    | 307  | 1/1   | 0.94 | 0.18 | 51,51,51,51                 | 0     |
| 54  | MG    | 1A    | 3910 | 1/1   | 0.94 | 0.33 | 33,33,33,33                 | 0     |
| 54  | MG    | 1a    | 1756 | 1/1   | 0.94 | 0.12 | 42,42,42,42                 | 0     |
| 54  | MG    | 1A    | 3607 | 1/1   | 0.94 | 0.09 | 30,30,30,30                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 1A    | 3398 | 1/1   | 0.94 | 0.17 | 35,35,35,35                 | 0     |
| 54  | MG   | 1A    | 3689 | 1/1   | 0.94 | 0.26 | 29,29,29,29                 | 0     |
| 54  | MG   | 1A    | 3401 | 1/1   | 0.94 | 0.15 | 51,51,51,51                 | 0     |
| 54  | MG   | 2E    | 307  | 1/1   | 0.94 | 0.14 | 44,44,44,44                 | 0     |
| 54  | MG   | 1a    | 1762 | 1/1   | 0.94 | 0.08 | 60,60,60,60                 | 0     |
| 54  | MG   | 2F    | 302  | 1/1   | 0.94 | 0.14 | 33,33,33,33                 | 0     |
| 54  | MG   | 2A    | 3484 | 1/1   | 0.94 | 0.20 | 65,65,65,65                 | 0     |
| 54  | MG   | 1A    | 4043 | 1/1   | 0.94 | 0.14 | 58,58,58,58                 | 0     |
| 54  | MG   | 1A    | 3542 | 1/1   | 0.94 | 0.27 | 47,47,47,47                 | 0     |
| 54  | MG   | 2I    | 201  | 1/1   | 0.94 | 0.10 | 77,77,77,77                 | 0     |
| 54  | MG   | 2N    | 201  | 1/1   | 0.94 | 0.07 | 68,68,68,68                 | 0     |
| 54  | MG   | 1A    | 3333 | 1/1   | 0.94 | 0.13 | 33,33,33,33                 | 0     |
| 54  | MG   | 1a    | 1618 | 1/1   | 0.94 | 0.10 | 68,68,68,68                 | 0     |
| 54  | MG   | 1A    | 4048 | 1/1   | 0.94 | 0.14 | 44,44,44,44                 | 0     |
| 54  | MG   | 2A    | 3493 | 1/1   | 0.94 | 0.12 | 46,46,46,46                 | 0     |
| 54  | MG   | 1B    | 201  | 1/1   | 0.94 | 0.14 | 44,44,44,44                 | 0     |
| 54  | MG   | 2A    | 3229 | 1/1   | 0.94 | 0.34 | 38,38,38,38                 | 0     |
| 54  | MG   | 1A    | 3408 | 1/1   | 0.94 | 0.07 | 44,44,44,44                 | 0     |
| 54  | MG   | 2A    | 3019 | 1/1   | 0.94 | 0.09 | 32,32,32,32                 | 0     |
| 54  | MG   | 2A    | 3502 | 1/1   | 0.94 | 0.10 | 32,32,32,32                 | 0     |
| 54  | MG   | 1A    | 3086 | 1/1   | 0.94 | 0.06 | 34,34,34,34                 | 0     |
| 54  | MG   | 2A    | 3021 | 1/1   | 0.94 | 0.10 | 39,39,39,39                 | 0     |
| 54  | MG   | 1A    | 3617 | 1/1   | 0.94 | 0.06 | 41,41,41,41                 | 0     |
| 54  | MG   | 2A    | 3023 | 1/1   | 0.94 | 0.06 | 44,44,44,44                 | 0     |
| 54  | MG   | 1A    | 3619 | 1/1   | 0.94 | 0.12 | 11,11,11,11                 | 0     |
| 54  | MG   | 1A    | 3008 | 1/1   | 0.94 | 0.06 | 37,37,37,37                 | 0     |
| 54  | MG   | 2A    | 3243 | 1/1   | 0.94 | 0.20 | 32,32,32,32                 | 0     |
| 54  | MG   | 2A    | 3027 | 1/1   | 0.94 | 0.06 | 38,38,38,38                 | 0     |
| 54  | MG   | 2A    | 3246 | 1/1   | 0.94 | 0.17 | 48,48,48,48                 | 0     |
| 54  | MG   | 1A    | 3932 | 1/1   | 0.94 | 0.08 | 49,49,49,49                 | 0     |
| 54  | MG   | 1A    | 3341 | 1/1   | 0.94 | 0.12 | 46,46,46,46                 | 0     |
| 54  | MG   | 1A    | 3934 | 1/1   | 0.94 | 0.08 | 51,51,51,51                 | 0     |
| 54  | MG   | 2A    | 3256 | 1/1   | 0.94 | 0.11 | 67,67,67,67                 | 0     |
| 54  | MG   | 2A    | 3032 | 1/1   | 0.94 | 0.26 | 47,47,47,47                 | 0     |
| 54  | MG   | 2A    | 3033 | 1/1   | 0.94 | 0.15 | 59,59,59,59                 | 0     |
| 54  | MG   | 2A    | 3262 | 1/1   | 0.94 | 0.09 | 29,29,29,29                 | 0     |
| 54  | MG   | 1A    | 3935 | 1/1   | 0.94 | 0.06 | 29,29,29,29                 | 0     |
| 54  | MG   | 1A    | 3231 | 1/1   | 0.94 | 0.38 | 31,31,31,31                 | 0     |
| 54  | MG   | 1a    | 1635 | 1/1   | 0.94 | 0.16 | 44,44,44,44                 | 0     |
| 54  | MG   | 2A    | 3531 | 1/1   | 0.94 | 0.08 | 59,59,59,59                 | 0     |
| 54  | MG   | 2A    | 3533 | 1/1   | 0.94 | 0.09 | 63,63,63,63                 | 0     |
| 54  | MG   | 1a    | 1636 | 1/1   | 0.94 | 0.13 | 48,48,48,48                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 2A    | 3537 | 1/1   | 0.94 | 0.09 | 55,55,55,55                 | 0     |
| 54  | MG   | 1a    | 1782 | 1/1   | 0.94 | 0.07 | 62,62,62,62                 | 0     |
| 54  | MG   | 2A    | 3043 | 1/1   | 0.94 | 0.10 | 51,51,51,51                 | 0     |
| 54  | MG   | 2A    | 3044 | 1/1   | 0.94 | 0.13 | 53,53,53,53                 | 0     |
| 54  | MG   | 2A    | 3045 | 1/1   | 0.94 | 0.07 | 50,50,50,50                 | 0     |
| 54  | MG   | 1A    | 3800 | 1/1   | 0.94 | 0.07 | 43,43,43,43                 | 0     |
| 54  | MG   | 2A    | 3047 | 1/1   | 0.94 | 0.12 | 45,45,45,45                 | 0     |
| 54  | MG   | 2A    | 3552 | 1/1   | 0.94 | 0.12 | 29,29,29,29                 | 0     |
| 54  | MG   | 1A    | 3939 | 1/1   | 0.94 | 0.07 | 38,38,38,38                 | 0     |
| 54  | MG   | 2A    | 3555 | 1/1   | 0.94 | 0.08 | 26,26,26,26                 | 0     |
| 54  | MG   | 1A    | 3234 | 1/1   | 0.94 | 0.18 | 26,26,26,26                 | 0     |
| 54  | MG   | 2a    | 3031 | 1/1   | 0.94 | 0.15 | 78,78,78,78                 | 0     |
| 54  | MG   | 2a    | 3032 | 1/1   | 0.94 | 0.26 | 45,45,45,45                 | 0     |
| 54  | MG   | 1A    | 3475 | 1/1   | 0.94 | 0.07 | 26,26,26,26                 | 0     |
| 54  | MG   | 1A    | 3351 | 1/1   | 0.94 | 0.09 | 34,34,34,34                 | 0     |
| 54  | MG   | 2A    | 3053 | 1/1   | 0.94 | 0.23 | 47,47,47,47                 | 0     |
| 54  | MG   | 1A    | 3052 | 1/1   | 0.94 | 0.17 | 35,35,35,35                 | 0     |
| 54  | MG   | 2A    | 3564 | 1/1   | 0.94 | 0.07 | 28,28,28,28                 | 0     |
| 54  | MG   | 1A    | 3483 | 1/1   | 0.94 | 0.09 | 58,58,58,58                 | 0     |
| 54  | MG   | 1a    | 1794 | 1/1   | 0.94 | 0.08 | 55,55,55,55                 | 0     |
| 54  | MG   | 1D    | 309  | 1/1   | 0.94 | 0.07 | 30,30,30,30                 | 0     |
| 54  | MG   | 1D    | 313  | 1/1   | 0.94 | 0.19 | 27,27,27,27                 | 0     |
| 54  | MG   | 2a    | 3043 | 1/1   | 0.94 | 0.18 | 71,71,71,71                 | 0     |
| 54  | MG   | 2A    | 3298 | 1/1   | 0.94 | 0.10 | 44,44,44,44                 | 0     |
| 54  | MG   | 2a    | 3045 | 1/1   | 0.94 | 0.16 | 44,44,44,44                 | 0     |
| 54  | MG   | 2A    | 3299 | 1/1   | 0.94 | 0.10 | 32,32,32,32                 | 0     |
| 54  | MG   | 1A    | 3484 | 1/1   | 0.94 | 0.07 | 26,26,26,26                 | 0     |
| 54  | MG   | 1A    | 3809 | 1/1   | 0.94 | 0.13 | 50,50,50,50                 | 0     |
| 54  | MG   | 2A    | 3304 | 1/1   | 0.94 | 0.08 | 30,30,30,30                 | 0     |
| 54  | MG   | 1D    | 316  | 1/1   | 0.94 | 0.10 | 28,28,28,28                 | 0     |
| 54  | MG   | 1D    | 317  | 1/1   | 0.94 | 0.23 | 29,29,29,29                 | 0     |
| 54  | MG   | 2A    | 3311 | 1/1   | 0.94 | 0.09 | 26,26,26,26                 | 0     |
| 54  | MG   | 2a    | 3054 | 1/1   | 0.94 | 0.10 | 56,56,56,56                 | 0     |
| 54  | MG   | 1A    | 3714 | 1/1   | 0.94 | 0.12 | 16,16,16,16                 | 0     |
| 54  | MG   | 2a    | 3056 | 1/1   | 0.94 | 0.22 | 60,60,60,60                 | 0     |
| 54  | MG   | 1A    | 3147 | 1/1   | 0.94 | 0.05 | 28,28,28,28                 | 0     |
| 54  | MG   | 1a    | 1811 | 1/1   | 0.94 | 0.15 | 60,60,60,60                 | 0     |
| 54  | MG   | 2A    | 3321 | 1/1   | 0.94 | 0.06 | 32,32,32,32                 | 0     |
| 54  | MG   | 2a    | 3060 | 1/1   | 0.94 | 0.10 | 54,54,54,54                 | 0     |
| 54  | MG   | 2A    | 3598 | 1/1   | 0.94 | 0.08 | 23,23,23,23                 | 0     |
| 54  | MG   | 1a    | 1812 | 1/1   | 0.94 | 0.07 | 64,64,64,64                 | 0     |
| 54  | MG   | 2A    | 3325 | 1/1   | 0.94 | 0.10 | 24,24,24,24                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 1a    | 1813 | 1/1   | 0.94 | 0.15 | 57,57,57,57                 | 0     |
| 54  | MG   | 1A    | 3004 | 1/1   | 0.94 | 0.08 | 33,33,33,33                 | 0     |
| 54  | MG   | 2A    | 3077 | 1/1   | 0.94 | 0.11 | 43,43,43,43                 | 0     |
| 54  | MG   | 1A    | 3956 | 1/1   | 0.94 | 0.08 | 41,41,41,41                 | 0     |
| 54  | MG   | 1A    | 3957 | 1/1   | 0.94 | 0.10 | 40,40,40,40                 | 0     |
| 54  | MG   | 2a    | 3071 | 1/1   | 0.94 | 0.14 | 54,54,54,54                 | 0     |
| 54  | MG   | 1A    | 3175 | 1/1   | 0.94 | 0.17 | 32,32,32,32                 | 0     |
| 54  | MG   | 1A    | 3149 | 1/1   | 0.94 | 0.12 | 36,36,36,36                 | 0     |
| 54  | MG   | 1E    | 308  | 1/1   | 0.94 | 0.07 | 30,30,30,30                 | 0     |
| 54  | MG   | 1a    | 1822 | 1/1   | 0.94 | 0.08 | 52,52,52,52                 | 0     |
| 54  | MG   | 1A    | 3965 | 1/1   | 0.94 | 0.20 | 33,33,33,33                 | 0     |
| 54  | MG   | 2A    | 3341 | 1/1   | 0.94 | 0.12 | 47,47,47,47                 | 0     |
| 54  | MG   | 1A    | 3119 | 1/1   | 0.94 | 0.07 | 24,24,24,24                 | 0     |
| 54  | MG   | 1A    | 3500 | 1/1   | 0.94 | 0.08 | 41,41,41,41                 | 0     |
| 54  | MG   | 1a    | 1665 | 1/1   | 0.94 | 0.33 | 52,52,52,52                 | 0     |
| 54  | MG   | 1F    | 310  | 1/1   | 0.94 | 0.12 | 21,21,21,21                 | 0     |
| 54  | MG   | 2A    | 3625 | 1/1   | 0.94 | 0.06 | 50,50,50,50                 | 0     |
| 54  | MG   | 1A    | 3501 | 1/1   | 0.94 | 0.12 | 39,39,39,39                 | 0     |
| 54  | MG   | 2A    | 3354 | 1/1   | 0.94 | 0.10 | 56,56,56,56                 | 0     |
| 54  | MG   | 2a    | 3088 | 1/1   | 0.94 | 0.08 | 82,82,82,82                 | 0     |
| 54  | MG   | 1A    | 3827 | 1/1   | 0.94 | 0.08 | 43,43,43,43                 | 0     |
| 54  | MG   | 1A    | 3017 | 1/1   | 0.94 | 0.18 | 33,33,33,33                 | 0     |
| 54  | MG   | 1A    | 3202 | 1/1   | 0.94 | 0.28 | 43,43,43,43                 | 0     |
| 54  | MG   | 2A    | 3640 | 1/1   | 0.94 | 0.08 | 49,49,49,49                 | 0     |
| 54  | MG   | 2A    | 3361 | 1/1   | 0.94 | 0.12 | 49,49,49,49                 | 0     |
| 54  | MG   | 2A    | 3101 | 1/1   | 0.94 | 0.21 | 40,40,40,40                 | 0     |
| 54  | MG   | 1A    | 3732 | 1/1   | 0.94 | 0.07 | 20,20,20,20                 | 0     |
| 54  | MG   | 1A    | 3577 | 1/1   | 0.94 | 0.08 | 35,35,35,35                 | 0     |
| 54  | MG   | 1A    | 3506 | 1/1   | 0.94 | 0.06 | 30,30,30,30                 | 0     |
| 54  | MG   | 2A    | 3109 | 1/1   | 0.94 | 0.19 | 53,53,53,53                 | 0     |
| 54  | MG   | 1a    | 1678 | 1/1   | 0.94 | 0.26 | 47,47,47,47                 | 0     |
| 54  | MG   | 2A    | 3652 | 1/1   | 0.94 | 0.09 | 40,40,40,40                 | 0     |
| 54  | MG   | 1A    | 3581 | 1/1   | 0.94 | 0.09 | 44,44,44,44                 | 0     |
| 54  | MG   | 1a    | 1680 | 1/1   | 0.94 | 0.20 | 45,45,45,45                 | 0     |
| 54  | MG   | 1A    | 3740 | 1/1   | 0.94 | 0.05 | 31,31,31,31                 | 0     |
| 54  | MG   | 2A    | 3668 | 1/1   | 0.94 | 0.07 | 65,65,65,65                 | 0     |
| 54  | MG   | 2a    | 3112 | 1/1   | 0.94 | 0.14 | 56,56,56,56                 | 0     |
| 54  | MG   | 2A    | 3670 | 1/1   | 0.94 | 0.06 | 41,41,41,41                 | 0     |
| 54  | MG   | 1A    | 3741 | 1/1   | 0.94 | 0.09 | 23,23,23,23                 | 0     |
| 54  | MG   | 2a    | 3115 | 1/1   | 0.94 | 0.16 | 64,64,64,64                 | 0     |
| 54  | MG   | 2A    | 3674 | 1/1   | 0.94 | 0.09 | 44,44,44,44                 | 0     |
| 54  | MG   | 1A    | 3508 | 1/1   | 0.94 | 0.09 | 16,16,16,16                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 1A    | 3058 | 1/1   | 0.94 | 0.06 | 28,28,28,28                 | 0     |
| 54  | MG   | 2a    | 3120 | 1/1   | 0.94 | 0.10 | 62,62,62,62                 | 0     |
| 54  | MG   | 2A    | 3378 | 1/1   | 0.94 | 0.19 | 59,59,59,59                 | 0     |
| 54  | MG   | 1a    | 1687 | 1/1   | 0.94 | 0.13 | 50,50,50,50                 | 0     |
| 54  | MG   | 1P    | 201  | 1/1   | 0.94 | 0.41 | 24,24,24,24                 | 0     |
| 54  | MG   | 1A    | 3745 | 1/1   | 0.94 | 0.08 | 41,41,41,41                 | 0     |
| 54  | MG   | 2A    | 3387 | 1/1   | 0.94 | 0.10 | 24,24,24,24                 | 0     |
| 54  | MG   | 2a    | 3128 | 1/1   | 0.94 | 0.11 | 52,52,52,52                 | 0     |
| 54  | MG   | 2a    | 3129 | 1/1   | 0.94 | 0.08 | 48,48,48,48                 | 0     |
| 54  | MG   | 2A    | 3685 | 1/1   | 0.94 | 0.08 | 56,56,56,56                 | 0     |
| 54  | MG   | 2a    | 3132 | 1/1   | 0.94 | 0.12 | 68,68,68,68                 | 0     |
| 54  | MG   | 2a    | 3133 | 1/1   | 0.94 | 0.08 | 64,64,64,64                 | 0     |
| 54  | MG   | 1a    | 1855 | 1/1   | 0.94 | 0.08 | 34,34,34,34                 | 0     |
| 54  | MG   | 1A    | 3433 | 1/1   | 0.94 | 0.13 | 42,42,42,42                 | 0     |
| 54  | MG   | 2A    | 3126 | 1/1   | 0.94 | 0.27 | 49,49,49,49                 | 0     |
| 54  | MG   | 2A    | 3127 | 1/1   | 0.94 | 0.06 | 33,33,33,33                 | 0     |
| 54  | MG   | 1A    | 3854 | 1/1   | 0.94 | 0.08 | 47,47,47,47                 | 0     |
| 54  | MG   | 2A    | 3696 | 1/1   | 0.94 | 0.10 | 52,52,52,52                 | 0     |
| 54  | MG   | 2A    | 3395 | 1/1   | 0.94 | 0.12 | 38,38,38,38                 | 0     |
| 54  | MG   | 2A    | 3398 | 1/1   | 0.94 | 0.21 | 59,59,59,59                 | 0     |
| 54  | MG   | 1A    | 3855 | 1/1   | 0.94 | 0.10 | 29,29,29,29                 | 0     |
| 54  | MG   | 1A    | 3856 | 1/1   | 0.94 | 0.17 | 22,22,22,22                 | 0     |
| 54  | MG   | 1Q    | 206  | 1/1   | 0.94 | 0.07 | 44,44,44,44                 | 0     |
| 54  | MG   | 2A    | 3136 | 1/1   | 0.94 | 0.08 | 27,27,27,27                 | 0     |
| 54  | MG   | 1A    | 3437 | 1/1   | 0.94 | 0.07 | 24,24,24,24                 | 0     |
| 54  | MG   | 1R    | 203  | 1/1   | 0.94 | 0.20 | 45,45,45,45                 | 0     |
| 54  | MG   | 1S    | 201  | 1/1   | 0.94 | 0.09 | 35,35,35,35                 | 0     |
| 54  | MG   | 1A    | 3515 | 1/1   | 0.94 | 0.09 | 15,15,15,15                 | 0     |
| 54  | MG   | 1a    | 1707 | 1/1   | 0.94 | 0.12 | 36,36,36,36                 | 0     |
| 54  | MG   | 2a    | 3164 | 1/1   | 0.94 | 0.12 | 60,60,60,60                 | 0     |
| 54  | MG   | 2a    | 3165 | 1/1   | 0.94 | 0.10 | 50,50,50,50                 | 0     |
| 54  | MG   | 1A    | 3661 | 1/1   | 0.94 | 0.07 | 57,57,57,57                 | 0     |
| 54  | MG   | 2A    | 3153 | 1/1   | 0.94 | 0.16 | 40,40,40,40                 | 0     |
| 54  | MG   | 1A    | 3752 | 1/1   | 0.94 | 0.08 | 44,44,44,44                 | 0     |
| 54  | MG   | 1A    | 3205 | 1/1   | 0.94 | 0.21 | 33,33,33,33                 | 0     |
| 54  | MG   | 1A    | 4004 | 1/1   | 0.94 | 0.10 | 19,19,19,19                 | 0     |
| 54  | MG   | 1U    | 201  | 1/1   | 0.94 | 0.10 | 22,22,22,22                 | 0     |
| 54  | MG   | 1a    | 1719 | 1/1   | 0.94 | 0.13 | 54,54,54,54                 | 0     |
| 54  | MG   | 2A    | 3725 | 1/1   | 0.94 | 0.11 | 54,54,54,54                 | 0     |
| 54  | MG   | 2A    | 3420 | 1/1   | 0.94 | 0.09 | 58,58,58,58                 | 0     |
| 54  | MG   | 1A    | 3756 | 1/1   | 0.94 | 0.11 | 26,26,26,26                 | 0     |
| 54  | MG   | 2A    | 3422 | 1/1   | 0.94 | 0.09 | 53,53,53,53                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 54  | MG   | 2a    | 3183 | 1/1   | 0.94 | 0.06 | 54,54,54,54                | 0     |
| 54  | MG   | 1A    | 4006 | 1/1   | 0.94 | 0.08 | 41,41,41,41                | 0     |
| 54  | MG   | 2A    | 3730 | 1/1   | 0.94 | 0.17 | 60,60,60,60                | 0     |
| 54  | MG   | 2A    | 3165 | 1/1   | 0.94 | 0.11 | 50,50,50,50                | 0     |
| 54  | MG   | 1A    | 3099 | 1/1   | 0.94 | 0.25 | 27,27,27,27                | 0     |
| 54  | MG   | 1a    | 1723 | 1/1   | 0.94 | 0.09 | 52,52,52,52                | 0     |
| 54  | MG   | 1A    | 3183 | 1/1   | 0.94 | 0.14 | 46,46,46,46                | 0     |
| 54  | MG   | 2A    | 3431 | 1/1   | 0.94 | 0.10 | 44,44,44,44                | 0     |
| 54  | MG   | 1A    | 4011 | 1/1   | 0.94 | 0.13 | 35,35,35,35                | 0     |
| 54  | MG   | 1A    | 4012 | 1/1   | 0.94 | 0.08 | 45,45,45,45                | 0     |
| 54  | MG   | 1A    | 3018 | 1/1   | 0.94 | 0.33 | 23,23,23,23                | 0     |
| 54  | MG   | 1A    | 3158 | 1/1   | 0.94 | 0.17 | 35,35,35,35                | 0     |
| 54  | MG   | 1A    | 3067 | 1/1   | 0.94 | 0.26 | 20,20,20,20                | 0     |
| 54  | MG   | 1A    | 3598 | 1/1   | 0.94 | 0.27 | 27,27,27,27                | 0     |
| 54  | MG   | 1d    | 305  | 1/1   | 0.94 | 0.07 | 86,86,86,86                | 0     |
| 54  | MG   | 2A    | 3181 | 1/1   | 0.94 | 0.17 | 45,45,45,45                | 0     |
| 54  | MG   | 2A    | 3749 | 1/1   | 0.94 | 0.12 | 53,53,53,53                | 0     |
| 54  | MG   | 1A    | 3137 | 1/1   | 0.94 | 0.14 | 39,39,39,39                | 0     |
| 54  | MG   | 2A    | 3443 | 1/1   | 0.94 | 0.11 | 62,62,62,62                | 0     |
| 54  | MG   | 1A    | 3882 | 1/1   | 0.94 | 0.11 | 41,41,41,41                | 0     |
| 54  | MG   | 15    | 102  | 1/1   | 0.94 | 0.20 | 25,25,25,25                | 0     |
| 54  | MG   | 1a    | 1739 | 1/1   | 0.94 | 0.16 | 66,66,66,66                | 0     |
| 54  | MG   | 1A    | 4020 | 1/1   | 0.94 | 0.04 | 50,50,50,50                | 0     |
| 54  | MG   | 1A    | 4021 | 1/1   | 0.94 | 0.11 | 51,51,51,51                | 0     |
| 54  | MG   | 2A    | 3450 | 1/1   | 0.94 | 0.10 | 44,44,44,44                | 0     |
| 54  | MG   | 17    | 101  | 1/1   | 0.94 | 0.17 | 23,23,23,23                | 0     |
| 54  | MG   | 1A    | 3600 | 1/1   | 0.94 | 0.14 | 44,44,44,44                | 0     |
| 54  | MG   | 1A    | 3889 | 1/1   | 0.94 | 0.06 | 49,49,49,49                | 0     |
| 54  | MG   | 2A    | 3455 | 1/1   | 0.94 | 0.11 | 49,49,49,49                | 0     |
| 54  | MG   | 2A    | 3424 | 1/1   | 0.95 | 0.06 | 50,50,50,50                | 0     |
| 54  | MG   | 1A    | 3507 | 1/1   | 0.95 | 0.09 | 44,44,44,44                | 0     |
| 54  | MG   | 1A    | 3830 | 1/1   | 0.95 | 0.09 | 39,39,39,39                | 0     |
| 54  | MG   | 1A    | 3266 | 1/1   | 0.95 | 0.22 | 35,35,35,35                | 0     |
| 54  | MG   | 1A    | 3981 | 1/1   | 0.95 | 0.09 | 53,53,53,53                | 0     |
| 54  | MG   | 2A    | 3164 | 1/1   | 0.95 | 0.23 | 48,48,48,48                | 0     |
| 54  | MG   | 1A    | 3837 | 1/1   | 0.95 | 0.13 | 50,50,50,50                | 0     |
| 54  | MG   | 1A    | 3323 | 1/1   | 0.95 | 0.16 | 31,31,31,31                | 0     |
| 54  | MG   | 1a    | 1697 | 1/1   | 0.95 | 0.05 | 45,45,45,45                | 0     |
| 54  | MG   | 1A    | 3413 | 1/1   | 0.95 | 0.05 | 20,20,20,20                | 0     |
| 54  | MG   | 1A    | 3065 | 1/1   | 0.95 | 0.22 | 39,39,39,39                | 0     |
| 54  | MG   | 2A    | 3173 | 1/1   | 0.95 | 0.13 | 59,59,59,59                | 0     |
| 54  | MG   | 1A    | 3330 | 1/1   | 0.95 | 0.09 | 41,41,41,41                | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 2A    | 3439 | 1/1   | 0.95 | 0.10 | 30,30,30,30                 | 0     |
| 54  | MG   | 2B    | 210  | 1/1   | 0.95 | 0.08 | 52,52,52,52                 | 0     |
| 54  | MG   | 1A    | 3209 | 1/1   | 0.95 | 0.14 | 23,23,23,23                 | 0     |
| 54  | MG   | 1A    | 3332 | 1/1   | 0.95 | 0.07 | 36,36,36,36                 | 0     |
| 54  | MG   | 1A    | 3991 | 1/1   | 0.95 | 0.09 | 62,62,62,62                 | 0     |
| 54  | MG   | 1R    | 204  | 1/1   | 0.95 | 0.08 | 30,30,30,30                 | 0     |
| 54  | MG   | 1A    | 3845 | 1/1   | 0.95 | 0.06 | 47,47,47,47                 | 0     |
| 54  | MG   | 1A    | 3523 | 1/1   | 0.95 | 0.07 | 49,49,49,49                 | 0     |
| 54  | MG   | 1A    | 3035 | 1/1   | 0.95 | 0.07 | 47,47,47,47                 | 0     |
| 54  | MG   | 1a    | 1718 | 1/1   | 0.95 | 0.07 | 49,49,49,49                 | 0     |
| 54  | MG   | 1A    | 3849 | 1/1   | 0.95 | 0.09 | 51,51,51,51                 | 0     |
| 54  | MG   | 2A    | 3449 | 1/1   | 0.95 | 0.23 | 58,58,58,58                 | 0     |
| 54  | MG   | 1A    | 3335 | 1/1   | 0.95 | 0.12 | 44,44,44,44                 | 0     |
| 54  | MG   | 1A    | 3997 | 1/1   | 0.95 | 0.15 | 8,8,8,8                     | 0     |
| 54  | MG   | 1A    | 3620 | 1/1   | 0.95 | 0.09 | 38,38,38,38                 | 0     |
| 54  | MG   | 2A    | 3189 | 1/1   | 0.95 | 0.08 | 36,36,36,36                 | 0     |
| 54  | MG   | 1A    | 4000 | 1/1   | 0.95 | 0.08 | 35,35,35,35                 | 0     |
| 54  | MG   | 1A    | 3012 | 1/1   | 0.95 | 0.24 | 33,33,33,33                 | 0     |
| 54  | MG   | 1A    | 3422 | 1/1   | 0.95 | 0.10 | 16,16,16,16                 | 0     |
| 54  | MG   | 1V    | 206  | 1/1   | 0.95 | 0.04 | 47,47,47,47                 | 0     |
| 54  | MG   | 1a    | 1728 | 1/1   | 0.95 | 0.11 | 47,47,47,47                 | 0     |
| 54  | MG   | 1A    | 3339 | 1/1   | 0.95 | 0.10 | 16,16,16,16                 | 0     |
| 54  | MG   | 1A    | 3857 | 1/1   | 0.95 | 0.04 | 48,48,48,48                 | 0     |
| 54  | MG   | 1A    | 3858 | 1/1   | 0.95 | 0.07 | 28,28,28,28                 | 0     |
| 54  | MG   | 2A    | 3201 | 1/1   | 0.95 | 0.14 | 40,40,40,40                 | 0     |
| 54  | MG   | 2A    | 3467 | 1/1   | 0.95 | 0.15 | 63,63,63,63                 | 0     |
| 54  | MG   | 2A    | 3202 | 1/1   | 0.95 | 0.18 | 49,49,49,49                 | 0     |
| 54  | MG   | 1A    | 3733 | 1/1   | 0.95 | 0.08 | 36,36,36,36                 | 0     |
| 54  | MG   | 10    | 103  | 1/1   | 0.95 | 0.06 | 38,38,38,38                 | 0     |
| 54  | MG   | 10    | 105  | 1/1   | 0.95 | 0.05 | 39,39,39,39                 | 0     |
| 54  | MG   | 1A    | 3116 | 1/1   | 0.95 | 0.08 | 17,17,17,17                 | 0     |
| 54  | MG   | 1A    | 3216 | 1/1   | 0.95 | 0.27 | 27,27,27,27                 | 0     |
| 54  | MG   | 1A    | 3342 | 1/1   | 0.95 | 0.09 | 21,21,21,21                 | 0     |
| 54  | MG   | 1A    | 3537 | 1/1   | 0.95 | 0.12 | 25,25,25,25                 | 0     |
| 54  | MG   | 13    | 101  | 1/1   | 0.95 | 0.12 | 27,27,27,27                 | 0     |
| 54  | MG   | 2Q    | 204  | 1/1   | 0.95 | 0.09 | 70,70,70,70                 | 0     |
| 54  | MG   | 1A    | 3218 | 1/1   | 0.95 | 0.22 | 28,28,28,28                 | 0     |
| 54  | MG   | 2T    | 202  | 1/1   | 0.95 | 0.06 | 47,47,47,47                 | 0     |
| 54  | MG   | 1A    | 3347 | 1/1   | 0.95 | 0.06 | 20,20,20,20                 | 0     |
| 54  | MG   | 2A    | 3213 | 1/1   | 0.95 | 0.23 | 50,50,50,50                 | 0     |
| 54  | MG   | 1A    | 3541 | 1/1   | 0.95 | 0.22 | 44,44,44,44                 | 0     |
| 54  | MG   | 2A    | 3486 | 1/1   | 0.95 | 0.06 | 63,63,63,63                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 2A    | 3487 | 1/1   | 0.95 | 0.06 | 64,64,64,64                 | 0     |
| 54  | MG   | 2A    | 3004 | 1/1   | 0.95 | 0.05 | 36,36,36,36                 | 0     |
| 54  | MG   | 2A    | 3216 | 1/1   | 0.95 | 0.28 | 31,31,31,31                 | 0     |
| 54  | MG   | 21    | 101  | 1/1   | 0.95 | 0.07 | 68,68,68,68                 | 0     |
| 54  | MG   | 2A    | 3217 | 1/1   | 0.95 | 0.30 | 45,45,45,45                 | 0     |
| 54  | MG   | 2A    | 3005 | 1/1   | 0.95 | 0.11 | 49,49,49,49                 | 0     |
| 54  | MG   | 15    | 107  | 1/1   | 0.95 | 0.07 | 46,46,46,46                 | 0     |
| 54  | MG   | 2A    | 3008 | 1/1   | 0.95 | 0.07 | 32,32,32,32                 | 0     |
| 54  | MG   | 2A    | 3222 | 1/1   | 0.95 | 0.24 | 56,56,56,56                 | 0     |
| 54  | MG   | 2A    | 3223 | 1/1   | 0.95 | 0.10 | 40,40,40,40                 | 0     |
| 54  | MG   | 2A    | 3500 | 1/1   | 0.95 | 0.10 | 18,18,18,18                 | 0     |
| 54  | MG   | 1A    | 3348 | 1/1   | 0.95 | 0.11 | 12,12,12,12                 | 0     |
| 54  | MG   | 2A    | 3225 | 1/1   | 0.95 | 0.10 | 53,53,53,53                 | 0     |
| 54  | MG   | 2A    | 3010 | 1/1   | 0.95 | 0.07 | 35,35,35,35                 | 0     |
| 54  | MG   | 16    | 101  | 1/1   | 0.95 | 0.06 | 35,35,35,35                 | 0     |
| 54  | MG   | 2A    | 3228 | 1/1   | 0.95 | 0.09 | 47,47,47,47                 | 0     |
| 54  | MG   | 1A    | 3070 | 1/1   | 0.95 | 0.08 | 25,25,25,25                 | 0     |
| 54  | MG   | 1a    | 1751 | 1/1   | 0.95 | 0.12 | 42,42,42,42                 | 0     |
| 54  | MG   | 1A    | 3544 | 1/1   | 0.95 | 0.09 | 40,40,40,40                 | 0     |
| 54  | MG   | 2A    | 3234 | 1/1   | 0.95 | 0.14 | 48,48,48,48                 | 0     |
| 54  | MG   | 1A    | 3120 | 1/1   | 0.95 | 0.18 | 37,37,37,37                 | 0     |
| 54  | MG   | 2a    | 3014 | 1/1   | 0.95 | 0.16 | 54,54,54,54                 | 0     |
| 54  | MG   | 2a    | 3015 | 1/1   | 0.95 | 0.19 | 39,39,39,39                 | 0     |
| 54  | MG   | 18    | 101  | 1/1   | 0.95 | 0.13 | 44,44,44,44                 | 0     |
| 54  | MG   | 1A    | 3880 | 1/1   | 0.95 | 0.09 | 37,37,37,37                 | 0     |
| 54  | MG   | 1A    | 3440 | 1/1   | 0.95 | 0.11 | 54,54,54,54                 | 0     |
| 54  | MG   | 2a    | 3020 | 1/1   | 0.95 | 0.08 | 47,47,47,47                 | 0     |
| 54  | MG   | 1A    | 3053 | 1/1   | 0.95 | 0.10 | 43,43,43,43                 | 0     |
| 54  | MG   | 2A    | 3240 | 1/1   | 0.95 | 0.20 | 48,48,48,48                 | 0     |
| 54  | MG   | 2A    | 3241 | 1/1   | 0.95 | 0.07 | 53,53,53,53                 | 0     |
| 54  | MG   | 2A    | 3523 | 1/1   | 0.95 | 0.15 | 25,25,25,25                 | 0     |
| 54  | MG   | 1A    | 3125 | 1/1   | 0.95 | 0.04 | 32,32,32,32                 | 0     |
| 54  | MG   | 1a    | 1601 | 1/1   | 0.95 | 0.07 | 58,58,58,58                 | 0     |
| 54  | MG   | 1A    | 3096 | 1/1   | 0.95 | 0.20 | 23,23,23,23                 | 0     |
| 54  | MG   | 2A    | 3245 | 1/1   | 0.95 | 0.07 | 42,42,42,42                 | 0     |
| 54  | MG   | 1a    | 1761 | 1/1   | 0.95 | 0.09 | 61,61,61,61                 | 0     |
| 54  | MG   | 2A    | 3248 | 1/1   | 0.95 | 0.36 | 44,44,44,44                 | 0     |
| 54  | MG   | 1a    | 1603 | 1/1   | 0.95 | 0.10 | 51,51,51,51                 | 0     |
| 54  | MG   | 2A    | 3252 | 1/1   | 0.95 | 0.29 | 42,42,42,42                 | 0     |
| 54  | MG   | 1A    | 3446 | 1/1   | 0.95 | 0.07 | 29,29,29,29                 | 0     |
| 54  | MG   | 2A    | 3538 | 1/1   | 0.95 | 0.10 | 69,69,69,69                 | 0     |
| 54  | MG   | 2A    | 3028 | 1/1   | 0.95 | 0.13 | 23,23,23,23                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 54  | MG   | 1A    | 3447 | 1/1   | 0.95 | 0.07 | 34,34,34,34                | 0     |
| 54  | MG   | 2A    | 3257 | 1/1   | 0.95 | 0.09 | 51,51,51,51                | 0     |
| 54  | MG   | 1A    | 3359 | 1/1   | 0.95 | 0.12 | 49,49,49,49                | 0     |
| 54  | MG   | 2A    | 3260 | 1/1   | 0.95 | 0.15 | 41,41,41,41                | 0     |
| 54  | MG   | 2A    | 3549 | 1/1   | 0.95 | 0.08 | 23,23,23,23                | 0     |
| 54  | MG   | 1A    | 3899 | 1/1   | 0.95 | 0.12 | 11,11,11,11                | 0     |
| 54  | MG   | 1A    | 4033 | 1/1   | 0.95 | 0.07 | 36,36,36,36                | 0     |
| 54  | MG   | 1A    | 4034 | 1/1   | 0.95 | 0.06 | 35,35,35,35                | 0     |
| 54  | MG   | 2A    | 3266 | 1/1   | 0.95 | 0.17 | 17,17,17,17                | 0     |
| 54  | MG   | 1A    | 3020 | 1/1   | 0.95 | 0.23 | 24,24,24,24                | 0     |
| 54  | MG   | 1A    | 3130 | 1/1   | 0.95 | 0.24 | 27,27,27,27                | 0     |
| 54  | MG   | 1A    | 3767 | 1/1   | 0.95 | 0.05 | 17,17,17,17                | 0     |
| 54  | MG   | 2A    | 3037 | 1/1   | 0.95 | 0.11 | 44,44,44,44                | 0     |
| 54  | MG   | 2A    | 3038 | 1/1   | 0.95 | 0.12 | 42,42,42,42                | 0     |
| 54  | MG   | 1A    | 3907 | 1/1   | 0.95 | 0.11 | 36,36,36,36                | 0     |
| 54  | MG   | 2a    | 3053 | 1/1   | 0.95 | 0.18 | 51,51,51,51                | 0     |
| 54  | MG   | 1A    | 4042 | 1/1   | 0.95 | 0.12 | 50,50,50,50                | 0     |
| 54  | MG   | 2A    | 3041 | 1/1   | 0.95 | 0.12 | 46,46,46,46                | 0     |
| 54  | MG   | 2A    | 3281 | 1/1   | 0.95 | 0.10 | 25,25,25,25                | 0     |
| 54  | MG   | 2A    | 3571 | 1/1   | 0.95 | 0.09 | 67,67,67,67                | 0     |
| 54  | MG   | 1a    | 1616 | 1/1   | 0.95 | 0.10 | 60,60,60,60                | 0     |
| 54  | MG   | 2A    | 3283 | 1/1   | 0.95 | 0.17 | 44,44,44,44                | 0     |
| 54  | MG   | 1a    | 1617 | 1/1   | 0.95 | 0.16 | 60,60,60,60                | 0     |
| 54  | MG   | 1A    | 3362 | 1/1   | 0.95 | 0.12 | 27,27,27,27                | 0     |
| 54  | MG   | 1A    | 4044 | 1/1   | 0.95 | 0.08 | 28,28,28,28                | 0     |
| 54  | MG   | 1A    | 3563 | 1/1   | 0.95 | 0.16 | 32,32,32,32                | 0     |
| 54  | MG   | 2A    | 3048 | 1/1   | 0.95 | 0.10 | 38,38,38,38                | 0     |
| 54  | MG   | 1A    | 4046 | 1/1   | 0.95 | 0.09 | 34,34,34,34                | 0     |
| 54  | MG   | 1a    | 1622 | 1/1   | 0.95 | 0.06 | 45,45,45,45                | 0     |
| 54  | MG   | 2a    | 3067 | 1/1   | 0.95 | 0.29 | 56,56,56,56                | 0     |
| 54  | MG   | 1A    | 3288 | 1/1   | 0.95 | 0.32 | 32,32,32,32                | 0     |
| 54  | MG   | 1a    | 1624 | 1/1   | 0.95 | 0.18 | 47,47,47,47                | 0     |
| 54  | MG   | 1a    | 1784 | 1/1   | 0.95 | 0.07 | 43,43,43,43                | 0     |
| 54  | MG   | 1A    | 3292 | 1/1   | 0.95 | 0.06 | 44,44,44,44                | 0     |
| 54  | MG   | 1a    | 1786 | 1/1   | 0.95 | 0.06 | 73,73,73,73                | 0     |
| 54  | MG   | 1A    | 3566 | 1/1   | 0.95 | 0.15 | 54,54,54,54                | 0     |
| 54  | MG   | 1a    | 1788 | 1/1   | 0.95 | 0.09 | 47,47,47,47                | 0     |
| 54  | MG   | 1A    | 3166 | 1/1   | 0.95 | 0.04 | 29,29,29,29                | 0     |
| 54  | MG   | 2A    | 3602 | 1/1   | 0.95 | 0.10 | 50,50,50,50                | 0     |
| 54  | MG   | 1A    | 3777 | 1/1   | 0.95 | 0.08 | 39,39,39,39                | 0     |
| 54  | MG   | 2A    | 3605 | 1/1   | 0.95 | 0.08 | 76,76,76,76                | 0     |
| 54  | MG   | 2A    | 3306 | 1/1   | 0.95 | 0.12 | 52,52,52,52                | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 54  | MG   | 1a    | 1791 | 1/1   | 0.95 | 0.09 | 61,61,61,61                | 0     |
| 54  | MG   | 2A    | 3066 | 1/1   | 0.95 | 0.13 | 27,27,27,27                | 0     |
| 54  | MG   | 2A    | 3067 | 1/1   | 0.95 | 0.07 | 47,47,47,47                | 0     |
| 54  | MG   | 2A    | 3610 | 1/1   | 0.95 | 0.07 | 53,53,53,53                | 0     |
| 54  | MG   | 1A    | 3667 | 1/1   | 0.95 | 0.06 | 53,53,53,53                | 0     |
| 54  | MG   | 1A    | 3924 | 1/1   | 0.95 | 0.09 | 41,41,41,41                | 0     |
| 54  | MG   | 2A    | 3320 | 1/1   | 0.95 | 0.08 | 30,30,30,30                | 0     |
| 54  | MG   | 1A    | 3925 | 1/1   | 0.95 | 0.08 | 53,53,53,53                | 0     |
| 54  | MG   | 1a    | 1795 | 1/1   | 0.95 | 0.09 | 50,50,50,50                | 0     |
| 54  | MG   | 1A    | 3668 | 1/1   | 0.95 | 0.09 | 49,49,49,49                | 0     |
| 54  | MG   | 2A    | 3618 | 1/1   | 0.95 | 0.09 | 73,73,73,73                | 0     |
| 54  | MG   | 1A    | 3236 | 1/1   | 0.95 | 0.19 | 22,22,22,22                | 0     |
| 54  | MG   | 2A    | 3620 | 1/1   | 0.95 | 0.10 | 47,47,47,47                | 0     |
| 54  | MG   | 1A    | 3369 | 1/1   | 0.95 | 0.07 | 44,44,44,44                | 0     |
| 54  | MG   | 2A    | 3328 | 1/1   | 0.95 | 0.07 | 22,22,22,22                | 0     |
| 54  | MG   | 1B    | 216  | 1/1   | 0.95 | 0.07 | 40,40,40,40                | 0     |
| 54  | MG   | 1a    | 1804 | 1/1   | 0.95 | 0.05 | 57,57,57,57                | 0     |
| 54  | MG   | 1a    | 1805 | 1/1   | 0.95 | 0.06 | 55,55,55,55                | 0     |
| 54  | MG   | 2a    | 3106 | 1/1   | 0.95 | 0.13 | 40,40,40,40                | 0     |
| 54  | MG   | 1A    | 3571 | 1/1   | 0.95 | 0.06 | 21,21,21,21                | 0     |
| 54  | MG   | 2A    | 3334 | 1/1   | 0.95 | 0.05 | 30,30,30,30                | 0     |
| 54  | MG   | 1A    | 3237 | 1/1   | 0.95 | 0.06 | 56,56,56,56                | 0     |
| 54  | MG   | 2a    | 3111 | 1/1   | 0.95 | 0.08 | 67,67,67,67                | 0     |
| 54  | MG   | 2A    | 3081 | 1/1   | 0.95 | 0.19 | 46,46,46,46                | 0     |
| 54  | MG   | 2A    | 3641 | 1/1   | 0.95 | 0.08 | 48,48,48,48                | 0     |
| 54  | MG   | 1A    | 3785 | 1/1   | 0.95 | 0.10 | 61,61,61,61                | 0     |
| 54  | MG   | 1A    | 3466 | 1/1   | 0.95 | 0.09 | 32,32,32,32                | 0     |
| 54  | MG   | 2a    | 3116 | 1/1   | 0.95 | 0.09 | 49,49,49,49                | 0     |
| 54  | MG   | 1A    | 3373 | 1/1   | 0.95 | 0.07 | 22,22,22,22                | 0     |
| 54  | MG   | 2A    | 3342 | 1/1   | 0.95 | 0.06 | 45,45,45,45                | 0     |
| 54  | MG   | 2A    | 3647 | 1/1   | 0.95 | 0.07 | 39,39,39,39                | 0     |
| 54  | MG   | 1A    | 3374 | 1/1   | 0.95 | 0.05 | 25,25,25,25                | 0     |
| 54  | MG   | 2A    | 3346 | 1/1   | 0.95 | 0.09 | 60,60,60,60                | 0     |
| 54  | MG   | 2A    | 3347 | 1/1   | 0.95 | 0.15 | 42,42,42,42                | 0     |
| 54  | MG   | 2A    | 3087 | 1/1   | 0.95 | 0.07 | 41,41,41,41                | 0     |
| 54  | MG   | 1A    | 3098 | 1/1   | 0.95 | 0.21 | 28,28,28,28                | 0     |
| 54  | MG   | 1a    | 1645 | 1/1   | 0.95 | 0.14 | 52,52,52,52                | 0     |
| 54  | MG   | 1A    | 3938 | 1/1   | 0.95 | 0.16 | 50,50,50,50                | 0     |
| 54  | MG   | 2A    | 3353 | 1/1   | 0.95 | 0.05 | 30,30,30,30                | 0     |
| 54  | MG   | 2A    | 3669 | 1/1   | 0.95 | 0.10 | 54,54,54,54                | 0     |
| 54  | MG   | 1A    | 3007 | 1/1   | 0.95 | 0.14 | 37,37,37,37                | 0     |
| 54  | MG   | 1a    | 1818 | 1/1   | 0.95 | 0.15 | 45,45,45,45                | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 2a    | 3136 | 1/1   | 0.95 | 0.07 | 69,69,69,69                 | 0     |
| 54  | MG   | 2A    | 3673 | 1/1   | 0.95 | 0.08 | 47,47,47,47                 | 0     |
| 54  | MG   | 2a    | 3140 | 1/1   | 0.95 | 0.06 | 62,62,62,62                 | 0     |
| 54  | MG   | 1a    | 1650 | 1/1   | 0.95 | 0.15 | 47,47,47,47                 | 0     |
| 54  | MG   | 2A    | 3095 | 1/1   | 0.95 | 0.11 | 44,44,44,44                 | 0     |
| 54  | MG   | 2A    | 3360 | 1/1   | 0.95 | 0.09 | 65,65,65,65                 | 0     |
| 54  | MG   | 2A    | 3678 | 1/1   | 0.95 | 0.07 | 29,29,29,29                 | 0     |
| 54  | MG   | 2A    | 3096 | 1/1   | 0.95 | 0.13 | 32,32,32,32                 | 0     |
| 54  | MG   | 1D    | 307  | 1/1   | 0.95 | 0.11 | 26,26,26,26                 | 0     |
| 54  | MG   | 2a    | 3149 | 1/1   | 0.95 | 0.09 | 33,33,33,33                 | 0     |
| 54  | MG   | 2A    | 3098 | 1/1   | 0.95 | 0.32 | 52,52,52,52                 | 0     |
| 54  | MG   | 1A    | 3302 | 1/1   | 0.95 | 0.54 | 37,37,37,37                 | 0     |
| 54  | MG   | 1D    | 312  | 1/1   | 0.95 | 0.19 | 24,24,24,24                 | 0     |
| 54  | MG   | 2A    | 3102 | 1/1   | 0.95 | 0.07 | 25,25,25,25                 | 0     |
| 54  | MG   | 1A    | 3378 | 1/1   | 0.95 | 0.07 | 21,21,21,21                 | 0     |
| 54  | MG   | 2A    | 3106 | 1/1   | 0.95 | 0.15 | 43,43,43,43                 | 0     |
| 54  | MG   | 1A    | 3583 | 1/1   | 0.95 | 0.12 | 47,47,47,47                 | 0     |
| 54  | MG   | 1A    | 3045 | 1/1   | 0.95 | 0.33 | 39,39,39,39                 | 0     |
| 54  | MG   | 2a    | 3160 | 1/1   | 0.95 | 0.08 | 70,70,70,70                 | 0     |
| 54  | MG   | 1A    | 3944 | 1/1   | 0.95 | 0.06 | 23,23,23,23                 | 0     |
| 54  | MG   | 1A    | 3248 | 1/1   | 0.95 | 0.20 | 31,31,31,31                 | 0     |
| 54  | MG   | 1A    | 3171 | 1/1   | 0.95 | 0.19 | 16,16,16,16                 | 0     |
| 54  | MG   | 1A    | 3804 | 1/1   | 0.95 | 0.16 | 26,26,26,26                 | 0     |
| 54  | MG   | 1D    | 320  | 1/1   | 0.95 | 0.14 | 59,59,59,59                 | 0     |
| 54  | MG   | 2A    | 3380 | 1/1   | 0.95 | 0.05 | 28,28,28,28                 | 0     |
| 54  | MG   | 2a    | 3170 | 1/1   | 0.95 | 0.09 | 66,66,66,66                 | 0     |
| 54  | MG   | 1A    | 3950 | 1/1   | 0.95 | 0.12 | 55,55,55,55                 | 0     |
| 54  | MG   | 2A    | 3384 | 1/1   | 0.95 | 0.07 | 50,50,50,50                 | 0     |
| 54  | MG   | 1A    | 3951 | 1/1   | 0.95 | 0.07 | 43,43,43,43                 | 0     |
| 54  | MG   | 1A    | 3172 | 1/1   | 0.95 | 0.08 | 49,49,49,49                 | 0     |
| 54  | MG   | 1A    | 3102 | 1/1   | 0.95 | 0.28 | 32,32,32,32                 | 0     |
| 54  | MG   | 1a    | 1666 | 1/1   | 0.95 | 0.19 | 49,49,49,49                 | 0     |
| 54  | MG   | 2A    | 3121 | 1/1   | 0.95 | 0.27 | 36,36,36,36                 | 0     |
| 54  | MG   | 1A    | 3394 | 1/1   | 0.95 | 0.11 | 17,17,17,17                 | 0     |
| 54  | MG   | 2A    | 3712 | 1/1   | 0.95 | 0.07 | 28,28,28,28                 | 0     |
| 54  | MG   | 2A    | 3713 | 1/1   | 0.95 | 0.14 | 49,49,49,49                 | 0     |
| 54  | MG   | 1A    | 3142 | 1/1   | 0.95 | 0.07 | 23,23,23,23                 | 0     |
| 54  | MG   | 1A    | 3498 | 1/1   | 0.95 | 0.07 | 15,15,15,15                 | 0     |
| 54  | MG   | 2A    | 3397 | 1/1   | 0.95 | 0.23 | 54,54,54,54                 | 0     |
| 54  | MG   | 2A    | 3125 | 1/1   | 0.95 | 0.27 | 62,62,62,62                 | 0     |
| 54  | MG   | 2A    | 3719 | 1/1   | 0.95 | 0.10 | 47,47,47,47                 | 0     |
| 54  | MG   | 1a    | 1848 | 1/1   | 0.95 | 0.13 | 50,50,50,50                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 2A    | 3721 | 1/1   | 0.95 | 0.12 | 45,45,45,45                 | 0     |
| 54  | MG   | 2A    | 3722 | 1/1   | 0.95 | 0.07 | 52,52,52,52                 | 0     |
| 54  | MG   | 2A    | 3400 | 1/1   | 0.95 | 0.10 | 39,39,39,39                 | 0     |
| 54  | MG   | 1A    | 3959 | 1/1   | 0.95 | 0.12 | 69,69,69,69                 | 0     |
| 54  | MG   | 1F    | 304  | 1/1   | 0.95 | 0.33 | 35,35,35,35                 | 0     |
| 54  | MG   | 1A    | 3499 | 1/1   | 0.95 | 0.14 | 59,59,59,59                 | 0     |
| 54  | MG   | 1A    | 3962 | 1/1   | 0.95 | 0.11 | 34,34,34,34                 | 0     |
| 54  | MG   | 1a    | 1676 | 1/1   | 0.95 | 0.14 | 47,47,47,47                 | 0     |
| 54  | MG   | 1A    | 3814 | 1/1   | 0.95 | 0.10 | 35,35,35,35                 | 0     |
| 54  | MG   | 1F    | 313  | 1/1   | 0.95 | 0.05 | 37,37,37,37                 | 0     |
| 54  | MG   | 1A    | 3046 | 1/1   | 0.95 | 0.33 | 35,35,35,35                 | 0     |
| 54  | MG   | 2A    | 3143 | 1/1   | 0.95 | 0.11 | 39,39,39,39                 | 0     |
| 54  | MG   | 2A    | 3411 | 1/1   | 0.95 | 0.22 | 45,45,45,45                 | 0     |
| 54  | MG   | 1A    | 3403 | 1/1   | 0.95 | 0.07 | 29,29,29,29                 | 0     |
| 54  | MG   | 1A    | 3701 | 1/1   | 0.95 | 0.15 | 62,62,62,62                 | 0     |
| 54  | MG   | 1a    | 1683 | 1/1   | 0.95 | 0.06 | 43,43,43,43                 | 0     |
| 54  | MG   | 1A    | 3703 | 1/1   | 0.95 | 0.13 | 29,29,29,29                 | 0     |
| 54  | MG   | 2A    | 3150 | 1/1   | 0.95 | 0.09 | 57,57,57,57                 | 0     |
| 54  | MG   | 1A    | 3263 | 1/1   | 0.95 | 0.25 | 20,20,20,20                 | 0     |
| 54  | MG   | 1A    | 3062 | 1/1   | 0.95 | 0.06 | 34,34,34,34                 | 0     |
| 57  | ARG  | 1B    | 231  | 12/12 | 0.95 | 0.09 | 26,36,49,52                 | 0     |
| 54  | MG   | 1A    | 3707 | 1/1   | 0.95 | 0.10 | 37,37,37,37                 | 0     |
| 54  | MG   | 1A    | 3319 | 1/1   | 0.95 | 0.10 | 19,19,19,19                 | 0     |
| 54  | MG   | 1A    | 3254 | 1/1   | 0.96 | 0.06 | 68,68,68,68                 | 0     |
| 54  | MG   | 2A    | 3518 | 1/1   | 0.96 | 0.06 | 35,35,35,35                 | 0     |
| 54  | MG   | 1a    | 1694 | 1/1   | 0.96 | 0.07 | 40,40,40,40                 | 0     |
| 54  | MG   | 2F    | 303  | 1/1   | 0.96 | 0.06 | 33,33,33,33                 | 0     |
| 54  | MG   | 2F    | 304  | 1/1   | 0.96 | 0.17 | 47,47,47,47                 | 0     |
| 54  | MG   | 2F    | 305  | 1/1   | 0.96 | 0.12 | 42,42,42,42                 | 0     |
| 54  | MG   | 2A    | 3300 | 1/1   | 0.96 | 0.07 | 39,39,39,39                 | 0     |
| 54  | MG   | 2A    | 3522 | 1/1   | 0.96 | 0.07 | 30,30,30,30                 | 0     |
| 54  | MG   | 1A    | 3469 | 1/1   | 0.96 | 0.07 | 13,13,13,13                 | 0     |
| 54  | MG   | 1V    | 202  | 1/1   | 0.96 | 0.11 | 22,22,22,22                 | 0     |
| 54  | MG   | 1A    | 3311 | 1/1   | 0.96 | 0.13 | 12,12,12,12                 | 0     |
| 54  | MG   | 1V    | 204  | 1/1   | 0.96 | 0.07 | 35,35,35,35                 | 0     |
| 54  | MG   | 1V    | 205  | 1/1   | 0.96 | 0.16 | 45,45,45,45                 | 0     |
| 54  | MG   | 2A    | 3529 | 1/1   | 0.96 | 0.07 | 55,55,55,55                 | 0     |
| 54  | MG   | 2A    | 3115 | 1/1   | 0.96 | 0.18 | 59,59,59,59                 | 0     |
| 54  | MG   | 2Q    | 201  | 1/1   | 0.96 | 0.08 | 48,48,48,48                 | 0     |
| 54  | MG   | 2A    | 3309 | 1/1   | 0.96 | 0.09 | 22,22,22,22                 | 0     |
| 54  | MG   | 1A    | 3030 | 1/1   | 0.96 | 0.19 | 16,16,16,16                 | 0     |
| 54  | MG   | 1W    | 201  | 1/1   | 0.96 | 0.08 | 37,37,37,37                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 1A    | 3473 | 1/1   | 0.96 | 0.08 | 19,19,19,19                 | 0     |
| 54  | MG   | 2A    | 3316 | 1/1   | 0.96 | 0.09 | 22,22,22,22                 | 0     |
| 54  | MG   | 2A    | 3539 | 1/1   | 0.96 | 0.07 | 37,37,37,37                 | 0     |
| 54  | MG   | 2V    | 202  | 1/1   | 0.96 | 0.09 | 50,50,50,50                 | 0     |
| 54  | MG   | 2A    | 3542 | 1/1   | 0.96 | 0.08 | 59,59,59,59                 | 0     |
| 54  | MG   | 2A    | 3317 | 1/1   | 0.96 | 0.14 | 23,23,23,23                 | 0     |
| 54  | MG   | 2A    | 3318 | 1/1   | 0.96 | 0.12 | 40,40,40,40                 | 0     |
| 54  | MG   | 1A    | 3259 | 1/1   | 0.96 | 0.06 | 46,46,46,46                 | 0     |
| 54  | MG   | 1A    | 3904 | 1/1   | 0.96 | 0.08 | 9,9,9,9                     | 0     |
| 54  | MG   | 1Y    | 201  | 1/1   | 0.96 | 0.07 | 64,64,64,64                 | 0     |
| 54  | MG   | 1A    | 3664 | 1/1   | 0.96 | 0.06 | 23,23,23,23                 | 0     |
| 54  | MG   | 23    | 101  | 1/1   | 0.96 | 0.11 | 52,52,52,52                 | 0     |
| 54  | MG   | 2A    | 3323 | 1/1   | 0.96 | 0.13 | 43,43,43,43                 | 0     |
| 54  | MG   | 10    | 102  | 1/1   | 0.96 | 0.13 | 41,41,41,41                 | 0     |
| 54  | MG   | 1A    | 3906 | 1/1   | 0.96 | 0.11 | 12,12,12,12                 | 0     |
| 54  | MG   | 27    | 102  | 1/1   | 0.96 | 0.06 | 39,39,39,39                 | 0     |
| 54  | MG   | 1A    | 3570 | 1/1   | 0.96 | 0.09 | 17,17,17,17                 | 0     |
| 54  | MG   | 10    | 106  | 1/1   | 0.96 | 0.10 | 57,57,57,57                 | 0     |
| 54  | MG   | 1A    | 3118 | 1/1   | 0.96 | 0.08 | 33,33,33,33                 | 0     |
| 54  | MG   | 1A    | 3210 | 1/1   | 0.96 | 0.21 | 32,32,32,32                 | 0     |
| 54  | MG   | 1A    | 4031 | 1/1   | 0.96 | 0.06 | 35,35,35,35                 | 0     |
| 54  | MG   | 2A    | 3562 | 1/1   | 0.96 | 0.06 | 33,33,33,33                 | 0     |
| 54  | MG   | 2A    | 3332 | 1/1   | 0.96 | 0.07 | 33,33,33,33                 | 0     |
| 54  | MG   | 2A    | 3131 | 1/1   | 0.96 | 0.06 | 37,37,37,37                 | 0     |
| 54  | MG   | 1A    | 3389 | 1/1   | 0.96 | 0.06 | 29,29,29,29                 | 0     |
| 54  | MG   | 2A    | 3133 | 1/1   | 0.96 | 0.10 | 39,39,39,39                 | 0     |
| 54  | MG   | 1A    | 3393 | 1/1   | 0.96 | 0.05 | 14,14,14,14                 | 0     |
| 54  | MG   | 2A    | 3135 | 1/1   | 0.96 | 0.09 | 34,34,34,34                 | 0     |
| 54  | MG   | 1a    | 1882 | 1/1   | 0.96 | 0.12 | 49,49,49,49                 | 0     |
| 54  | MG   | 2a    | 3013 | 1/1   | 0.96 | 0.14 | 49,49,49,49                 | 0     |
| 54  | MG   | 2A    | 3137 | 1/1   | 0.96 | 0.06 | 27,27,27,27                 | 0     |
| 54  | MG   | 2A    | 3138 | 1/1   | 0.96 | 0.11 | 52,52,52,52                 | 0     |
| 54  | MG   | 13    | 102  | 1/1   | 0.96 | 0.14 | 72,72,72,72                 | 0     |
| 54  | MG   | 2A    | 3140 | 1/1   | 0.96 | 0.05 | 45,45,45,45                 | 0     |
| 54  | MG   | 1A    | 3317 | 1/1   | 0.96 | 0.08 | 51,51,51,51                 | 0     |
| 54  | MG   | 1A    | 4036 | 1/1   | 0.96 | 0.08 | 42,42,42,42                 | 0     |
| 54  | MG   | 2A    | 3144 | 1/1   | 0.96 | 0.10 | 44,44,44,44                 | 0     |
| 54  | MG   | 15    | 104  | 1/1   | 0.96 | 0.26 | 20,20,20,20                 | 0     |
| 54  | MG   | 1A    | 4037 | 1/1   | 0.96 | 0.10 | 39,39,39,39                 | 0     |
| 54  | MG   | 2A    | 3352 | 1/1   | 0.96 | 0.15 | 50,50,50,50                 | 0     |
| 54  | MG   | 1A    | 3087 | 1/1   | 0.96 | 0.12 | 32,32,32,32                 | 0     |
| 54  | MG   | 1A    | 3213 | 1/1   | 0.96 | 0.13 | 25,25,25,25                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 2A    | 3597 | 1/1   | 0.96 | 0.07 | 35,35,35,35                 | 0     |
| 54  | MG   | 1a    | 1735 | 1/1   | 0.96 | 0.06 | 44,44,44,44                 | 0     |
| 54  | MG   | 2A    | 3151 | 1/1   | 0.96 | 0.12 | 41,41,41,41                 | 0     |
| 54  | MG   | 2A    | 3358 | 1/1   | 0.96 | 0.05 | 56,56,56,56                 | 0     |
| 54  | MG   | 2A    | 3152 | 1/1   | 0.96 | 0.25 | 67,67,67,67                 | 0     |
| 54  | MG   | 1A    | 3320 | 1/1   | 0.96 | 0.07 | 43,43,43,43                 | 0     |
| 54  | MG   | 2A    | 3154 | 1/1   | 0.96 | 0.14 | 46,46,46,46                 | 0     |
| 54  | MG   | 2A    | 3604 | 1/1   | 0.96 | 0.07 | 45,45,45,45                 | 0     |
| 54  | MG   | 1A    | 3923 | 1/1   | 0.96 | 0.10 | 26,26,26,26                 | 0     |
| 54  | MG   | 1A    | 3495 | 1/1   | 0.96 | 0.06 | 38,38,38,38                 | 0     |
| 54  | MG   | 17    | 104  | 1/1   | 0.96 | 0.14 | 48,48,48,48                 | 0     |
| 54  | MG   | 1A    | 3265 | 1/1   | 0.96 | 0.25 | 46,46,46,46                 | 0     |
| 54  | MG   | 1a    | 1742 | 1/1   | 0.96 | 0.11 | 37,37,37,37                 | 0     |
| 54  | MG   | 1A    | 3407 | 1/1   | 0.96 | 0.06 | 30,30,30,30                 | 0     |
| 54  | MG   | 2A    | 3368 | 1/1   | 0.96 | 0.11 | 33,33,33,33                 | 0     |
| 54  | MG   | 1A    | 3100 | 1/1   | 0.96 | 0.07 | 55,55,55,55                 | 0     |
| 54  | MG   | 1l    | 202  | 1/1   | 0.96 | 0.04 | 48,48,48,48                 | 0     |
| 54  | MG   | 1A    | 3326 | 1/1   | 0.96 | 0.05 | 22,22,22,22                 | 0     |
| 54  | MG   | 1A    | 3181 | 1/1   | 0.96 | 0.20 | 34,34,34,34                 | 0     |
| 54  | MG   | 2A    | 3373 | 1/1   | 0.96 | 0.07 | 27,27,27,27                 | 0     |
| 54  | MG   | 1A    | 3798 | 1/1   | 0.96 | 0.10 | 52,52,52,52                 | 0     |
| 54  | MG   | 2A    | 3168 | 1/1   | 0.96 | 0.17 | 54,54,54,54                 | 0     |
| 54  | MG   | 2A    | 3377 | 1/1   | 0.96 | 0.07 | 36,36,36,36                 | 0     |
| 54  | MG   | 1A    | 4049 | 1/1   | 0.96 | 0.17 | 42,42,42,42                 | 0     |
| 54  | MG   | 2A    | 3623 | 1/1   | 0.96 | 0.06 | 68,68,68,68                 | 0     |
| 54  | MG   | 1A    | 3502 | 1/1   | 0.96 | 0.09 | 13,13,13,13                 | 0     |
| 54  | MG   | 1A    | 3088 | 1/1   | 0.96 | 0.08 | 34,34,34,34                 | 0     |
| 54  | MG   | 1B    | 203  | 1/1   | 0.96 | 0.16 | 38,38,38,38                 | 0     |
| 54  | MG   | 2A    | 3627 | 1/1   | 0.96 | 0.14 | 56,56,56,56                 | 0     |
| 54  | MG   | 1B    | 205  | 1/1   | 0.96 | 0.34 | 37,37,37,37                 | 0     |
| 54  | MG   | 1A    | 3217 | 1/1   | 0.96 | 0.07 | 36,36,36,36                 | 0     |
| 54  | MG   | 2A    | 3634 | 1/1   | 0.96 | 0.08 | 70,70,70,70                 | 0     |
| 54  | MG   | 2A    | 3635 | 1/1   | 0.96 | 0.09 | 35,35,35,35                 | 0     |
| 54  | MG   | 2A    | 3636 | 1/1   | 0.96 | 0.12 | 75,75,75,75                 | 0     |
| 54  | MG   | 1A    | 3272 | 1/1   | 0.96 | 0.07 | 29,29,29,29                 | 0     |
| 54  | MG   | 1A    | 3027 | 1/1   | 0.96 | 0.17 | 23,23,23,23                 | 0     |
| 54  | MG   | 1A    | 3219 | 1/1   | 0.96 | 0.06 | 30,30,30,30                 | 0     |
| 54  | MG   | 2A    | 3390 | 1/1   | 0.96 | 0.06 | 33,33,33,33                 | 0     |
| 54  | MG   | 2A    | 3003 | 1/1   | 0.96 | 0.06 | 56,56,56,56                 | 0     |
| 54  | MG   | 1A    | 3079 | 1/1   | 0.96 | 0.06 | 23,23,23,23                 | 0     |
| 54  | MG   | 1a    | 1611 | 1/1   | 0.96 | 0.13 | 38,38,38,38                 | 0     |
| 54  | MG   | 1A    | 3223 | 1/1   | 0.96 | 0.22 | 22,22,22,22                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 2A    | 3185 | 1/1   | 0.96 | 0.17 | 49,49,49,49                 | 0     |
| 54  | MG   | 1A    | 3697 | 1/1   | 0.96 | 0.15 | 47,47,47,47                 | 0     |
| 54  | MG   | 1A    | 3022 | 1/1   | 0.96 | 0.21 | 24,24,24,24                 | 0     |
| 54  | MG   | 1A    | 3512 | 1/1   | 0.96 | 0.09 | 15,15,15,15                 | 0     |
| 54  | MG   | 2A    | 3401 | 1/1   | 0.96 | 0.12 | 39,39,39,39                 | 0     |
| 54  | MG   | 2A    | 3653 | 1/1   | 0.96 | 0.07 | 31,31,31,31                 | 0     |
| 54  | MG   | 1A    | 3811 | 1/1   | 0.96 | 0.08 | 16,16,16,16                 | 0     |
| 54  | MG   | 2A    | 3663 | 1/1   | 0.96 | 0.05 | 54,54,54,54                 | 0     |
| 54  | MG   | 1A    | 3812 | 1/1   | 0.96 | 0.14 | 21,21,21,21                 | 0     |
| 54  | MG   | 1A    | 3603 | 1/1   | 0.96 | 0.20 | 25,25,25,25                 | 0     |
| 54  | MG   | 1A    | 3948 | 1/1   | 0.96 | 0.11 | 35,35,35,35                 | 0     |
| 54  | MG   | 2A    | 3194 | 1/1   | 0.96 | 0.09 | 46,46,46,46                 | 0     |
| 54  | MG   | 1A    | 3514 | 1/1   | 0.96 | 0.07 | 41,41,41,41                 | 0     |
| 54  | MG   | 2a    | 3087 | 1/1   | 0.96 | 0.07 | 75,75,75,75                 | 0     |
| 54  | MG   | 1A    | 3605 | 1/1   | 0.96 | 0.11 | 43,43,43,43                 | 0     |
| 54  | MG   | 1A    | 3106 | 1/1   | 0.96 | 0.09 | 52,52,52,52                 | 0     |
| 54  | MG   | 1A    | 3131 | 1/1   | 0.96 | 0.05 | 18,18,18,18                 | 0     |
| 54  | MG   | 1D    | 302  | 1/1   | 0.96 | 0.06 | 33,33,33,33                 | 0     |
| 54  | MG   | 1D    | 303  | 1/1   | 0.96 | 0.07 | 50,50,50,50                 | 0     |
| 54  | MG   | 1a    | 1773 | 1/1   | 0.96 | 0.08 | 74,74,74,74                 | 0     |
| 54  | MG   | 2a    | 3095 | 1/1   | 0.96 | 0.06 | 56,56,56,56                 | 0     |
| 54  | MG   | 2A    | 3679 | 1/1   | 0.96 | 0.06 | 33,33,33,33                 | 0     |
| 54  | MG   | 1A    | 3953 | 1/1   | 0.96 | 0.10 | 55,55,55,55                 | 0     |
| 54  | MG   | 2A    | 3415 | 1/1   | 0.96 | 0.14 | 49,49,49,49                 | 0     |
| 54  | MG   | 1A    | 3424 | 1/1   | 0.96 | 0.09 | 43,43,43,43                 | 0     |
| 54  | MG   | 1A    | 3521 | 1/1   | 0.96 | 0.07 | 21,21,21,21                 | 0     |
| 54  | MG   | 1A    | 3160 | 1/1   | 0.96 | 0.10 | 35,35,35,35                 | 0     |
| 54  | MG   | 1A    | 3426 | 1/1   | 0.96 | 0.07 | 43,43,43,43                 | 0     |
| 54  | MG   | 2A    | 3687 | 1/1   | 0.96 | 0.10 | 39,39,39,39                 | 0     |
| 54  | MG   | 2a    | 3105 | 1/1   | 0.96 | 0.13 | 50,50,50,50                 | 0     |
| 54  | MG   | 1a    | 1631 | 1/1   | 0.96 | 0.09 | 49,49,49,49                 | 0     |
| 54  | MG   | 1a    | 1632 | 1/1   | 0.96 | 0.20 | 38,38,38,38                 | 0     |
| 54  | MG   | 1A    | 3828 | 1/1   | 0.96 | 0.11 | 22,22,22,22                 | 0     |
| 54  | MG   | 1A    | 3132 | 1/1   | 0.96 | 0.09 | 52,52,52,52                 | 0     |
| 54  | MG   | 1A    | 3284 | 1/1   | 0.96 | 0.12 | 14,14,14,14                 | 0     |
| 54  | MG   | 1A    | 3833 | 1/1   | 0.96 | 0.10 | 36,36,36,36                 | 0     |
| 54  | MG   | 1A    | 3107 | 1/1   | 0.96 | 0.11 | 22,22,22,22                 | 0     |
| 54  | MG   | 2A    | 3699 | 1/1   | 0.96 | 0.10 | 51,51,51,51                 | 0     |
| 54  | MG   | 1A    | 3134 | 1/1   | 0.96 | 0.24 | 24,24,24,24                 | 0     |
| 54  | MG   | 1A    | 3718 | 1/1   | 0.96 | 0.09 | 43,43,43,43                 | 0     |
| 54  | MG   | 1A    | 3432 | 1/1   | 0.96 | 0.05 | 12,12,12,12                 | 0     |
| 54  | MG   | 2A    | 3218 | 1/1   | 0.96 | 0.16 | 44,44,44,44                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 1A    | 3109 | 1/1   | 0.96 | 0.20 | 33,33,33,33                 | 0     |
| 54  | MG   | 1A    | 3974 | 1/1   | 0.96 | 0.07 | 55,55,55,55                 | 0     |
| 54  | MG   | 1A    | 3353 | 1/1   | 0.96 | 0.15 | 41,41,41,41                 | 0     |
| 54  | MG   | 2A    | 3042 | 1/1   | 0.96 | 0.17 | 50,50,50,50                 | 0     |
| 54  | MG   | 1E    | 306  | 1/1   | 0.96 | 0.10 | 22,22,22,22                 | 0     |
| 54  | MG   | 1E    | 307  | 1/1   | 0.96 | 0.04 | 40,40,40,40                 | 0     |
| 54  | MG   | 2a    | 3126 | 1/1   | 0.96 | 0.04 | 65,65,65,65                 | 0     |
| 54  | MG   | 1a    | 1646 | 1/1   | 0.96 | 0.12 | 40,40,40,40                 | 0     |
| 54  | MG   | 1A    | 3289 | 1/1   | 0.96 | 0.07 | 40,40,40,40                 | 0     |
| 54  | MG   | 1a    | 1797 | 1/1   | 0.96 | 0.06 | 62,62,62,62                 | 0     |
| 54  | MG   | 1A    | 3724 | 1/1   | 0.96 | 0.11 | 32,32,32,32                 | 0     |
| 54  | MG   | 1a    | 1649 | 1/1   | 0.96 | 0.08 | 45,45,45,45                 | 0     |
| 54  | MG   | 1F    | 302  | 1/1   | 0.96 | 0.29 | 20,20,20,20                 | 0     |
| 54  | MG   | 1A    | 3290 | 1/1   | 0.96 | 0.10 | 36,36,36,36                 | 0     |
| 54  | MG   | 1A    | 3358 | 1/1   | 0.96 | 0.09 | 8,8,8,8                     | 0     |
| 54  | MG   | 1A    | 3071 | 1/1   | 0.96 | 0.06 | 38,38,38,38                 | 0     |
| 54  | MG   | 2a    | 3141 | 1/1   | 0.96 | 0.08 | 70,70,70,70                 | 0     |
| 54  | MG   | 2a    | 3142 | 1/1   | 0.96 | 0.06 | 67,67,67,67                 | 0     |
| 54  | MG   | 1A    | 3628 | 1/1   | 0.96 | 0.09 | 37,37,37,37                 | 0     |
| 54  | MG   | 1F    | 311  | 1/1   | 0.96 | 0.34 | 33,33,33,33                 | 0     |
| 54  | MG   | 1A    | 3850 | 1/1   | 0.96 | 0.06 | 35,35,35,35                 | 0     |
| 54  | MG   | 1A    | 3082 | 1/1   | 0.96 | 0.17 | 29,29,29,29                 | 0     |
| 54  | MG   | 1a    | 1810 | 1/1   | 0.96 | 0.07 | 61,61,61,61                 | 0     |
| 54  | MG   | 1A    | 3294 | 1/1   | 0.96 | 0.06 | 32,32,32,32                 | 0     |
| 54  | MG   | 1A    | 3632 | 1/1   | 0.96 | 0.20 | 44,44,44,44                 | 0     |
| 54  | MG   | 1A    | 3139 | 1/1   | 0.96 | 0.18 | 14,14,14,14                 | 0     |
| 54  | MG   | 1F    | 317  | 1/1   | 0.96 | 0.05 | 31,31,31,31                 | 0     |
| 54  | MG   | 1A    | 3296 | 1/1   | 0.96 | 0.16 | 26,26,26,26                 | 0     |
| 54  | MG   | 2A    | 3461 | 1/1   | 0.96 | 0.06 | 39,39,39,39                 | 0     |
| 54  | MG   | 2a    | 3154 | 1/1   | 0.96 | 0.06 | 53,53,53,53                 | 0     |
| 54  | MG   | 1A    | 3297 | 1/1   | 0.96 | 0.06 | 26,26,26,26                 | 0     |
| 54  | MG   | 2A    | 3247 | 1/1   | 0.96 | 0.11 | 19,19,19,19                 | 0     |
| 54  | MG   | 1A    | 3242 | 1/1   | 0.96 | 0.26 | 24,24,24,24                 | 0     |
| 54  | MG   | 2A    | 3466 | 1/1   | 0.96 | 0.08 | 34,34,34,34                 | 0     |
| 54  | MG   | 1A    | 3367 | 1/1   | 0.96 | 0.05 | 16,16,16,16                 | 0     |
| 54  | MG   | 1A    | 3141 | 1/1   | 0.96 | 0.07 | 25,25,25,25                 | 0     |
| 54  | MG   | 2A    | 3253 | 1/1   | 0.96 | 0.05 | 56,56,56,56                 | 0     |
| 54  | MG   | 2A    | 3743 | 1/1   | 0.96 | 0.17 | 41,41,41,41                 | 0     |
| 54  | MG   | 1A    | 3247 | 1/1   | 0.96 | 0.08 | 35,35,35,35                 | 0     |
| 54  | MG   | 1A    | 3640 | 1/1   | 0.96 | 0.09 | 32,32,32,32                 | 0     |
| 54  | MG   | 1a    | 1669 | 1/1   | 0.96 | 0.10 | 43,43,43,43                 | 0     |
| 54  | MG   | 1a    | 1670 | 1/1   | 0.96 | 0.21 | 44,44,44,44                 | 0     |

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| Mol | Type  | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|-------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG    | 2a    | 3171 | 1/1   | 0.96 | 0.10 | 72,72,72,72                 | 0     |
| 54  | MG    | 1A    | 3863 | 1/1   | 0.96 | 0.05 | 31,31,31,31                 | 0     |
| 54  | MG    | 2A    | 3750 | 1/1   | 0.96 | 0.14 | 38,38,38,38                 | 0     |
| 54  | MG    | 2A    | 3259 | 1/1   | 0.96 | 0.06 | 35,35,35,35                 | 0     |
| 54  | MG    | 1A    | 3641 | 1/1   | 0.96 | 0.08 | 42,42,42,42                 | 0     |
| 54  | MG    | 1A    | 3066 | 1/1   | 0.96 | 0.47 | 31,31,31,31                 | 0     |
| 54  | MG    | 1A    | 3644 | 1/1   | 0.96 | 0.14 | 51,51,51,51                 | 0     |
| 54  | MG    | 2A    | 3483 | 1/1   | 0.96 | 0.13 | 60,60,60,60                 | 0     |
| 54  | MG    | 1A    | 3114 | 1/1   | 0.96 | 0.07 | 19,19,19,19                 | 0     |
| 54  | MG    | 2A    | 3264 | 1/1   | 0.96 | 0.06 | 21,21,21,21                 | 0     |
| 54  | MG    | 1P    | 206  | 1/1   | 0.96 | 0.04 | 33,33,33,33                 | 0     |
| 54  | MG    | 1A    | 3871 | 1/1   | 0.96 | 0.06 | 21,21,21,21                 | 0     |
| 54  | MG    | 2A    | 3488 | 1/1   | 0.96 | 0.04 | 32,32,32,32                 | 0     |
| 54  | MG    | 1a    | 1833 | 1/1   | 0.96 | 0.12 | 63,63,63,63                 | 0     |
| 54  | MG    | 1A    | 3647 | 1/1   | 0.96 | 0.13 | 45,45,45,45                 | 0     |
| 54  | MG    | 2B    | 208  | 1/1   | 0.96 | 0.15 | 49,49,49,49                 | 0     |
| 54  | MG    | 2A    | 3088 | 1/1   | 0.96 | 0.14 | 43,43,43,43                 | 0     |
| 54  | MG    | 1Q    | 204  | 1/1   | 0.96 | 0.15 | 35,35,35,35                 | 0     |
| 54  | MG    | 1a    | 1836 | 1/1   | 0.96 | 0.06 | 45,45,45,45                 | 0     |
| 54  | MG    | 1A    | 3144 | 1/1   | 0.96 | 0.07 | 17,17,17,17                 | 0     |
| 54  | MG    | 2A    | 3495 | 1/1   | 0.96 | 0.11 | 48,48,48,48                 | 0     |
| 54  | MG    | 1A    | 4007 | 1/1   | 0.96 | 0.08 | 20,20,20,20                 | 0     |
| 54  | MG    | 1a    | 1682 | 1/1   | 0.96 | 0.19 | 62,62,62,62                 | 0     |
| 54  | MG    | 1a    | 1840 | 1/1   | 0.96 | 0.06 | 80,80,80,80                 | 0     |
| 54  | MG    | 1A    | 3757 | 1/1   | 0.96 | 0.08 | 32,32,32,32                 | 0     |
| 54  | MG    | 1A    | 3651 | 1/1   | 0.96 | 0.09 | 14,14,14,14                 | 0     |
| 54  | MG    | 2D    | 301  | 1/1   | 0.96 | 0.12 | 36,36,36,36                 | 0     |
| 54  | MG    | 1A    | 3759 | 1/1   | 0.96 | 0.04 | 17,17,17,17                 | 0     |
| 54  | MG    | 1A    | 3305 | 1/1   | 0.96 | 0.14 | 13,13,13,13                 | 0     |
| 54  | MG    | 2A    | 3507 | 1/1   | 0.96 | 0.11 | 34,34,34,34                 | 0     |
| 55  | A1CQ5 | 1A    | 4050 | 45/45 | 0.96 | 0.11 | 16,22,50,60                 | 0     |
| 54  | MG    | 1A    | 3560 | 1/1   | 0.96 | 0.08 | 11,11,11,11                 | 0     |
| 54  | MG    | 2A    | 3100 | 1/1   | 0.96 | 0.15 | 44,44,44,44                 | 0     |
| 54  | MG    | 1A    | 3307 | 1/1   | 0.96 | 0.10 | 31,31,31,31                 | 0     |
| 56  | MPD   | 18    | 104  | 8/8   | 0.96 | 0.12 | 24,26,28,30                 | 0     |
| 54  | MG    | 1A    | 3884 | 1/1   | 0.96 | 0.27 | 20,20,20,20                 | 0     |
| 54  | MG    | 2A    | 3103 | 1/1   | 0.96 | 0.12 | 61,61,61,61                 | 0     |
| 54  | MG    | 2A    | 3292 | 1/1   | 0.96 | 0.15 | 31,31,31,31                 | 0     |
| 54  | MG    | 2E    | 301  | 1/1   | 0.96 | 0.13 | 37,37,37,37                 | 0     |
| 54  | MG    | 1A    | 3253 | 1/1   | 0.96 | 0.33 | 26,26,26,26                 | 0     |
| 54  | MG    | 2A    | 3294 | 1/1   | 0.96 | 0.07 | 50,50,50,50                 | 0     |
| 54  | MG    | 1A    | 3890 | 1/1   | 0.96 | 0.07 | 39,39,39,39                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 1a    | 1861 | 1/1   | 0.97 | 0.05 | 83,83,83,83                 | 0     |
| 54  | MG   | 1A    | 3471 | 1/1   | 0.97 | 0.06 | 16,16,16,16                 | 0     |
| 54  | MG   | 1A    | 3821 | 1/1   | 0.97 | 0.07 | 32,32,32,32                 | 0     |
| 54  | MG   | 2A    | 3335 | 1/1   | 0.97 | 0.06 | 23,23,23,23                 | 0     |
| 54  | MG   | 1A    | 3123 | 1/1   | 0.97 | 0.04 | 48,48,48,48                 | 0     |
| 54  | MG   | 2Q    | 203  | 1/1   | 0.97 | 0.08 | 47,47,47,47                 | 0     |
| 54  | MG   | 1a    | 1865 | 1/1   | 0.97 | 0.11 | 51,51,51,51                 | 0     |
| 54  | MG   | 2A    | 3560 | 1/1   | 0.97 | 0.12 | 52,52,52,52                 | 0     |
| 54  | MG   | 1A    | 3823 | 1/1   | 0.97 | 0.08 | 35,35,35,35                 | 0     |
| 54  | MG   | 1A    | 3262 | 1/1   | 0.97 | 0.30 | 28,28,28,28                 | 0     |
| 54  | MG   | 2T    | 204  | 1/1   | 0.97 | 0.07 | 32,32,32,32                 | 0     |
| 54  | MG   | 1a    | 1868 | 1/1   | 0.97 | 0.05 | 42,42,42,42                 | 0     |
| 54  | MG   | 1a    | 1690 | 1/1   | 0.97 | 0.15 | 58,58,58,58                 | 0     |
| 54  | MG   | 1A    | 3474 | 1/1   | 0.97 | 0.09 | 26,26,26,26                 | 0     |
| 54  | MG   | 1A    | 3576 | 1/1   | 0.97 | 0.06 | 38,38,38,38                 | 0     |
| 54  | MG   | 1A    | 3983 | 1/1   | 0.97 | 0.05 | 15,15,15,15                 | 0     |
| 54  | MG   | 2X    | 101  | 1/1   | 0.97 | 0.11 | 49,49,49,49                 | 0     |
| 54  | MG   | 1Q    | 203  | 1/1   | 0.97 | 0.10 | 29,29,29,29                 | 0     |
| 54  | MG   | 1A    | 3381 | 1/1   | 0.97 | 0.05 | 13,13,13,13                 | 0     |
| 54  | MG   | 2A    | 3573 | 1/1   | 0.97 | 0.08 | 26,26,26,26                 | 0     |
| 54  | MG   | 1A    | 3578 | 1/1   | 0.97 | 0.04 | 30,30,30,30                 | 0     |
| 54  | MG   | 2A    | 3145 | 1/1   | 0.97 | 0.12 | 51,51,51,51                 | 0     |
| 54  | MG   | 1A    | 3476 | 1/1   | 0.97 | 0.09 | 14,14,14,14                 | 0     |
| 54  | MG   | 1a    | 1698 | 1/1   | 0.97 | 0.04 | 22,22,22,22                 | 0     |
| 54  | MG   | 1A    | 3477 | 1/1   | 0.97 | 0.06 | 20,20,20,20                 | 0     |
| 54  | MG   | 1A    | 3834 | 1/1   | 0.97 | 0.12 | 40,40,40,40                 | 0     |
| 54  | MG   | 28    | 101  | 1/1   | 0.97 | 0.06 | 52,52,52,52                 | 0     |
| 54  | MG   | 1a    | 1704 | 1/1   | 0.97 | 0.06 | 45,45,45,45                 | 0     |
| 54  | MG   | 1A    | 3124 | 1/1   | 0.97 | 0.07 | 53,53,53,53                 | 0     |
| 54  | MG   | 1A    | 3024 | 1/1   | 0.97 | 0.25 | 33,33,33,33                 | 0     |
| 54  | MG   | 1A    | 3386 | 1/1   | 0.97 | 0.07 | 11,11,11,11                 | 0     |
| 54  | MG   | 1A    | 3839 | 1/1   | 0.97 | 0.05 | 39,39,39,39                 | 0     |
| 54  | MG   | 2A    | 3594 | 1/1   | 0.97 | 0.11 | 73,73,73,73                 | 0     |
| 54  | MG   | 1a    | 1709 | 1/1   | 0.97 | 0.10 | 71,71,71,71                 | 0     |
| 54  | MG   | 1A    | 3025 | 1/1   | 0.97 | 0.16 | 19,19,19,19                 | 0     |
| 54  | MG   | 1a    | 1712 | 1/1   | 0.97 | 0.14 | 61,61,61,61                 | 0     |
| 54  | MG   | 1a    | 1714 | 1/1   | 0.97 | 0.08 | 53,53,53,53                 | 0     |
| 54  | MG   | 1A    | 3586 | 1/1   | 0.97 | 0.12 | 40,40,40,40                 | 0     |
| 54  | MG   | 1A    | 3588 | 1/1   | 0.97 | 0.08 | 36,36,36,36                 | 0     |
| 54  | MG   | 2A    | 3162 | 1/1   | 0.97 | 0.13 | 49,49,49,49                 | 0     |
| 54  | MG   | 1U    | 202  | 1/1   | 0.97 | 0.27 | 22,22,22,22                 | 0     |
| 54  | MG   | 1U    | 204  | 1/1   | 0.97 | 0.11 | 25,25,25,25                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 1A    | 3704 | 1/1   | 0.97 | 0.04 | 24,24,24,24                 | 0     |
| 54  | MG   | 1A    | 3388 | 1/1   | 0.97 | 0.06 | 18,18,18,18                 | 0     |
| 54  | MG   | 1V    | 201  | 1/1   | 0.97 | 0.10 | 16,16,16,16                 | 0     |
| 54  | MG   | 1A    | 3999 | 1/1   | 0.97 | 0.07 | 21,21,21,21                 | 0     |
| 54  | MG   | 1A    | 3085 | 1/1   | 0.97 | 0.08 | 42,42,42,42                 | 0     |
| 54  | MG   | 2A    | 3376 | 1/1   | 0.97 | 0.07 | 26,26,26,26                 | 0     |
| 54  | MG   | 1k    | 201  | 1/1   | 0.97 | 0.11 | 43,43,43,43                 | 0     |
| 54  | MG   | 2A    | 3612 | 1/1   | 0.97 | 0.05 | 52,52,52,52                 | 0     |
| 54  | MG   | 2a    | 3024 | 1/1   | 0.97 | 0.18 | 57,57,57,57                 | 0     |
| 54  | MG   | 2A    | 3171 | 1/1   | 0.97 | 0.06 | 38,38,38,38                 | 0     |
| 54  | MG   | 2A    | 3172 | 1/1   | 0.97 | 0.12 | 41,41,41,41                 | 0     |
| 54  | MG   | 1A    | 3487 | 1/1   | 0.97 | 0.05 | 41,41,41,41                 | 0     |
| 54  | MG   | 1A    | 3592 | 1/1   | 0.97 | 0.07 | 21,21,21,21                 | 0     |
| 54  | MG   | 1A    | 3391 | 1/1   | 0.97 | 0.07 | 10,10,10,10                 | 0     |
| 54  | MG   | 1A    | 3491 | 1/1   | 0.97 | 0.06 | 26,26,26,26                 | 0     |
| 54  | MG   | 2A    | 3177 | 1/1   | 0.97 | 0.18 | 47,47,47,47                 | 0     |
| 54  | MG   | 1A    | 3154 | 1/1   | 0.97 | 0.07 | 28,28,28,28                 | 0     |
| 54  | MG   | 1A    | 3494 | 1/1   | 0.97 | 0.06 | 48,48,48,48                 | 0     |
| 54  | MG   | 2a    | 3034 | 1/1   | 0.97 | 0.17 | 36,36,36,36                 | 0     |
| 54  | MG   | 1A    | 3269 | 1/1   | 0.97 | 0.09 | 44,44,44,44                 | 0     |
| 54  | MG   | 2A    | 3391 | 1/1   | 0.97 | 0.05 | 33,33,33,33                 | 0     |
| 54  | MG   | 1A    | 3322 | 1/1   | 0.97 | 0.09 | 16,16,16,16                 | 0     |
| 54  | MG   | 1A    | 3399 | 1/1   | 0.97 | 0.10 | 30,30,30,30                 | 0     |
| 54  | MG   | 1A    | 3185 | 1/1   | 0.97 | 0.15 | 25,25,25,25                 | 0     |
| 54  | MG   | 1A    | 3325 | 1/1   | 0.97 | 0.06 | 18,18,18,18                 | 0     |
| 54  | MG   | 1a    | 1737 | 1/1   | 0.97 | 0.17 | 50,50,50,50                 | 0     |
| 54  | MG   | 2A    | 3631 | 1/1   | 0.97 | 0.06 | 53,53,53,53                 | 0     |
| 54  | MG   | 10    | 104  | 1/1   | 0.97 | 0.05 | 35,35,35,35                 | 0     |
| 54  | MG   | 1A    | 3187 | 1/1   | 0.97 | 0.21 | 34,34,34,34                 | 0     |
| 54  | MG   | 1A    | 4016 | 1/1   | 0.97 | 0.20 | 51,51,51,51                 | 0     |
| 54  | MG   | 1A    | 3222 | 1/1   | 0.97 | 0.34 | 22,22,22,22                 | 0     |
| 54  | MG   | 1A    | 3329 | 1/1   | 0.97 | 0.12 | 25,25,25,25                 | 0     |
| 54  | MG   | 1A    | 3409 | 1/1   | 0.97 | 0.07 | 20,20,20,20                 | 0     |
| 54  | MG   | 2A    | 3007 | 1/1   | 0.97 | 0.06 | 38,38,38,38                 | 0     |
| 54  | MG   | 11    | 104  | 1/1   | 0.97 | 0.06 | 30,30,30,30                 | 0     |
| 54  | MG   | 1A    | 3727 | 1/1   | 0.97 | 0.13 | 35,35,35,35                 | 0     |
| 54  | MG   | 1A    | 3129 | 1/1   | 0.97 | 0.14 | 26,26,26,26                 | 0     |
| 54  | MG   | 1A    | 3274 | 1/1   | 0.97 | 0.27 | 18,18,18,18                 | 0     |
| 54  | MG   | 2A    | 3012 | 1/1   | 0.97 | 0.10 | 25,25,25,25                 | 0     |
| 54  | MG   | 1A    | 3015 | 1/1   | 0.97 | 0.15 | 28,28,28,28                 | 0     |
| 54  | MG   | 1A    | 3731 | 1/1   | 0.97 | 0.05 | 32,32,32,32                 | 0     |
| 54  | MG   | 15    | 103  | 1/1   | 0.97 | 0.26 | 31,31,31,31                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 1A    | 3037 | 1/1   | 0.97 | 0.06 | 31,31,31,31                 | 0     |
| 54  | MG   | 1A    | 3872 | 1/1   | 0.97 | 0.06 | 10,10,10,10                 | 0     |
| 54  | MG   | 1A    | 3334 | 1/1   | 0.97 | 0.05 | 20,20,20,20                 | 0     |
| 54  | MG   | 2A    | 3656 | 1/1   | 0.97 | 0.09 | 56,56,56,56                 | 0     |
| 54  | MG   | 2A    | 3657 | 1/1   | 0.97 | 0.12 | 63,63,63,63                 | 0     |
| 54  | MG   | 2A    | 3660 | 1/1   | 0.97 | 0.07 | 56,56,56,56                 | 0     |
| 54  | MG   | 1A    | 3734 | 1/1   | 0.97 | 0.14 | 31,31,31,31                 | 0     |
| 54  | MG   | 1A    | 3612 | 1/1   | 0.97 | 0.11 | 40,40,40,40                 | 0     |
| 54  | MG   | 1A    | 3736 | 1/1   | 0.97 | 0.12 | 32,32,32,32                 | 0     |
| 54  | MG   | 2A    | 3667 | 1/1   | 0.97 | 0.05 | 30,30,30,30                 | 0     |
| 54  | MG   | 2a    | 3068 | 1/1   | 0.97 | 0.19 | 32,32,32,32                 | 0     |
| 54  | MG   | 1A    | 3879 | 1/1   | 0.97 | 0.07 | 43,43,43,43                 | 0     |
| 54  | MG   | 17    | 103  | 1/1   | 0.97 | 0.10 | 40,40,40,40                 | 0     |
| 54  | MG   | 1A    | 3227 | 1/1   | 0.97 | 0.08 | 35,35,35,35                 | 0     |
| 54  | MG   | 2A    | 3423 | 1/1   | 0.97 | 0.07 | 46,46,46,46                 | 0     |
| 54  | MG   | 2A    | 3025 | 1/1   | 0.97 | 0.10 | 27,27,27,27                 | 0     |
| 54  | MG   | 2A    | 3425 | 1/1   | 0.97 | 0.13 | 50,50,50,50                 | 0     |
| 54  | MG   | 1A    | 3738 | 1/1   | 0.97 | 0.10 | 34,34,34,34                 | 0     |
| 54  | MG   | 2A    | 3676 | 1/1   | 0.97 | 0.05 | 68,68,68,68                 | 0     |
| 54  | MG   | 1A    | 3016 | 1/1   | 0.97 | 0.16 | 10,10,10,10                 | 0     |
| 54  | MG   | 1A    | 4035 | 1/1   | 0.97 | 0.07 | 30,30,30,30                 | 0     |
| 54  | MG   | 1A    | 3513 | 1/1   | 0.97 | 0.08 | 23,23,23,23                 | 0     |
| 54  | MG   | 1A    | 3337 | 1/1   | 0.97 | 0.10 | 40,40,40,40                 | 0     |
| 54  | MG   | 1A    | 3886 | 1/1   | 0.97 | 0.05 | 16,16,16,16                 | 0     |
| 54  | MG   | 1A    | 3072 | 1/1   | 0.97 | 0.22 | 31,31,31,31                 | 0     |
| 54  | MG   | 1A    | 3193 | 1/1   | 0.97 | 0.25 | 33,33,33,33                 | 0     |
| 54  | MG   | 2a    | 3084 | 1/1   | 0.97 | 0.18 | 43,43,43,43                 | 0     |
| 54  | MG   | 1A    | 3518 | 1/1   | 0.97 | 0.04 | 23,23,23,23                 | 0     |
| 54  | MG   | 1A    | 3896 | 1/1   | 0.97 | 0.06 | 28,28,28,28                 | 0     |
| 54  | MG   | 1A    | 3073 | 1/1   | 0.97 | 0.34 | 24,24,24,24                 | 0     |
| 54  | MG   | 1A    | 3232 | 1/1   | 0.97 | 0.11 | 32,32,32,32                 | 0     |
| 54  | MG   | 1A    | 3522 | 1/1   | 0.97 | 0.08 | 37,37,37,37                 | 0     |
| 54  | MG   | 1A    | 3900 | 1/1   | 0.97 | 0.05 | 25,25,25,25                 | 0     |
| 54  | MG   | 1A    | 3283 | 1/1   | 0.97 | 0.16 | 14,14,14,14                 | 0     |
| 54  | MG   | 2A    | 3692 | 1/1   | 0.97 | 0.10 | 65,65,65,65                 | 0     |
| 54  | MG   | 2A    | 3693 | 1/1   | 0.97 | 0.09 | 50,50,50,50                 | 0     |
| 54  | MG   | 2a    | 3096 | 1/1   | 0.97 | 0.09 | 34,34,34,34                 | 0     |
| 54  | MG   | 1A    | 3346 | 1/1   | 0.97 | 0.05 | 14,14,14,14                 | 0     |
| 54  | MG   | 1A    | 3629 | 1/1   | 0.97 | 0.11 | 24,24,24,24                 | 0     |
| 54  | MG   | 1A    | 3233 | 1/1   | 0.97 | 0.19 | 30,30,30,30                 | 0     |
| 54  | MG   | 2A    | 3698 | 1/1   | 0.97 | 0.08 | 66,66,66,66                 | 0     |
| 54  | MG   | 1A    | 3526 | 1/1   | 0.97 | 0.09 | 30,30,30,30                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 1A    | 3527 | 1/1   | 0.97 | 0.08 | 48,48,48,48                 | 0     |
| 54  | MG   | 1A    | 3908 | 1/1   | 0.97 | 0.06 | 15,15,15,15                 | 0     |
| 54  | MG   | 1A    | 3528 | 1/1   | 0.97 | 0.07 | 50,50,50,50                 | 0     |
| 54  | MG   | 1A    | 3165 | 1/1   | 0.97 | 0.20 | 27,27,27,27                 | 0     |
| 54  | MG   | 1A    | 3761 | 1/1   | 0.97 | 0.09 | 41,41,41,41                 | 0     |
| 54  | MG   | 1A    | 3349 | 1/1   | 0.97 | 0.08 | 21,21,21,21                 | 0     |
| 54  | MG   | 1A    | 3916 | 1/1   | 0.97 | 0.05 | 40,40,40,40                 | 0     |
| 54  | MG   | 1A    | 3917 | 1/1   | 0.97 | 0.06 | 46,46,46,46                 | 0     |
| 54  | MG   | 1B    | 212  | 1/1   | 0.97 | 0.05 | 52,52,52,52                 | 0     |
| 54  | MG   | 1A    | 3764 | 1/1   | 0.97 | 0.04 | 29,29,29,29                 | 0     |
| 54  | MG   | 1A    | 3429 | 1/1   | 0.97 | 0.06 | 35,35,35,35                 | 0     |
| 54  | MG   | 1A    | 3532 | 1/1   | 0.97 | 0.11 | 22,22,22,22                 | 0     |
| 54  | MG   | 1A    | 3093 | 1/1   | 0.97 | 0.10 | 10,10,10,10                 | 0     |
| 54  | MG   | 1B    | 219  | 1/1   | 0.97 | 0.06 | 32,32,32,32                 | 0     |
| 54  | MG   | 2A    | 3061 | 1/1   | 0.97 | 0.12 | 48,48,48,48                 | 0     |
| 54  | MG   | 1A    | 3768 | 1/1   | 0.97 | 0.10 | 10,10,10,10                 | 0     |
| 54  | MG   | 2A    | 3063 | 1/1   | 0.97 | 0.04 | 38,38,38,38                 | 0     |
| 54  | MG   | 2A    | 3064 | 1/1   | 0.97 | 0.27 | 45,45,45,45                 | 0     |
| 54  | MG   | 1A    | 3074 | 1/1   | 0.97 | 0.16 | 24,24,24,24                 | 0     |
| 54  | MG   | 1A    | 3113 | 1/1   | 0.97 | 0.09 | 34,34,34,34                 | 0     |
| 54  | MG   | 1B    | 224  | 1/1   | 0.97 | 0.07 | 48,48,48,48                 | 0     |
| 54  | MG   | 1A    | 3536 | 1/1   | 0.97 | 0.10 | 33,33,33,33                 | 0     |
| 54  | MG   | 2A    | 3724 | 1/1   | 0.97 | 0.06 | 42,42,42,42                 | 0     |
| 54  | MG   | 1A    | 3056 | 1/1   | 0.97 | 0.08 | 55,55,55,55                 | 0     |
| 54  | MG   | 1A    | 3643 | 1/1   | 0.97 | 0.04 | 31,31,31,31                 | 0     |
| 54  | MG   | 1A    | 3434 | 1/1   | 0.97 | 0.06 | 30,30,30,30                 | 0     |
| 54  | MG   | 1B    | 229  | 1/1   | 0.97 | 0.05 | 44,44,44,44                 | 0     |
| 54  | MG   | 1B    | 230  | 1/1   | 0.97 | 0.07 | 50,50,50,50                 | 0     |
| 54  | MG   | 1A    | 3776 | 1/1   | 0.97 | 0.08 | 35,35,35,35                 | 0     |
| 54  | MG   | 1A    | 3291 | 1/1   | 0.97 | 0.10 | 23,23,23,23                 | 0     |
| 54  | MG   | 1A    | 3355 | 1/1   | 0.97 | 0.09 | 9,9,9,9                     | 0     |
| 54  | MG   | 1A    | 3041 | 1/1   | 0.97 | 0.12 | 11,11,11,11                 | 0     |
| 54  | MG   | 2A    | 3269 | 1/1   | 0.97 | 0.07 | 35,35,35,35                 | 0     |
| 54  | MG   | 1D    | 311  | 1/1   | 0.97 | 0.05 | 36,36,36,36                 | 0     |
| 54  | MG   | 2A    | 3737 | 1/1   | 0.97 | 0.12 | 51,51,51,51                 | 0     |
| 54  | MG   | 2A    | 3738 | 1/1   | 0.97 | 0.11 | 52,52,52,52                 | 0     |
| 54  | MG   | 1A    | 3357 | 1/1   | 0.97 | 0.08 | 12,12,12,12                 | 0     |
| 54  | MG   | 1A    | 3243 | 1/1   | 0.97 | 0.08 | 33,33,33,33                 | 0     |
| 54  | MG   | 2A    | 3274 | 1/1   | 0.97 | 0.17 | 38,38,38,38                 | 0     |
| 54  | MG   | 1A    | 3545 | 1/1   | 0.97 | 0.05 | 21,21,21,21                 | 0     |
| 54  | MG   | 1A    | 3117 | 1/1   | 0.97 | 0.09 | 17,17,17,17                 | 0     |
| 54  | MG   | 2A    | 3084 | 1/1   | 0.97 | 0.05 | 25,25,25,25                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 2A    | 3745 | 1/1   | 0.97 | 0.05 | 42,42,42,42                 | 0     |
| 54  | MG   | 1A    | 3784 | 1/1   | 0.97 | 0.08 | 32,32,32,32                 | 0     |
| 54  | MG   | 2A    | 3280 | 1/1   | 0.97 | 0.04 | 32,32,32,32                 | 0     |
| 54  | MG   | 1A    | 3246 | 1/1   | 0.97 | 0.25 | 35,35,35,35                 | 0     |
| 54  | MG   | 1A    | 3203 | 1/1   | 0.97 | 0.18 | 33,33,33,33                 | 0     |
| 54  | MG   | 1A    | 3013 | 1/1   | 0.97 | 0.17 | 35,35,35,35                 | 0     |
| 54  | MG   | 1A    | 3249 | 1/1   | 0.97 | 0.07 | 31,31,31,31                 | 0     |
| 54  | MG   | 2A    | 3498 | 1/1   | 0.97 | 0.07 | 47,47,47,47                 | 0     |
| 54  | MG   | 2a    | 3159 | 1/1   | 0.97 | 0.05 | 63,63,63,63                 | 0     |
| 54  | MG   | 1A    | 3031 | 1/1   | 0.97 | 0.06 | 24,24,24,24                 | 0     |
| 54  | MG   | 2a    | 3161 | 1/1   | 0.97 | 0.07 | 48,48,48,48                 | 0     |
| 54  | MG   | 1A    | 3791 | 1/1   | 0.97 | 0.05 | 28,28,28,28                 | 0     |
| 54  | MG   | 1A    | 3947 | 1/1   | 0.97 | 0.07 | 44,44,44,44                 | 0     |
| 54  | MG   | 1A    | 3452 | 1/1   | 0.97 | 0.09 | 13,13,13,13                 | 0     |
| 54  | MG   | 1A    | 3662 | 1/1   | 0.97 | 0.13 | 43,43,43,43                 | 0     |
| 54  | MG   | 2A    | 3505 | 1/1   | 0.97 | 0.08 | 39,39,39,39                 | 0     |
| 54  | MG   | 1A    | 3556 | 1/1   | 0.97 | 0.06 | 41,41,41,41                 | 0     |
| 54  | MG   | 2a    | 3169 | 1/1   | 0.97 | 0.05 | 69,69,69,69                 | 0     |
| 54  | MG   | 1A    | 3251 | 1/1   | 0.97 | 0.09 | 26,26,26,26                 | 0     |
| 54  | MG   | 1A    | 3206 | 1/1   | 0.97 | 0.32 | 34,34,34,34                 | 0     |
| 54  | MG   | 1a    | 1829 | 1/1   | 0.97 | 0.05 | 53,53,53,53                 | 0     |
| 54  | MG   | 1A    | 3666 | 1/1   | 0.97 | 0.15 | 29,29,29,29                 | 0     |
| 54  | MG   | 1A    | 3145 | 1/1   | 0.97 | 0.20 | 19,19,19,19                 | 0     |
| 54  | MG   | 2A    | 3297 | 1/1   | 0.97 | 0.09 | 44,44,44,44                 | 0     |
| 54  | MG   | 1A    | 3063 | 1/1   | 0.97 | 0.08 | 12,12,12,12                 | 0     |
| 54  | MG   | 1A    | 3561 | 1/1   | 0.97 | 0.05 | 28,28,28,28                 | 0     |
| 54  | MG   | 1F    | 305  | 1/1   | 0.97 | 0.04 | 28,28,28,28                 | 0     |
| 54  | MG   | 2A    | 3104 | 1/1   | 0.97 | 0.08 | 42,42,42,42                 | 0     |
| 54  | MG   | 1A    | 3371 | 1/1   | 0.97 | 0.07 | 22,22,22,22                 | 0     |
| 54  | MG   | 2A    | 3303 | 1/1   | 0.97 | 0.05 | 37,37,37,37                 | 0     |
| 54  | MG   | 1F    | 307  | 1/1   | 0.97 | 0.21 | 24,24,24,24                 | 0     |
| 54  | MG   | 1F    | 308  | 1/1   | 0.97 | 0.07 | 29,29,29,29                 | 0     |
| 54  | MG   | 2A    | 3521 | 1/1   | 0.97 | 0.07 | 34,34,34,34                 | 0     |
| 54  | MG   | 1F    | 309  | 1/1   | 0.97 | 0.10 | 26,26,26,26                 | 0     |
| 54  | MG   | 1A    | 3958 | 1/1   | 0.97 | 0.08 | 40,40,40,40                 | 0     |
| 54  | MG   | 2A    | 3524 | 1/1   | 0.97 | 0.06 | 38,38,38,38                 | 0     |
| 54  | MG   | 1A    | 3255 | 1/1   | 0.97 | 0.05 | 26,26,26,26                 | 0     |
| 54  | MG   | 2A    | 3111 | 1/1   | 0.97 | 0.13 | 45,45,45,45                 | 0     |
| 54  | MG   | 1a    | 1841 | 1/1   | 0.97 | 0.07 | 42,42,42,42                 | 0     |
| 54  | MG   | 2A    | 3313 | 1/1   | 0.97 | 0.07 | 27,27,27,27                 | 0     |
| 54  | MG   | 1a    | 1844 | 1/1   | 0.97 | 0.06 | 44,44,44,44                 | 0     |
| 54  | MG   | 2D    | 310  | 1/1   | 0.97 | 0.13 | 57,57,57,57                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 1A    | 3462 | 1/1   | 0.97 | 0.05 | 18,18,18,18                 | 0     |
| 54  | MG   | 2k    | 201  | 1/1   | 0.97 | 0.13 | 51,51,51,51                 | 0     |
| 54  | MG   | 1A    | 3674 | 1/1   | 0.97 | 0.05 | 15,15,15,15                 | 0     |
| 54  | MG   | 2E    | 302  | 1/1   | 0.97 | 0.10 | 38,38,38,38                 | 0     |
| 54  | MG   | 1A    | 3306 | 1/1   | 0.97 | 0.25 | 24,24,24,24                 | 0     |
| 54  | MG   | 1A    | 3964 | 1/1   | 0.97 | 0.09 | 48,48,48,48                 | 0     |
| 54  | MG   | 1A    | 3464 | 1/1   | 0.97 | 0.04 | 35,35,35,35                 | 0     |
| 54  | MG   | 1A    | 3966 | 1/1   | 0.97 | 0.07 | 49,49,49,49                 | 0     |
| 54  | MG   | 1A    | 3256 | 1/1   | 0.97 | 0.14 | 26,26,26,26                 | 0     |
| 54  | MG   | 2A    | 3540 | 1/1   | 0.97 | 0.05 | 58,58,58,58                 | 0     |
| 54  | MG   | 2A    | 3541 | 1/1   | 0.97 | 0.06 | 24,24,24,24                 | 0     |
| 54  | MG   | 1A    | 3005 | 1/1   | 0.97 | 0.09 | 21,21,21,21                 | 0     |
| 54  | MG   | 1A    | 3258 | 1/1   | 0.97 | 0.19 | 22,22,22,22                 | 0     |
| 54  | MG   | 1G    | 203  | 1/1   | 0.97 | 0.05 | 56,56,56,56                 | 0     |
| 54  | MG   | 1A    | 3211 | 1/1   | 0.97 | 0.08 | 52,52,52,52                 | 0     |
| 54  | MG   | 1A    | 3973 | 1/1   | 0.97 | 0.06 | 27,27,27,27                 | 0     |
| 54  | MG   | 1A    | 3684 | 1/1   | 0.97 | 0.04 | 29,29,29,29                 | 0     |
| 54  | MG   | 1A    | 3178 | 1/1   | 0.97 | 0.22 | 25,25,25,25                 | 0     |
| 54  | MG   | 2O    | 201  | 1/1   | 0.97 | 0.04 | 33,33,33,33                 | 0     |
| 58  | ZN   | 2Y    | 202  | 1/1   | 0.97 | 0.04 | 99,99,99,99                 | 0     |
| 54  | MG   | 2A    | 3128 | 1/1   | 0.97 | 0.08 | 47,47,47,47                 | 0     |
| 58  | ZN   | 2n    | 102  | 1/1   | 0.97 | 0.06 | 95,95,95,95                 | 0     |
| 54  | MG   | 1a    | 1732 | 1/1   | 0.98 | 0.06 | 49,49,49,49                 | 0     |
| 54  | MG   | 1A    | 3702 | 1/1   | 0.98 | 0.07 | 38,38,38,38                 | 0     |
| 54  | MG   | 1A    | 3169 | 1/1   | 0.98 | 0.12 | 33,33,33,33                 | 0     |
| 54  | MG   | 1A    | 3444 | 1/1   | 0.98 | 0.04 | 15,15,15,15                 | 0     |
| 54  | MG   | 2A    | 3694 | 1/1   | 0.98 | 0.04 | 51,51,51,51                 | 0     |
| 54  | MG   | 1A    | 3885 | 1/1   | 0.98 | 0.06 | 30,30,30,30                 | 0     |
| 54  | MG   | 1A    | 3069 | 1/1   | 0.98 | 0.15 | 21,21,21,21                 | 0     |
| 54  | MG   | 1A    | 3343 | 1/1   | 0.98 | 0.05 | 28,28,28,28                 | 0     |
| 54  | MG   | 1A    | 3009 | 1/1   | 0.98 | 0.12 | 23,23,23,23                 | 0     |
| 54  | MG   | 1A    | 3790 | 1/1   | 0.98 | 0.05 | 69,69,69,69                 | 0     |
| 54  | MG   | 1A    | 3345 | 1/1   | 0.98 | 0.04 | 24,24,24,24                 | 0     |
| 54  | MG   | 1A    | 4001 | 1/1   | 0.98 | 0.06 | 26,26,26,26                 | 0     |
| 54  | MG   | 1A    | 3792 | 1/1   | 0.98 | 0.05 | 18,18,18,18                 | 0     |
| 54  | MG   | 1A    | 3010 | 1/1   | 0.98 | 0.09 | 25,25,25,25                 | 0     |
| 54  | MG   | 1A    | 3267 | 1/1   | 0.98 | 0.07 | 31,31,31,31                 | 0     |
| 54  | MG   | 1A    | 3795 | 1/1   | 0.98 | 0.05 | 30,30,30,30                 | 0     |
| 54  | MG   | 1A    | 3453 | 1/1   | 0.98 | 0.10 | 35,35,35,35                 | 0     |
| 54  | MG   | 2A    | 3707 | 1/1   | 0.98 | 0.04 | 55,55,55,55                 | 0     |
| 54  | MG   | 1A    | 3712 | 1/1   | 0.98 | 0.07 | 12,12,12,12                 | 0     |
| 54  | MG   | 1A    | 4009 | 1/1   | 0.98 | 0.05 | 54,54,54,54                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 1A    | 3395 | 1/1   | 0.98 | 0.04 | 14,14,14,14                 | 0     |
| 54  | MG   | 1A    | 3397 | 1/1   | 0.98 | 0.04 | 25,25,25,25                 | 0     |
| 54  | MG   | 1A    | 3715 | 1/1   | 0.98 | 0.07 | 34,34,34,34                 | 0     |
| 54  | MG   | 1A    | 3716 | 1/1   | 0.98 | 0.06 | 73,73,73,73                 | 0     |
| 54  | MG   | 1A    | 3803 | 1/1   | 0.98 | 0.07 | 38,38,38,38                 | 0     |
| 54  | MG   | 2A    | 3232 | 1/1   | 0.98 | 0.08 | 45,45,45,45                 | 0     |
| 54  | MG   | 2A    | 3532 | 1/1   | 0.98 | 0.04 | 69,69,69,69                 | 0     |
| 54  | MG   | 1A    | 3122 | 1/1   | 0.98 | 0.14 | 25,25,25,25                 | 0     |
| 54  | MG   | 2A    | 3718 | 1/1   | 0.98 | 0.06 | 36,36,36,36                 | 0     |
| 54  | MG   | 2A    | 3534 | 1/1   | 0.98 | 0.04 | 80,80,80,80                 | 0     |
| 54  | MG   | 1A    | 3103 | 1/1   | 0.98 | 0.28 | 32,32,32,32                 | 0     |
| 54  | MG   | 2A    | 3536 | 1/1   | 0.98 | 0.05 | 58,58,58,58                 | 0     |
| 54  | MG   | 2A    | 3381 | 1/1   | 0.98 | 0.15 | 40,40,40,40                 | 0     |
| 54  | MG   | 1A    | 3912 | 1/1   | 0.98 | 0.04 | 44,44,44,44                 | 0     |
| 54  | MG   | 1G    | 204  | 1/1   | 0.98 | 0.11 | 45,45,45,45                 | 0     |
| 54  | MG   | 1A    | 3517 | 1/1   | 0.98 | 0.03 | 36,36,36,36                 | 0     |
| 54  | MG   | 2A    | 3386 | 1/1   | 0.98 | 0.07 | 36,36,36,36                 | 0     |
| 54  | MG   | 1A    | 3235 | 1/1   | 0.98 | 0.20 | 17,17,17,17                 | 0     |
| 54  | MG   | 2A    | 3543 | 1/1   | 0.98 | 0.06 | 45,45,45,45                 | 0     |
| 54  | MG   | 1A    | 3059 | 1/1   | 0.98 | 0.06 | 28,28,28,28                 | 0     |
| 54  | MG   | 1A    | 3580 | 1/1   | 0.98 | 0.03 | 22,22,22,22                 | 0     |
| 54  | MG   | 1N    | 202  | 1/1   | 0.98 | 0.09 | 50,50,50,50                 | 0     |
| 54  | MG   | 1O    | 201  | 1/1   | 0.98 | 0.03 | 37,37,37,37                 | 0     |
| 54  | MG   | 1A    | 3723 | 1/1   | 0.98 | 0.05 | 37,37,37,37                 | 0     |
| 54  | MG   | 1A    | 3646 | 1/1   | 0.98 | 0.09 | 47,47,47,47                 | 0     |
| 54  | MG   | 1P    | 202  | 1/1   | 0.98 | 0.20 | 15,15,15,15                 | 0     |
| 54  | MG   | 2A    | 3736 | 1/1   | 0.98 | 0.09 | 52,52,52,52                 | 0     |
| 54  | MG   | 2A    | 3551 | 1/1   | 0.98 | 0.04 | 57,57,57,57                 | 0     |
| 54  | MG   | 1A    | 3520 | 1/1   | 0.98 | 0.08 | 38,38,38,38                 | 0     |
| 54  | MG   | 2A    | 3396 | 1/1   | 0.98 | 0.05 | 41,41,41,41                 | 0     |
| 54  | MG   | 1A    | 3813 | 1/1   | 0.98 | 0.17 | 35,35,35,35                 | 0     |
| 54  | MG   | 1A    | 3648 | 1/1   | 0.98 | 0.11 | 33,33,33,33                 | 0     |
| 54  | MG   | 1A    | 3060 | 1/1   | 0.98 | 0.04 | 24,24,24,24                 | 0     |
| 54  | MG   | 2A    | 3250 | 1/1   | 0.98 | 0.11 | 22,22,22,22                 | 0     |
| 54  | MG   | 2A    | 3251 | 1/1   | 0.98 | 0.06 | 35,35,35,35                 | 0     |
| 54  | MG   | 2a    | 3086 | 1/1   | 0.98 | 0.06 | 61,61,61,61                 | 0     |
| 54  | MG   | 1A    | 3650 | 1/1   | 0.98 | 0.04 | 19,19,19,19                 | 0     |
| 54  | MG   | 1A    | 3817 | 1/1   | 0.98 | 0.12 | 13,13,13,13                 | 0     |
| 54  | MG   | 1A    | 3927 | 1/1   | 0.98 | 0.08 | 32,32,32,32                 | 0     |
| 54  | MG   | 1A    | 3310 | 1/1   | 0.98 | 0.06 | 30,30,30,30                 | 0     |
| 54  | MG   | 1Q    | 205  | 1/1   | 0.98 | 0.05 | 25,25,25,25                 | 0     |
| 54  | MG   | 2a    | 3092 | 1/1   | 0.98 | 0.11 | 38,38,38,38                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 2A    | 3566 | 1/1   | 0.98 | 0.11 | 38,38,38,38                 | 0     |
| 54  | MG   | 2A    | 3567 | 1/1   | 0.98 | 0.06 | 49,49,49,49                 | 0     |
| 54  | MG   | 1A    | 3929 | 1/1   | 0.98 | 0.05 | 52,52,52,52                 | 0     |
| 54  | MG   | 1A    | 3819 | 1/1   | 0.98 | 0.09 | 22,22,22,22                 | 0     |
| 54  | MG   | 2A    | 3570 | 1/1   | 0.98 | 0.05 | 57,57,57,57                 | 0     |
| 54  | MG   | 2A    | 3755 | 1/1   | 0.98 | 0.07 | 37,37,37,37                 | 0     |
| 54  | MG   | 1R    | 202  | 1/1   | 0.98 | 0.07 | 35,35,35,35                 | 0     |
| 54  | MG   | 1A    | 3047 | 1/1   | 0.98 | 0.15 | 22,22,22,22                 | 0     |
| 54  | MG   | 1A    | 3239 | 1/1   | 0.98 | 0.34 | 28,28,28,28                 | 0     |
| 54  | MG   | 1A    | 3240 | 1/1   | 0.98 | 0.27 | 31,31,31,31                 | 0     |
| 54  | MG   | 1A    | 3314 | 1/1   | 0.98 | 0.07 | 15,15,15,15                 | 0     |
| 54  | MG   | 1A    | 3656 | 1/1   | 0.98 | 0.04 | 42,42,42,42                 | 0     |
| 54  | MG   | 2A    | 3578 | 1/1   | 0.98 | 0.04 | 57,57,57,57                 | 0     |
| 54  | MG   | 2A    | 3579 | 1/1   | 0.98 | 0.07 | 52,52,52,52                 | 0     |
| 54  | MG   | 2A    | 3580 | 1/1   | 0.98 | 0.04 | 56,56,56,56                 | 0     |
| 54  | MG   | 2A    | 3582 | 1/1   | 0.98 | 0.04 | 34,34,34,34                 | 0     |
| 54  | MG   | 2A    | 3265 | 1/1   | 0.98 | 0.07 | 42,42,42,42                 | 0     |
| 54  | MG   | 2a    | 3110 | 1/1   | 0.98 | 0.08 | 56,56,56,56                 | 0     |
| 54  | MG   | 1A    | 3825 | 1/1   | 0.98 | 0.04 | 42,42,42,42                 | 0     |
| 54  | MG   | 2A    | 3267 | 1/1   | 0.98 | 0.08 | 51,51,51,51                 | 0     |
| 54  | MG   | 1A    | 3090 | 1/1   | 0.98 | 0.23 | 17,17,17,17                 | 0     |
| 54  | MG   | 2A    | 3419 | 1/1   | 0.98 | 0.03 | 43,43,43,43                 | 0     |
| 54  | MG   | 2B    | 215  | 1/1   | 0.98 | 0.04 | 58,58,58,58                 | 0     |
| 54  | MG   | 2A    | 3589 | 1/1   | 0.98 | 0.04 | 51,51,51,51                 | 0     |
| 54  | MG   | 1A    | 3128 | 1/1   | 0.98 | 0.10 | 22,22,22,22                 | 0     |
| 54  | MG   | 1A    | 3152 | 1/1   | 0.98 | 0.11 | 31,31,31,31                 | 0     |
| 54  | MG   | 1A    | 3108 | 1/1   | 0.98 | 0.17 | 31,31,31,31                 | 0     |
| 54  | MG   | 1U    | 203  | 1/1   | 0.98 | 0.22 | 24,24,24,24                 | 0     |
| 54  | MG   | 1A    | 3245 | 1/1   | 0.98 | 0.15 | 25,25,25,25                 | 0     |
| 54  | MG   | 1A    | 3832 | 1/1   | 0.98 | 0.05 | 29,29,29,29                 | 0     |
| 54  | MG   | 1A    | 3363 | 1/1   | 0.98 | 0.07 | 24,24,24,24                 | 0     |
| 54  | MG   | 2a    | 3124 | 1/1   | 0.98 | 0.04 | 51,51,51,51                 | 0     |
| 54  | MG   | 1A    | 3742 | 1/1   | 0.98 | 0.06 | 27,27,27,27                 | 0     |
| 54  | MG   | 2A    | 3278 | 1/1   | 0.98 | 0.07 | 30,30,30,30                 | 0     |
| 54  | MG   | 1A    | 3023 | 1/1   | 0.98 | 0.13 | 11,11,11,11                 | 0     |
| 54  | MG   | 1A    | 3092 | 1/1   | 0.98 | 0.06 | 21,21,21,21                 | 0     |
| 54  | MG   | 2A    | 3142 | 1/1   | 0.98 | 0.09 | 45,45,45,45                 | 0     |
| 54  | MG   | 2A    | 3432 | 1/1   | 0.98 | 0.07 | 41,41,41,41                 | 0     |
| 54  | MG   | 1A    | 3050 | 1/1   | 0.98 | 0.07 | 33,33,33,33                 | 0     |
| 54  | MG   | 1A    | 3064 | 1/1   | 0.98 | 0.04 | 21,21,21,21                 | 0     |
| 54  | MG   | 2a    | 3135 | 1/1   | 0.98 | 0.04 | 60,60,60,60                 | 0     |
| 54  | MG   | 1A    | 3479 | 1/1   | 0.98 | 0.06 | 49,49,49,49                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 1B    | 204  | 1/1   | 0.98 | 0.04 | 35,35,35,35                 | 0     |
| 54  | MG   | 2a    | 3139 | 1/1   | 0.98 | 0.05 | 58,58,58,58                 | 0     |
| 54  | MG   | 1a    | 1802 | 1/1   | 0.98 | 0.05 | 77,77,77,77                 | 0     |
| 54  | MG   | 1A    | 3186 | 1/1   | 0.98 | 0.08 | 32,32,32,32                 | 0     |
| 54  | MG   | 2E    | 306  | 1/1   | 0.98 | 0.05 | 25,25,25,25                 | 0     |
| 54  | MG   | 1A    | 3481 | 1/1   | 0.98 | 0.05 | 10,10,10,10                 | 0     |
| 54  | MG   | 1A    | 3751 | 1/1   | 0.98 | 0.05 | 26,26,26,26                 | 0     |
| 54  | MG   | 1A    | 3602 | 1/1   | 0.98 | 0.33 | 26,26,26,26                 | 0     |
| 54  | MG   | 1A    | 3753 | 1/1   | 0.98 | 0.05 | 34,34,34,34                 | 0     |
| 54  | MG   | 10    | 101  | 1/1   | 0.98 | 0.10 | 38,38,38,38                 | 0     |
| 54  | MG   | 1A    | 3846 | 1/1   | 0.98 | 0.12 | 47,47,47,47                 | 0     |
| 54  | MG   | 1A    | 3754 | 1/1   | 0.98 | 0.14 | 46,46,46,46                 | 0     |
| 54  | MG   | 2A    | 3156 | 1/1   | 0.98 | 0.05 | 46,46,46,46                 | 0     |
| 54  | MG   | 2A    | 3296 | 1/1   | 0.98 | 0.08 | 43,43,43,43                 | 0     |
| 54  | MG   | 1A    | 3540 | 1/1   | 0.98 | 0.06 | 42,42,42,42                 | 0     |
| 54  | MG   | 1B    | 214  | 1/1   | 0.98 | 0.04 | 35,35,35,35                 | 0     |
| 54  | MG   | 1A    | 3482 | 1/1   | 0.98 | 0.04 | 19,19,19,19                 | 0     |
| 54  | MG   | 1A    | 3159 | 1/1   | 0.98 | 0.14 | 18,18,18,18                 | 0     |
| 54  | MG   | 1A    | 3370 | 1/1   | 0.98 | 0.07 | 36,36,36,36                 | 0     |
| 54  | MG   | 11    | 102  | 1/1   | 0.98 | 0.04 | 35,35,35,35                 | 0     |
| 54  | MG   | 1A    | 3961 | 1/1   | 0.98 | 0.09 | 49,49,49,49                 | 0     |
| 54  | MG   | 1A    | 3287 | 1/1   | 0.98 | 0.29 | 24,24,24,24                 | 0     |
| 54  | MG   | 1A    | 3853 | 1/1   | 0.98 | 0.06 | 31,31,31,31                 | 0     |
| 54  | MG   | 1A    | 3040 | 1/1   | 0.98 | 0.11 | 25,25,25,25                 | 0     |
| 54  | MG   | 1A    | 3161 | 1/1   | 0.98 | 0.07 | 29,29,29,29                 | 0     |
| 54  | MG   | 2R    | 201  | 1/1   | 0.98 | 0.06 | 30,30,30,30                 | 0     |
| 54  | MG   | 1B    | 223  | 1/1   | 0.98 | 0.04 | 43,43,43,43                 | 0     |
| 54  | MG   | 2A    | 3310 | 1/1   | 0.98 | 0.04 | 26,26,26,26                 | 0     |
| 54  | MG   | 1A    | 3489 | 1/1   | 0.98 | 0.05 | 10,10,10,10                 | 0     |
| 54  | MG   | 1a    | 1699 | 1/1   | 0.98 | 0.10 | 29,29,29,29                 | 0     |
| 54  | MG   | 2a    | 3168 | 1/1   | 0.98 | 0.05 | 59,59,59,59                 | 0     |
| 54  | MG   | 1A    | 3034 | 1/1   | 0.98 | 0.12 | 22,22,22,22                 | 0     |
| 54  | MG   | 1A    | 3968 | 1/1   | 0.98 | 0.04 | 15,15,15,15                 | 0     |
| 54  | MG   | 2A    | 3315 | 1/1   | 0.98 | 0.07 | 40,40,40,40                 | 0     |
| 54  | MG   | 15    | 105  | 1/1   | 0.98 | 0.19 | 23,23,23,23                 | 0     |
| 54  | MG   | 2a    | 3173 | 1/1   | 0.98 | 0.04 | 54,54,54,54                 | 0     |
| 54  | MG   | 1A    | 3221 | 1/1   | 0.98 | 0.06 | 25,25,25,25                 | 0     |
| 54  | MG   | 1A    | 3685 | 1/1   | 0.98 | 0.13 | 30,30,30,30                 | 0     |
| 54  | MG   | 1A    | 3163 | 1/1   | 0.98 | 0.06 | 17,17,17,17                 | 0     |
| 54  | MG   | 1A    | 3614 | 1/1   | 0.98 | 0.06 | 16,16,16,16                 | 0     |
| 54  | MG   | 2A    | 3649 | 1/1   | 0.98 | 0.09 | 37,37,37,37                 | 0     |
| 54  | MG   | 1A    | 3769 | 1/1   | 0.98 | 0.05 | 31,31,31,31                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 2A    | 3475 | 1/1   | 0.98 | 0.04 | 65,65,65,65                 | 0     |
| 54  | MG   | 2a    | 3181 | 1/1   | 0.98 | 0.08 | 61,61,61,61                 | 0     |
| 54  | MG   | 1A    | 3493 | 1/1   | 0.98 | 0.04 | 37,37,37,37                 | 0     |
| 54  | MG   | 2A    | 3477 | 1/1   | 0.98 | 0.04 | 20,20,20,20                 | 0     |
| 54  | MG   | 1D    | 306  | 1/1   | 0.98 | 0.07 | 35,35,35,35                 | 0     |
| 54  | MG   | 2A    | 3655 | 1/1   | 0.98 | 0.06 | 58,58,58,58                 | 0     |
| 54  | MG   | 1a    | 1713 | 1/1   | 0.98 | 0.05 | 34,34,34,34                 | 0     |
| 54  | MG   | 1A    | 3115 | 1/1   | 0.98 | 0.15 | 23,23,23,23                 | 0     |
| 54  | MG   | 2A    | 3658 | 1/1   | 0.98 | 0.04 | 52,52,52,52                 | 0     |
| 54  | MG   | 1A    | 3618 | 1/1   | 0.98 | 0.09 | 40,40,40,40                 | 0     |
| 54  | MG   | 2A    | 3662 | 1/1   | 0.98 | 0.04 | 35,35,35,35                 | 0     |
| 54  | MG   | 1A    | 3866 | 1/1   | 0.98 | 0.06 | 39,39,39,39                 | 0     |
| 54  | MG   | 2A    | 3056 | 1/1   | 0.98 | 0.04 | 29,29,29,29                 | 0     |
| 54  | MG   | 2A    | 3665 | 1/1   | 0.98 | 0.04 | 56,56,56,56                 | 0     |
| 54  | MG   | 2A    | 3057 | 1/1   | 0.98 | 0.06 | 42,42,42,42                 | 0     |
| 54  | MG   | 1A    | 3555 | 1/1   | 0.98 | 0.06 | 42,42,42,42                 | 0     |
| 54  | MG   | 1a    | 1843 | 1/1   | 0.98 | 0.04 | 62,62,62,62                 | 0     |
| 54  | MG   | 1A    | 3224 | 1/1   | 0.98 | 0.19 | 26,26,26,26                 | 0     |
| 54  | MG   | 1A    | 3870 | 1/1   | 0.98 | 0.04 | 27,27,27,27                 | 0     |
| 54  | MG   | 1a    | 1846 | 1/1   | 0.98 | 0.06 | 58,58,58,58                 | 0     |
| 54  | MG   | 2A    | 3672 | 1/1   | 0.98 | 0.05 | 49,49,49,49                 | 0     |
| 54  | MG   | 2A    | 3192 | 1/1   | 0.98 | 0.06 | 39,39,39,39                 | 0     |
| 54  | MG   | 1A    | 3496 | 1/1   | 0.98 | 0.07 | 28,28,28,28                 | 0     |
| 54  | MG   | 19    | 103  | 1/1   | 0.98 | 0.07 | 35,35,35,35                 | 0     |
| 54  | MG   | 1A    | 3694 | 1/1   | 0.98 | 0.04 | 38,38,38,38                 | 0     |
| 54  | MG   | 2a    | 3018 | 1/1   | 0.98 | 0.22 | 50,50,50,50                 | 0     |
| 54  | MG   | 1A    | 3622 | 1/1   | 0.98 | 0.09 | 16,16,16,16                 | 0     |
| 54  | MG   | 1a    | 1724 | 1/1   | 0.98 | 0.07 | 32,32,32,32                 | 0     |
| 54  | MG   | 1A    | 3435 | 1/1   | 0.98 | 0.15 | 36,36,36,36                 | 0     |
| 54  | MG   | 1A    | 3011 | 1/1   | 0.98 | 0.06 | 37,37,37,37                 | 0     |
| 54  | MG   | 1A    | 3044 | 1/1   | 0.98 | 0.07 | 18,18,18,18                 | 0     |
| 54  | MG   | 1A    | 3338 | 1/1   | 0.98 | 0.07 | 38,38,38,38                 | 0     |
| 54  | MG   | 2A    | 3072 | 1/1   | 0.98 | 0.11 | 48,48,48,48                 | 0     |
| 54  | MG   | 1A    | 3140 | 1/1   | 0.98 | 0.05 | 25,25,25,25                 | 0     |
| 58  | ZN   | 1Y    | 202  | 1/1   | 0.98 | 0.04 | 59,59,59,59                 | 0     |
| 54  | MG   | 2A    | 3504 | 1/1   | 0.98 | 0.06 | 41,41,41,41                 | 0     |
| 58  | ZN   | 1n    | 102  | 1/1   | 0.98 | 0.03 | 78,78,78,78                 | 0     |
| 54  | MG   | 1a    | 1857 | 1/1   | 0.98 | 0.05 | 52,52,52,52                 | 0     |
| 54  | MG   | 1A    | 3990 | 1/1   | 0.98 | 0.05 | 43,43,43,43                 | 0     |
| 54  | MG   | 1A    | 3083 | 1/1   | 0.98 | 0.35 | 37,37,37,37                 | 0     |
| 59  | SF4  | 1d    | 306  | 8/8   | 0.98 | 0.04 | 64,67,77,86                 | 0     |
| 59  | SF4  | 2d    | 501  | 8/8   | 0.98 | 0.04 | 67,74,83,87                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 2A    | 3661 | 1/1   | 0.99 | 0.05 | 49,49,49,49                 | 0     |
| 54  | MG   | 1A    | 3200 | 1/1   | 0.99 | 0.18 | 33,33,33,33                 | 0     |
| 54  | MG   | 1a    | 1803 | 1/1   | 0.99 | 0.04 | 51,51,51,51                 | 0     |
| 54  | MG   | 1A    | 3450 | 1/1   | 0.99 | 0.03 | 39,39,39,39                 | 0     |
| 54  | MG   | 1A    | 3921 | 1/1   | 0.99 | 0.03 | 42,42,42,42                 | 0     |
| 54  | MG   | 1A    | 3615 | 1/1   | 0.99 | 0.05 | 18,18,18,18                 | 0     |
| 54  | MG   | 1A    | 3451 | 1/1   | 0.99 | 0.07 | 29,29,29,29                 | 0     |
| 54  | MG   | 2A    | 3324 | 1/1   | 0.99 | 0.08 | 31,31,31,31                 | 0     |
| 54  | MG   | 1A    | 3423 | 1/1   | 0.99 | 0.03 | 17,17,17,17                 | 0     |
| 54  | MG   | 2a    | 3130 | 1/1   | 0.99 | 0.05 | 63,63,63,63                 | 0     |
| 54  | MG   | 1A    | 3868 | 1/1   | 0.99 | 0.03 | 21,21,21,21                 | 0     |
| 54  | MG   | 1A    | 3029 | 1/1   | 0.99 | 0.07 | 23,23,23,23                 | 0     |
| 54  | MG   | 1A    | 3400 | 1/1   | 0.99 | 0.06 | 17,17,17,17                 | 0     |
| 54  | MG   | 2a    | 3134 | 1/1   | 0.99 | 0.04 | 71,71,71,71                 | 0     |
| 54  | MG   | 2A    | 3576 | 1/1   | 0.99 | 0.07 | 25,25,25,25                 | 0     |
| 54  | MG   | 1A    | 3550 | 1/1   | 0.99 | 0.10 | 36,36,36,36                 | 0     |
| 54  | MG   | 1A    | 3324 | 1/1   | 0.99 | 0.03 | 12,12,12,12                 | 0     |
| 54  | MG   | 2a    | 3138 | 1/1   | 0.99 | 0.06 | 37,37,37,37                 | 0     |
| 54  | MG   | 1E    | 304  | 1/1   | 0.99 | 0.11 | 11,11,11,11                 | 0     |
| 54  | MG   | 1A    | 3402 | 1/1   | 0.99 | 0.05 | 12,12,12,12                 | 0     |
| 54  | MG   | 2A    | 3581 | 1/1   | 0.99 | 0.04 | 54,54,54,54                 | 0     |
| 54  | MG   | 2A    | 3496 | 1/1   | 0.99 | 0.07 | 47,47,47,47                 | 0     |
| 54  | MG   | 1A    | 3874 | 1/1   | 0.99 | 0.03 | 34,34,34,34                 | 0     |
| 54  | MG   | 1a    | 1817 | 1/1   | 0.99 | 0.03 | 70,70,70,70                 | 0     |
| 54  | MG   | 1A    | 3587 | 1/1   | 0.99 | 0.04 | 21,21,21,21                 | 0     |
| 54  | MG   | 1A    | 3876 | 1/1   | 0.99 | 0.04 | 57,57,57,57                 | 0     |
| 54  | MG   | 2A    | 3587 | 1/1   | 0.99 | 0.06 | 31,31,31,31                 | 0     |
| 54  | MG   | 1A    | 3488 | 1/1   | 0.99 | 0.08 | 45,45,45,45                 | 0     |
| 54  | MG   | 2A    | 3686 | 1/1   | 0.99 | 0.03 | 36,36,36,36                 | 0     |
| 54  | MG   | 1A    | 3554 | 1/1   | 0.99 | 0.03 | 40,40,40,40                 | 0     |
| 54  | MG   | 1A    | 3077 | 1/1   | 0.99 | 0.13 | 32,32,32,32                 | 0     |
| 54  | MG   | 2A    | 3591 | 1/1   | 0.99 | 0.06 | 28,28,28,28                 | 0     |
| 54  | MG   | 1A    | 3404 | 1/1   | 0.99 | 0.13 | 25,25,25,25                 | 0     |
| 54  | MG   | 1A    | 3459 | 1/1   | 0.99 | 0.04 | 36,36,36,36                 | 0     |
| 54  | MG   | 2A    | 3195 | 1/1   | 0.99 | 0.10 | 28,28,28,28                 | 0     |
| 54  | MG   | 2A    | 3344 | 1/1   | 0.99 | 0.04 | 30,30,30,30                 | 0     |
| 54  | MG   | 2A    | 3596 | 1/1   | 0.99 | 0.03 | 32,32,32,32                 | 0     |
| 54  | MG   | 2A    | 3345 | 1/1   | 0.99 | 0.04 | 27,27,27,27                 | 0     |
| 54  | MG   | 1A    | 3405 | 1/1   | 0.99 | 0.03 | 16,16,16,16                 | 0     |
| 54  | MG   | 1A    | 3461 | 1/1   | 0.99 | 0.04 | 28,28,28,28                 | 0     |
| 54  | MG   | 1A    | 3748 | 1/1   | 0.99 | 0.05 | 32,32,32,32                 | 0     |
| 54  | MG   | 1A    | 3383 | 1/1   | 0.99 | 0.03 | 28,28,28,28                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 1A    | 3001 | 1/1   | 0.99 | 0.04 | 26,26,26,26                 | 0     |
| 54  | MG   | 2A    | 3273 | 1/1   | 0.99 | 0.10 | 34,34,34,34                 | 0     |
| 54  | MG   | 1A    | 3888 | 1/1   | 0.99 | 0.04 | 32,32,32,32                 | 0     |
| 54  | MG   | 1A    | 3385 | 1/1   | 0.99 | 0.07 | 17,17,17,17                 | 0     |
| 54  | MG   | 1A    | 3135 | 1/1   | 0.99 | 0.05 | 29,29,29,29                 | 0     |
| 54  | MG   | 1A    | 4003 | 1/1   | 0.99 | 0.02 | 42,42,42,42                 | 0     |
| 54  | MG   | 2A    | 3356 | 1/1   | 0.99 | 0.12 | 37,37,37,37                 | 0     |
| 54  | MG   | 1A    | 3892 | 1/1   | 0.99 | 0.03 | 20,20,20,20                 | 0     |
| 54  | MG   | 1A    | 3671 | 1/1   | 0.99 | 0.07 | 57,57,57,57                 | 0     |
| 54  | MG   | 1a    | 1701 | 1/1   | 0.99 | 0.04 | 46,46,46,46                 | 0     |
| 54  | MG   | 1a    | 1702 | 1/1   | 0.99 | 0.05 | 31,31,31,31                 | 0     |
| 54  | MG   | 1B    | 213  | 1/1   | 0.99 | 0.08 | 39,39,39,39                 | 0     |
| 54  | MG   | 1A    | 3894 | 1/1   | 0.99 | 0.05 | 55,55,55,55                 | 0     |
| 54  | MG   | 1A    | 3895 | 1/1   | 0.99 | 0.08 | 40,40,40,40                 | 0     |
| 54  | MG   | 1A    | 3797 | 1/1   | 0.99 | 0.11 | 51,51,51,51                 | 0     |
| 54  | MG   | 1a    | 1842 | 1/1   | 0.99 | 0.03 | 63,63,63,63                 | 0     |
| 54  | MG   | 1A    | 3301 | 1/1   | 0.99 | 0.10 | 39,39,39,39                 | 0     |
| 54  | MG   | 1A    | 3057 | 1/1   | 0.99 | 0.10 | 16,16,16,16                 | 0     |
| 54  | MG   | 15    | 101  | 1/1   | 0.99 | 0.15 | 28,28,28,28                 | 0     |
| 54  | MG   | 2A    | 3621 | 1/1   | 0.99 | 0.04 | 59,59,59,59                 | 0     |
| 54  | MG   | 1A    | 3051 | 1/1   | 0.99 | 0.22 | 30,30,30,30                 | 0     |
| 54  | MG   | 1a    | 1711 | 1/1   | 0.99 | 0.06 | 31,31,31,31                 | 0     |
| 54  | MG   | 1A    | 3675 | 1/1   | 0.99 | 0.08 | 32,32,32,32                 | 0     |
| 54  | MG   | 1A    | 3901 | 1/1   | 0.99 | 0.02 | 47,47,47,47                 | 0     |
| 54  | MG   | 1A    | 3390 | 1/1   | 0.99 | 0.05 | 29,29,29,29                 | 0     |
| 54  | MG   | 2A    | 3453 | 1/1   | 0.99 | 0.03 | 58,58,58,58                 | 0     |
| 54  | MG   | 2A    | 3628 | 1/1   | 0.99 | 0.02 | 41,41,41,41                 | 0     |
| 54  | MG   | 1A    | 3677 | 1/1   | 0.99 | 0.04 | 33,33,33,33                 | 0     |
| 54  | MG   | 1A    | 3678 | 1/1   | 0.99 | 0.04 | 32,32,32,32                 | 0     |
| 54  | MG   | 1A    | 3207 | 1/1   | 0.99 | 0.10 | 24,24,24,24                 | 0     |
| 54  | MG   | 2A    | 3632 | 1/1   | 0.99 | 0.03 | 24,24,24,24                 | 0     |
| 54  | MG   | 2A    | 3633 | 1/1   | 0.99 | 0.05 | 28,28,28,28                 | 0     |
| 54  | MG   | 1A    | 3503 | 1/1   | 0.99 | 0.05 | 10,10,10,10                 | 0     |
| 54  | MG   | 1A    | 3763 | 1/1   | 0.99 | 0.03 | 28,28,28,28                 | 0     |
| 54  | MG   | 1A    | 3415 | 1/1   | 0.99 | 0.09 | 15,15,15,15                 | 0     |
| 54  | MG   | 1A    | 3909 | 1/1   | 0.99 | 0.06 | 40,40,40,40                 | 0     |
| 54  | MG   | 2A    | 3638 | 1/1   | 0.99 | 0.02 | 45,45,45,45                 | 0     |
| 54  | MG   | 1A    | 3392 | 1/1   | 0.99 | 0.10 | 9,9,9,9                     | 0     |
| 54  | MG   | 2A    | 3230 | 1/1   | 0.99 | 0.15 | 38,38,38,38                 | 0     |
| 54  | MG   | 2A    | 3383 | 1/1   | 0.99 | 0.09 | 27,27,27,27                 | 0     |
| 54  | MG   | 1D    | 301  | 1/1   | 0.99 | 0.18 | 24,24,24,24                 | 0     |
| 54  | MG   | 1A    | 3443 | 1/1   | 0.99 | 0.06 | 15,15,15,15                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 2A    | 3644 | 1/1   | 0.99 | 0.03 | 38,38,38,38                 | 0     |
| 54  | MG   | 1A    | 3156 | 1/1   | 0.99 | 0.18 | 24,24,24,24                 | 0     |
| 54  | MG   | 2A    | 3468 | 1/1   | 0.99 | 0.03 | 32,32,32,32                 | 0     |
| 54  | MG   | 1D    | 305  | 1/1   | 0.99 | 0.11 | 26,26,26,26                 | 0     |
| 54  | MG   | 2A    | 3308 | 1/1   | 0.99 | 0.07 | 28,28,28,28                 | 0     |
| 54  | MG   | 2A    | 3554 | 1/1   | 0.99 | 0.04 | 42,42,42,42                 | 0     |
| 54  | MG   | 1A    | 3913 | 1/1   | 0.99 | 0.12 | 47,47,47,47                 | 0     |
| 54  | MG   | 1A    | 3026 | 1/1   | 0.99 | 0.23 | 20,20,20,20                 | 0     |
| 54  | MG   | 1D    | 308  | 1/1   | 0.99 | 0.06 | 31,31,31,31                 | 0     |
| 54  | MG   | 2A    | 3558 | 1/1   | 0.99 | 0.05 | 49,49,49,49                 | 0     |
| 54  | MG   | 1a    | 1796 | 1/1   | 0.99 | 0.03 | 73,73,73,73                 | 0     |
| 58  | ZN   | 15    | 109  | 1/1   | 0.99 | 0.03 | 58,58,58,58                 | 0     |
| 58  | ZN   | 16    | 102  | 1/1   | 0.99 | 0.02 | 35,35,35,35                 | 0     |
| 54  | MG   | 1A    | 3726 | 1/1   | 0.99 | 0.04 | 40,40,40,40                 | 0     |
| 54  | MG   | 1D    | 310  | 1/1   | 0.99 | 0.05 | 15,15,15,15                 | 0     |
| 54  | MG   | 1A    | 3038 | 1/1   | 0.99 | 0.12 | 27,27,27,27                 | 0     |
| 58  | ZN   | 25    | 103  | 1/1   | 0.99 | 0.04 | 78,78,78,78                 | 0     |
| 58  | ZN   | 26    | 501  | 1/1   | 0.99 | 0.03 | 53,53,53,53                 | 0     |
| 58  | ZN   | 29    | 501  | 1/1   | 0.99 | 0.03 | 67,67,67,67                 | 0     |
| 54  | MG   | 1A    | 3396 | 1/1   | 0.99 | 0.07 | 17,17,17,17                 | 0     |
| 54  | MG   | 2A    | 3659 | 1/1   | 0.99 | 0.02 | 52,52,52,52                 | 0     |
| 54  | MG   | 1A    | 3048 | 1/1   | 0.99 | 0.15 | 23,23,23,23                 | 0     |
| 54  | MG   | 2A    | 3340 | 1/1   | 1.00 | 0.03 | 31,31,31,31                 | 0     |
| 54  | MG   | 1A    | 3006 | 1/1   | 1.00 | 0.04 | 12,12,12,12                 | 0     |
| 54  | MG   | 2A    | 3462 | 1/1   | 1.00 | 0.08 | 33,33,33,33                 | 0     |
| 54  | MG   | 1A    | 3043 | 1/1   | 1.00 | 0.02 | 10,10,10,10                 | 0     |
| 54  | MG   | 1D    | 304  | 1/1   | 1.00 | 0.04 | 16,16,16,16                 | 0     |
| 58  | ZN   | 19    | 104  | 1/1   | 1.00 | 0.03 | 43,43,43,43                 | 0     |
| 54  | MG   | 1A    | 3891 | 1/1   | 1.00 | 0.04 | 16,16,16,16                 | 0     |
| 54  | MG   | 2A    | 3479 | 1/1   | 1.00 | 0.04 | 25,25,25,25                 | 0     |
| 54  | MG   | 1A    | 3468 | 1/1   | 1.00 | 0.03 | 31,31,31,31                 | 0     |
| 54  | MG   | 1A    | 3436 | 1/1   | 1.00 | 0.03 | 14,14,14,14                 | 0     |
| 54  | MG   | 1A    | 3836 | 1/1   | 1.00 | 0.03 | 12,12,12,12                 | 0     |
| 54  | MG   | 1A    | 3328 | 1/1   | 1.00 | 0.06 | 18,18,18,18                 | 0     |
| 54  | MG   | 1A    | 3887 | 1/1   | 1.00 | 0.02 | 30,30,30,30                 | 0     |
| 54  | MG   | 1A    | 3969 | 1/1   | 1.00 | 0.04 | 15,15,15,15                 | 0     |
| 54  | MG   | 1A    | 3831 | 1/1   | 1.00 | 0.02 | 19,19,19,19                 | 0     |

## 6.5 Other polymers ⓘ

There are no such residues in this entry.