



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 20, 2016 – 02:59 AM GMT

PDB ID : 5DOY  
Title : Crystal structure of the *Thermus thermophilus* 70S ribosome in complex with antibiotic Hygromycin A, mRNA and three tRNAs in the A, P and E sites at 2.6Å resolution  
Authors : Polikanov, Y.S.; Starosta, A.L.; Juetten, M.F.; Altman, R.B.; Terry, D.S.; Lu, W.; Burnett, B.J.; Dinos, G.; Reynolds, K.; Blanchard, S.C.; Steitz, T.A.; Wilson, D.N.  
Deposited on : 2015-09-11  
Resolution : 2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026982  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20026982

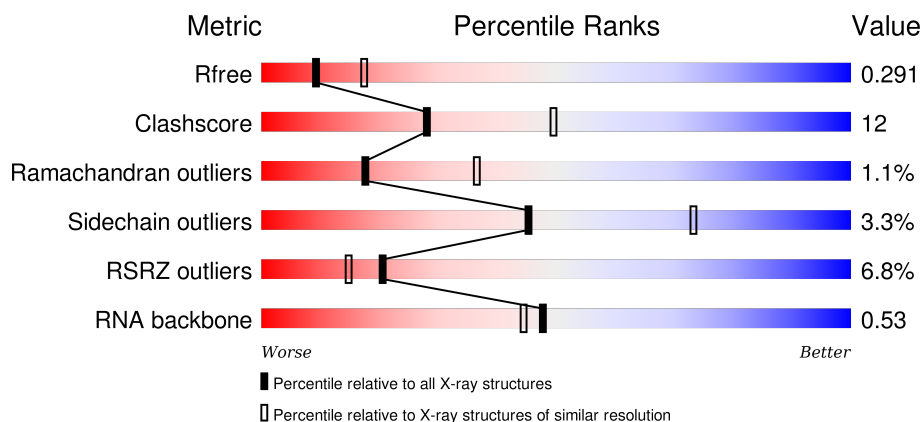
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 Å.

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



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 91344                       | 2328 (2.60-2.60)                                      |
| Clashscore            | 102246                      | 2679 (2.60-2.60)                                      |
| Ramachandran outliers | 100387                      | 2635 (2.60-2.60)                                      |
| Sidechain outliers    | 100360                      | 2635 (2.60-2.60)                                      |
| RSRZ outliers         | 91569                       | 2334 (2.60-2.60)                                      |
| RNA backbone          | 2183                        | 1022 (3.00-2.20)                                      |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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>2%</div> <div>57%</div> <div>33%</div> <div>8%</div> <div>.</div> </div>  |
| 1   | 2A    | 2915   | <div> <div>2%</div> <div>45%</div> <div>41%</div> <div>9%</div> <div>.</div> </div>  |
| 2   | 1B    | 121    | <div> <div>64%</div> <div>31%</div> <div>...</div> </div>                            |
| 2   | 2B    | 121    | <div> <div>2%</div> <div>28%</div> <div>53%</div> <div>18%</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  | 1v    | 27     |                  |
| 53  | 2v    | 27     |                  |
| 54  | 1w    | 76     |                  |
| 54  | 1y    | 76     |                  |
| 54  | 2w    | 76     |                  |
| 54  | 2y    | 76     |                  |
| 55  | 1x    | 77     |                  |
| 55  | 2x    | 77     |                  |

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

| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 56  | MG   | 17    | 101  | -         | -        | -       | X                |
| 56  | MG   | 18    | 101  | -         | -        | -       | X                |
| 56  | MG   | 1A    | 3030 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 3039 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 3094 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 3121 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 3123 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 3125 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 3126 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 3159 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 3162 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 3178 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 3192 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 3198 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 3199 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 3202 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 3234 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 3235 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 3249 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 3251 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 3268 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 3296 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 3313 | -         | -        | -       | X                |

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| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 56  | MG   | 1A    | 3314 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 3315 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 3317 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 3319 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 3362 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 3604 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 3652 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 3658 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 3670 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 3680 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 3736 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 3738 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 3762 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 3769 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 3770 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 3827 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 3897 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 3908 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 3910 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 3917 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 3919 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 3926 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 3929 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 3930 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 3934 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 3935 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 3940 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 3944 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 3947 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 3957 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 3958 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 3965 | -         | -        | -       | X                |
| 56  | MG   | 1B    | 3003 | -         | -        | -       | X                |
| 56  | MG   | 1B    | 3011 | -         | -        | -       | X                |
| 56  | MG   | 1B    | 3024 | -         | -        | -       | X                |
| 56  | MG   | 1F    | 304  | -         | -        | -       | X                |
| 56  | MG   | 1F    | 307  | -         | -        | -       | X                |
| 56  | MG   | 1N    | 3001 | -         | -        | -       | X                |
| 56  | MG   | 1N    | 3004 | -         | -        | -       | X                |
| 56  | MG   | 1N    | 3006 | -         | -        | -       | X                |
| 56  | MG   | 1S    | 3001 | -         | -        | -       | X                |
| 56  | MG   | 1X    | 3004 | -         | -        | -       | X                |

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| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 56  | MG   | 1a    | 1608 | -         | -        | -       | X                |
| 56  | MG   | 1a    | 1625 | -         | -        | -       | X                |
| 56  | MG   | 1a    | 1644 | -         | -        | -       | X                |
| 56  | MG   | 1a    | 1649 | -         | -        | -       | X                |
| 56  | MG   | 1a    | 1653 | -         | -        | -       | X                |
| 56  | MG   | 1a    | 1656 | -         | -        | -       | X                |
| 56  | MG   | 1a    | 1669 | -         | -        | -       | X                |
| 56  | MG   | 1a    | 1713 | -         | -        | -       | X                |
| 56  | MG   | 1a    | 1730 | -         | -        | -       | X                |
| 56  | MG   | 1a    | 1761 | -         | -        | -       | X                |
| 56  | MG   | 1a    | 1837 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3015 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3022 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3048 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3071 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3090 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3104 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3123 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3159 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3167 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3201 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3202 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3205 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3215 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3264 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3303 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3304 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3405 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3421 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3451 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3481 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3482 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3495 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3497 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3559 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3598 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3622 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3656 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3659 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3662 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3664 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3668 | -         | -        | -       | X                |

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| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 56  | MG   | 2A    | 3669 | -         | -        | -       | X                |
| 56  | MG   | 2D    | 301  | -         | -        | -       | X                |
| 56  | MG   | 2D    | 303  | -         | -        | -       | X                |
| 56  | MG   | 2F    | 302  | -         | -        | -       | X                |
| 56  | MG   | 2Q    | 201  | -         | -        | -       | X                |
| 56  | MG   | 2U    | 204  | -         | -        | -       | X                |
| 56  | MG   | 2a    | 1633 | -         | -        | -       | X                |
| 56  | MG   | 2a    | 1659 | -         | -        | -       | X                |
| 56  | MG   | 2a    | 1679 | -         | -        | -       | X                |
| 56  | MG   | 2a    | 1715 | -         | -        | -       | X                |
| 56  | MG   | 2a    | 1738 | -         | -        | -       | X                |
| 56  | MG   | 2a    | 1747 | -         | -        | -       | X                |
| 56  | MG   | 2a    | 1787 | -         | -        | -       | X                |

## 2 Entry composition [i](#)

There are 61 unique types of molecules in this entry. The entry contains 298925 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

- Molecule 3 is a protein called 50S Ribosomal Protein L2.

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

- Molecule 4 is a protein called 50S Ribosomal Protein L3.

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

- Molecule 5 is a protein called 50S Ribosomal Protein L4.

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

- Molecule 6 is a protein called 50S Ribosomal Protein L5.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 6   | 1G    | 181      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1429  | 916 | 256 | 253 | 4 |         |         |       |
| 6   | 2G    | 181      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1428  | 913 | 258 | 253 | 4 |         |         |       |

- Molecule 7 is a protein called 50S Ribosomal Protein L6.

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

- Molecule 8 is a protein called 50S Ribosomal Protein L9.

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

- Molecule 9 is a protein called 50S Ribosomal Protein L13.

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

- Molecule 10 is a protein called 50S Ribosomal Protein L14.

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

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

- Molecule 11 is a protein called 50S Ribosomal Protein L15.

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

- Molecule 12 is a protein called 50S Ribosomal Protein L16.

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

- Molecule 13 is a protein called 50S Ribosomal Protein L17.

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

- Molecule 14 is a protein called 50S Ribosomal Protein L18.

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

- Molecule 15 is a protein called 50S Ribosomal Protein L19.

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

- Molecule 16 is a protein called 50S Ribosomal Protein L20.

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

- Molecule 17 is a protein called 50S Ribosomal Protein L21.

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

- Molecule 18 is a protein called 50S Ribosomal Protein L22.

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

- Molecule 19 is a protein called 50S Ribosomal Protein L23.

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

- Molecule 20 is a protein called 50S Ribosomal Protein L24.

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

- Molecule 21 is a protein called 50S Ribosomal Protein L25.

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

- Molecule 22 is a protein called 50S Ribosomal Protein L27.

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

- Molecule 23 is a protein called 50S Ribosomal Protein L28.

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

- Molecule 24 is a protein called 50S Ribosomal Protein L29.

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

- Molecule 25 is a protein called 50S Ribosomal Protein L30.

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

- Molecule 26 is a protein called 50S Ribosomal Protein L31.

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

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

- Molecule 27 is a protein called 50S Ribosomal Protein L32.

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

- Molecule 28 is a protein called 50S Ribosomal Protein L33.

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

- Molecule 29 is a protein called 50S Ribosomal Protein L34.

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

- Molecule 30 is a protein called 50S Ribosomal Protein L35.

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

- Molecule 31 is a protein called 50S Ribosomal Protein L36.

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

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

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

- Molecule 33 is a protein called 30S Ribosomal Protein S2.

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

- Molecule 34 is a protein called 30S Ribosomal Protein S3.

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

- Molecule 35 is a protein called 30S Ribosomal Protein S4.

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

- Molecule 36 is a protein called 30S Ribosomal Protein S5.

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

- Molecule 37 is a protein called 30S Ribosomal Protein S6.

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

- Molecule 38 is a protein called 30S Ribosomal Protein S7.

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

- Molecule 39 is a protein called 30S Ribosomal Protein S8.

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

- Molecule 40 is a protein called 30S Ribosomal Protein S9.

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

- Molecule 41 is a protein called 30S Ribosomal Protein S10.

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

- Molecule 42 is a protein called 30S Ribosomal Protein S11.

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

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

- Molecule 43 is a protein called 30S Ribosomal Protein S12.

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

- Molecule 44 is a protein called 30S Ribosomal Protein S13.

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

- Molecule 45 is a protein called 30S Ribosomal Protein S14.

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

- Molecule 46 is a protein called 30S Ribosomal Protein S15.

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

- Molecule 47 is a protein called 30S Ribosomal Protein S16.

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

- Molecule 48 is a protein called 30S Ribosomal Protein S17.

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

- Molecule 49 is a protein called 30S Ribosomal Protein S18.

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

- Molecule 50 is a protein called 30S Ribosomal Protein S19.

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

- Molecule 51 is a protein called 30S Ribosomal Protein S20.

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

- Molecule 52 is a protein called 30S Ribosomal Protein THX.

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

- Molecule 53 is a RNA chain called mRNA.



| Mol | Chain | Residues | Atoms |     |    |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|----|---------|---------|-------|
| 53  | 1v    | 14       | Total | C   | N  | O  | P  | 0       | 0       | 0     |
|     |       |          | 281   | 125 | 51 | 91 | 14 |         |         |       |
| 53  | 2v    | 13       | Total | C   | N  | O  | P  | 0       | 0       | 0     |
|     |       |          | 277   | 125 | 51 | 88 | 13 |         |         |       |

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

| Mol | Chain | Residues | Atoms         |          |          |          |         |        | ZeroOcc | AltConf | Trace |
|-----|-------|----------|---------------|----------|----------|----------|---------|--------|---------|---------|-------|
| 54  | 1w    | 75       | Total<br>1574 | C<br>704 | N<br>283 | O<br>512 | P<br>73 | S<br>2 | 0       | 0       | 1     |
| 54  | 1y    | 74       | Total<br>1581 | C<br>707 | N<br>285 | O<br>515 | P<br>73 | S<br>1 | 0       | 0       | 0     |
| 54  | 2w    | 74       | Total<br>1547 | C<br>688 | N<br>278 | O<br>507 | P<br>73 | S<br>1 | 0       | 0       | 1     |
| 54  | 2y    | 73       | Total<br>1561 | C<br>698 | N<br>283 | O<br>507 | P<br>72 | S<br>1 | 0       | 0       | 0     |

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

| Mol | Chain | Residues | Atoms |     |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---|---------|---------|-------|
| 55  | 1x    | 76       | Total | C   | N   | O   | P  | S | 0       | 0       | 0     |
|     |       |          | 1635  | 731 | 295 | 531 | 76 | 2 |         |         |       |
| 55  | 2x    | 76       | Total | C   | N   | O   | P  | S | 0       | 0       | 0     |
|     |       |          | 1635  | 731 | 295 | 531 | 76 | 2 |         |         |       |

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

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 56  | 2E    | 5        | Total | Mg | 0       | 0       |
|     |       |          | 5     | 5  |         |         |
| 56  | 17    | 2        | Total | Mg | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 56  | 2d    | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 56  | 1T    | 3        | Total | Mg | 0       | 0       |
|     |       |          | 3     | 3  |         |         |
| 56  | 1N    | 7        | Total | Mg | 0       | 0       |
|     |       |          | 7     | 7  |         |         |
| 56  | 20    | 3        | Total | Mg | 0       | 0       |
|     |       |          | 3     | 3  |         |         |
| 56  | 18    | 2        | Total | Mg | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 56  | 1Y    | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

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| Mol | Chain | Residues | Atoms        |           | ZeroOcc | AltConf |
|-----|-------|----------|--------------|-----------|---------|---------|
| 56  | 13    | 3        | Total<br>3   | Mg<br>3   | 0       | 0       |
| 56  | 1f    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 56  | 1P    | 4        | Total<br>4   | Mg<br>4   | 0       | 0       |
| 56  | 2B    | 18       | Total<br>18  | Mg<br>18  | 0       | 0       |
| 56  | 2a    | 196      | Total<br>196 | Mg<br>196 | 0       | 0       |
| 56  | 1E    | 6        | Total<br>6   | Mg<br>6   | 0       | 0       |
| 56  | 1b    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 56  | 2l    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 56  | 2F    | 4        | Total<br>4   | Mg<br>4   | 0       | 0       |
| 56  | 16    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 56  | 28    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 56  | 2e    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 56  | 1W    | 6        | Total<br>6   | Mg<br>6   | 0       | 0       |
| 56  | 1A    | 963      | Total<br>963 | Mg<br>963 | 0       | 0       |
| 56  | 1t    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 56  | 2p    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 56  | 2P    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 56  | 1X    | 4        | Total<br>4   | Mg<br>4   | 0       | 0       |
| 56  | 12    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 56  | 1y    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 56  | 1S    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |

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| Mol | Chain | Residues | Atoms        |           | ZeroOcc | AltConf |
|-----|-------|----------|--------------|-----------|---------|---------|
| 56  | 2T    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 56  | 1D    | 5        | Total<br>5   | Mg<br>5   | 0       | 0       |
| 56  | 23    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 56  | 1e    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 56  | 2G    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 56  | 1I    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 56  | 2f    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 56  | 1V    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 56  | 2X    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 56  | 1w    | 6        | Total<br>6   | Mg<br>6   | 0       | 0       |
| 56  | 1a    | 239      | Total<br>239 | Mg<br>239 | 0       | 0       |
| 56  | 2Q    | 4        | Total<br>4   | Mg<br>4   | 0       | 0       |
| 56  | 15    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 56  | 1x    | 10       | Total<br>10  | Mg<br>10  | 0       | 0       |
| 56  | 2j    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 56  | 1R    | 3        | Total<br>3   | Mg<br>3   | 0       | 0       |
| 56  | 26    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 56  | 2v    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 56  | 2U    | 4        | Total<br>4   | Mg<br>4   | 0       | 0       |
| 56  | 1G    | 4        | Total<br>4   | Mg<br>4   | 0       | 0       |
| 56  | 2O    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |

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| Mol | Chain | Residues | Atoms        |           | ZeroOcc | AltConf |
|-----|-------|----------|--------------|-----------|---------|---------|
| 56  | 1l    | 3        | Total<br>3   | Mg<br>3   | 0       | 0       |
| 56  | 1d    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 56  | 2r    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 56  | 2g    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 56  | 1v    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 56  | 2x    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 56  | 2R    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 56  | 1Z    | 5        | Total<br>5   | Mg<br>5   | 0       | 0       |
| 56  | 2D    | 4        | Total<br>4   | Mg<br>4   | 0       | 0       |
| 56  | 2q    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 56  | 1U    | 5        | Total<br>5   | Mg<br>5   | 0       | 0       |
| 56  | 1O    | 6        | Total<br>6   | Mg<br>6   | 0       | 0       |
| 56  | 19    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 56  | 1l    | 3        | Total<br>3   | Mg<br>3   | 0       | 0       |
| 56  | 2V    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 56  | 1F    | 7        | Total<br>7   | Mg<br>7   | 0       | 0       |
| 56  | 10    | 4        | Total<br>4   | Mg<br>4   | 0       | 0       |
| 56  | 2t    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 56  | 1Q    | 6        | Total<br>6   | Mg<br>6   | 0       | 0       |
| 56  | 2A    | 673      | Total<br>673 | Mg<br>673 | 0       | 0       |
| 56  | 2Z    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |

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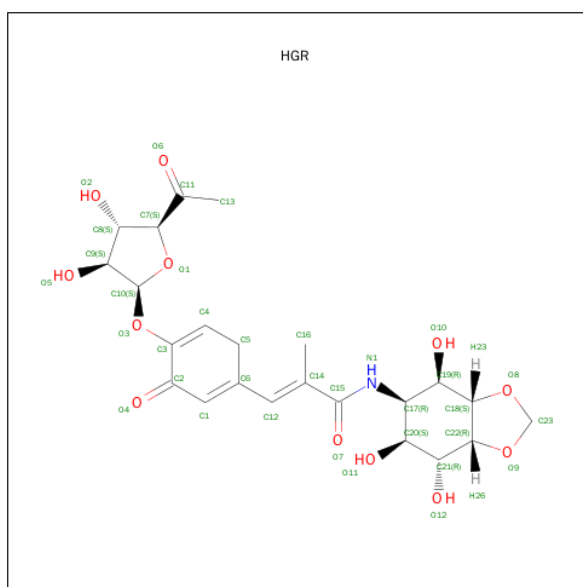
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| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 56  | 1B    | 29       | Total | Mg | 0       | 0       |
|     |       |          | 29    | 29 |         |         |
| 56  | 2w    | 3        | Total | Mg | 0       | 0       |
|     |       |          | 3     | 3  |         |         |

- Molecule 57 is POTASSIUM ION (three-letter code: K) (formula: K).

| Mol | Chain | Residues | Atoms |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---------|---------|
| 57  | 1A    | 1        | Total | K | 0       | 0       |
|     |       |          | 1     | 1 |         |         |
| 57  | 2A    | 1        | Total | K | 0       | 0       |
|     |       |          | 1     | 1 |         |         |

- Molecule 58 is Hygromycin A (three-letter code: HGR) (formula: C<sub>23</sub>H<sub>29</sub>NO<sub>12</sub>).



| Mol | Chain | Residues | Atoms |    |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---------|---------|
| 58  | 1A    | 1        | Total | C  | N | O  | 0       | 0       |
|     |       |          | 36    | 23 | 1 | 12 |         |         |
| 58  | 2A    | 1        | Total | C  | N | O  | 0       | 0       |
|     |       |          | 36    | 23 | 1 | 12 |         |         |

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

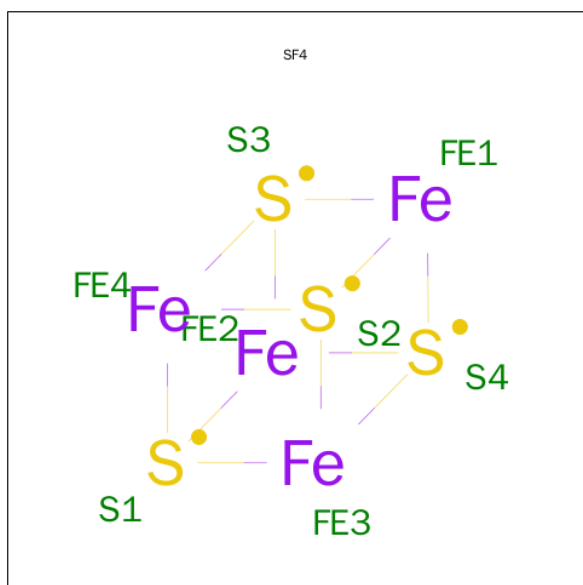
| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 59  | 1Y    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

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| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 59  | 14    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 59  | 1n    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 59  | 15    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 59  | 29    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 59  | 19    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 59  | 26    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 59  | 25    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 59  | 24    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 59  | 2n    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 59  | 2Y    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 59  | 16    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

- Molecule 60 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



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

- Molecule 61 is water.

| Mol | Chain | Residues | Atoms |      | ZeroOcc | AltConf |
|-----|-------|----------|-------|------|---------|---------|
| 61  | 1A    | 1577     | Total | O    | 0       | 0       |
|     |       |          | 1577  | 1577 |         |         |
| 61  | 1B    | 43       | Total | O    | 0       | 0       |
|     |       |          | 43    | 43   |         |         |
| 61  | 1D    | 23       | Total | O    | 0       | 0       |
|     |       |          | 23    | 23   |         |         |
| 61  | 1E    | 25       | Total | O    | 0       | 0       |
|     |       |          | 25    | 25   |         |         |
| 61  | 1F    | 17       | Total | O    | 0       | 0       |
|     |       |          | 17    | 17   |         |         |
| 61  | 1G    | 3        | Total | O    | 0       | 0       |
|     |       |          | 3     | 3    |         |         |
| 61  | 1H    | 1        | Total | O    | 0       | 0       |
|     |       |          | 1     | 1    |         |         |
| 61  | 1N    | 3        | Total | O    | 0       | 0       |
|     |       |          | 3     | 3    |         |         |
| 61  | 1O    | 4        | Total | O    | 0       | 0       |
|     |       |          | 4     | 4    |         |         |
| 61  | 1P    | 20       | Total | O    | 0       | 0       |
|     |       |          | 20    | 20   |         |         |
| 61  | 1Q    | 4        | Total | O    | 0       | 0       |
|     |       |          | 4     | 4    |         |         |
| 61  | 1R    | 5        | Total | O    | 0       | 0       |
|     |       |          | 5     | 5    |         |         |
| 61  | 1S    | 3        | Total | O    | 0       | 0       |
|     |       |          | 3     | 3    |         |         |
| 61  | 1T    | 4        | Total | O    | 0       | 0       |
|     |       |          | 4     | 4    |         |         |
| 61  | 1U    | 9        | Total | O    | 0       | 0       |
|     |       |          | 9     | 9    |         |         |
| 61  | 1V    | 5        | Total | O    | 0       | 0       |
|     |       |          | 5     | 5    |         |         |
| 61  | 1W    | 8        | Total | O    | 0       | 0       |
|     |       |          | 8     | 8    |         |         |
| 61  | 1X    | 7        | Total | O    | 0       | 0       |
|     |       |          | 7     | 7    |         |         |

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| Mol | Chain | Residues | Atoms        |          | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 61  | 1Y    | 2        | Total<br>2   | O<br>2   | 0       | 0       |
| 61  | 1Z    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 61  | 10    | 9        | Total<br>9   | O<br>9   | 0       | 0       |
| 61  | 11    | 3        | Total<br>3   | O<br>3   | 0       | 0       |
| 61  | 12    | 4        | Total<br>4   | O<br>4   | 0       | 0       |
| 61  | 13    | 3        | Total<br>3   | O<br>3   | 0       | 0       |
| 61  | 14    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 61  | 15    | 4        | Total<br>4   | O<br>4   | 0       | 0       |
| 61  | 16    | 2        | Total<br>2   | O<br>2   | 0       | 0       |
| 61  | 17    | 5        | Total<br>5   | O<br>5   | 0       | 0       |
| 61  | 18    | 10       | Total<br>10  | O<br>10  | 0       | 0       |
| 61  | 19    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 61  | 1a    | 287      | Total<br>287 | O<br>287 | 0       | 0       |
| 61  | 1e    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 61  | 1h    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 61  | 1i    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 61  | 1l    | 4        | Total<br>4   | O<br>4   | 0       | 0       |
| 61  | 1m    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 61  | 1n    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 61  | 1o    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 61  | 1p    | 1        | Total<br>1   | O<br>1   | 0       | 0       |

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| Mol | Chain | Residues | Atoms         |           | ZeroOcc | AltConf |
|-----|-------|----------|---------------|-----------|---------|---------|
| 61  | 1q    | 1        | Total<br>1    | O<br>1    | 0       | 0       |
| 61  | 1s    | 1        | Total<br>1    | O<br>1    | 0       | 0       |
| 61  | 1v    | 3        | Total<br>3    | O<br>3    | 0       | 0       |
| 61  | 1w    | 8        | Total<br>8    | O<br>8    | 0       | 0       |
| 61  | 1x    | 6        | Total<br>6    | O<br>6    | 0       | 0       |
| 61  | 1y    | 1        | Total<br>1    | O<br>1    | 0       | 0       |
| 61  | 2A    | 1063     | Total<br>1063 | O<br>1063 | 0       | 0       |
| 61  | 2B    | 10       | Total<br>10   | O<br>10   | 0       | 0       |
| 61  | 2D    | 20       | Total<br>20   | O<br>20   | 0       | 0       |
| 61  | 2E    | 9        | Total<br>9    | O<br>9    | 0       | 0       |
| 61  | 2F    | 7        | Total<br>7    | O<br>7    | 0       | 0       |
| 61  | 2I    | 1        | Total<br>1    | O<br>1    | 0       | 0       |
| 61  | 2N    | 2        | Total<br>2    | O<br>2    | 0       | 0       |
| 61  | 2O    | 1        | Total<br>1    | O<br>1    | 0       | 0       |
| 61  | 2P    | 14       | Total<br>14   | O<br>14   | 0       | 0       |
| 61  | 2Q    | 1        | Total<br>1    | O<br>1    | 0       | 0       |
| 61  | 2R    | 3        | Total<br>3    | O<br>3    | 0       | 0       |
| 61  | 2T    | 2        | Total<br>2    | O<br>2    | 0       | 0       |
| 61  | 2U    | 1        | Total<br>1    | O<br>1    | 0       | 0       |
| 61  | 2V    | 2        | Total<br>2    | O<br>2    | 0       | 0       |
| 61  | 2W    | 2        | Total<br>2    | O<br>2    | 0       | 0       |

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| Mol | Chain | Residues | Atoms        |          | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 61  | 2X    | 3        | Total<br>3   | O<br>3   | 0       | 0       |
| 61  | 2Y    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 61  | 2Z    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 61  | 20    | 4        | Total<br>4   | O<br>4   | 0       | 0       |
| 61  | 21    | 3        | Total<br>3   | O<br>3   | 0       | 0       |
| 61  | 23    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 61  | 25    | 2        | Total<br>2   | O<br>2   | 0       | 0       |
| 61  | 26    | 2        | Total<br>2   | O<br>2   | 0       | 0       |
| 61  | 28    | 5        | Total<br>5   | O<br>5   | 0       | 0       |
| 61  | 29    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 61  | 2a    | 213      | Total<br>213 | O<br>213 | 0       | 0       |
| 61  | 2d    | 3        | Total<br>3   | O<br>3   | 0       | 0       |
| 61  | 2g    | 2        | Total<br>2   | O<br>2   | 0       | 0       |
| 61  | 2i    | 2        | Total<br>2   | O<br>2   | 0       | 0       |
| 61  | 2j    | 5        | Total<br>5   | O<br>5   | 0       | 0       |
| 61  | 2l    | 3        | Total<br>3   | O<br>3   | 0       | 0       |
| 61  | 2n    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 61  | 2o    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 61  | 2p    | 3        | Total<br>3   | O<br>3   | 0       | 0       |
| 61  | 2r    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 61  | 2t    | 2        | Total<br>2   | O<br>2   | 0       | 0       |

*Continued on next page...*

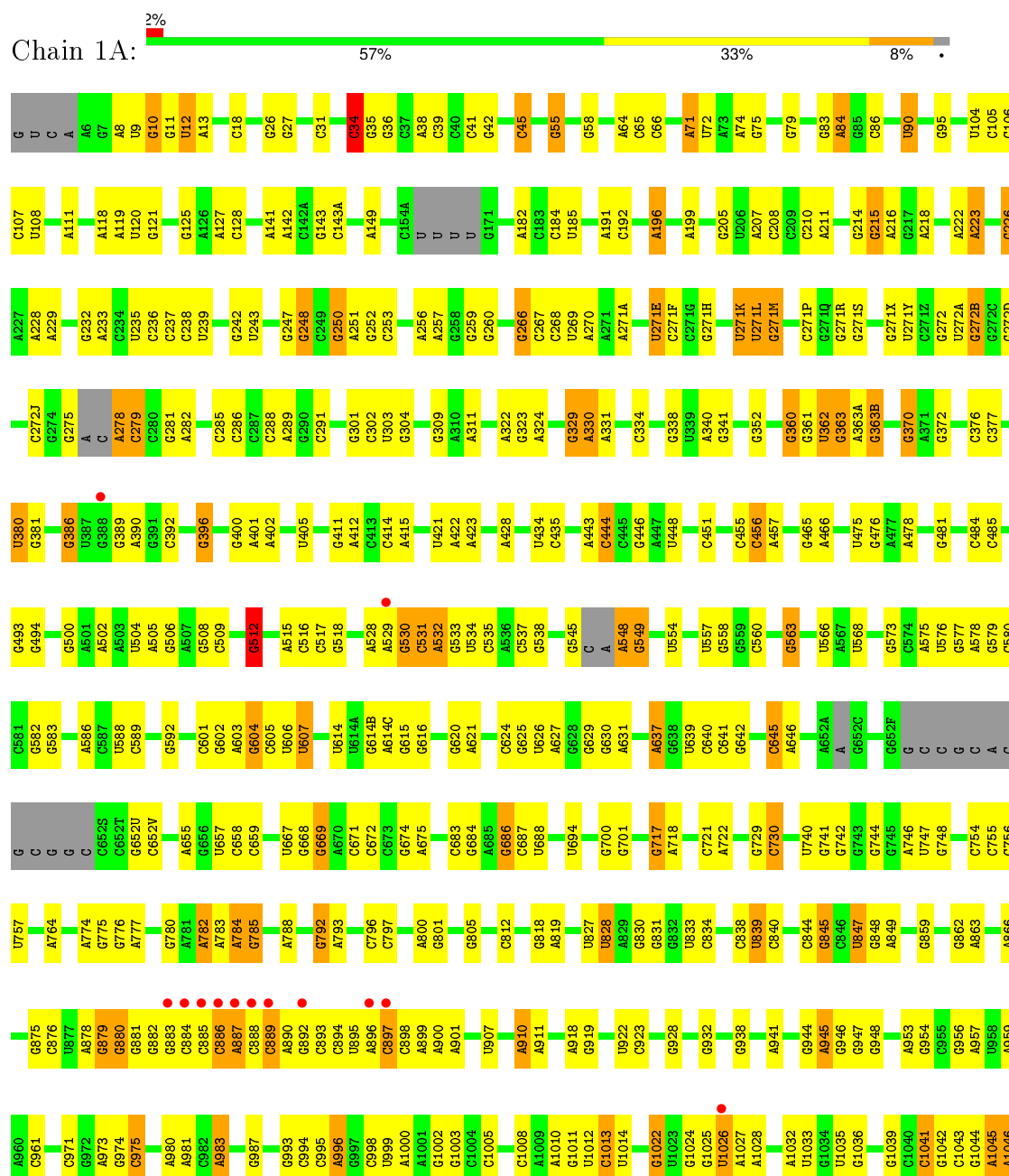
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| Mol | Chain | Residues | Atoms |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---------|---------|
| 61  | 2v    | 1        | Total | O | 0       | 0       |
|     |       |          | 1     | 1 |         |         |
| 61  | 2w    | 2        | Total | O | 0       | 0       |
|     |       |          | 2     | 2 |         |         |
| 61  | 2x    | 6        | Total | O | 0       | 0       |
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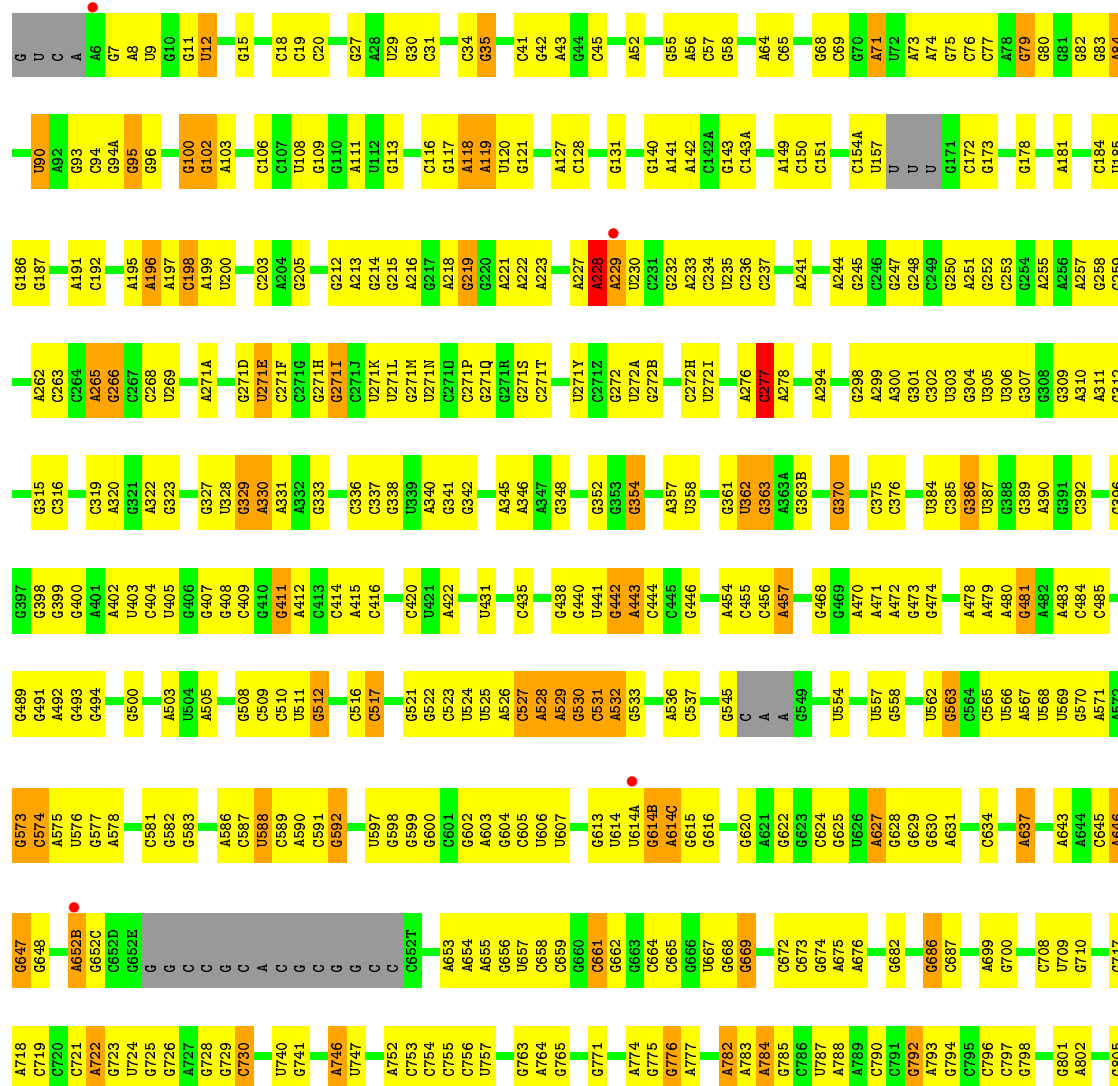
### 3 Residue-property plots

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

#### • Molecule 1: 23S Ribosomal RNA



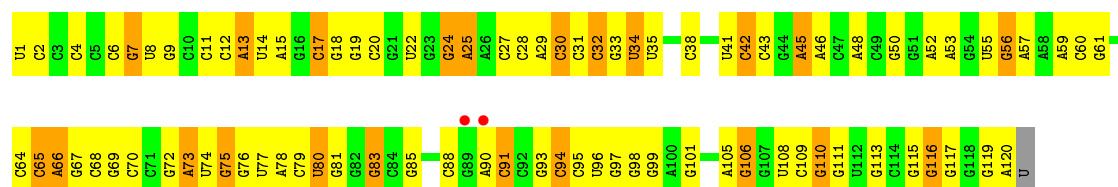
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| G2445 | G2340 | A2267 | G2156 | G2087 | C1967 | C1837 | A1608 | C1493  | C1387 | C1293 | G1201 | C1109 | A1048 |
| G2446 | G2341 | A2268 | G2157 | G2093 | G1968 | C1837 | A1609 | A1494  | U1394 | A1494 | A1204 | G1110 | G1051 |
| G2447 | G2342 | A2269 | G2158 | G2096 | A1969 | C1837 | A1610 | A1495  | U1395 | C1297 | U1205 | G1112 | C1052 |
| A2448 | C2347 | G2270 | G2159 | U2096 | A1970 | C1843 | G1746 | A1508  | U1396 | C1299 | G1206 | G1113 | C1053 |
| G2448 | C2350 | G2271 | C2161 | C2097 | A1971 | G1846 | G1756 | C1509  | G1400 | U1300 | A1210 | G1114 | A1054 |
| G2451 | G2351 | U2272 | C2162 | U2098 | A1972 | A1847 | G1766 | C1509A | G1401 | A1301 | U1211 | G1115 | G1055 |
| C2452 | G2352 | A2273 | C2163 | U2099 | G1985 | G1848 | A1759 | A1509B | C1402 | C1302 | G1218 | G1116 | A1057 |
| G2453 | G2353 | A2274 | C2164 | G2100 | A1986 | G1849 | G1762 | U1512  | C1403 | G1303 | G1219 | G1122 | U1058 |
| G2454 | G2354 | G2275 | G2165 | G2101 | G1987 | U1850 | G1763 | U1513  | G1404 | C1306 | A1220 | G1125 | G1059 |
| G2455 | C2355 | A2276 | U2167 | U2102 | G1989 | U1851 | G1764 | U1514  | U1405 | U1301 | G1219 | G1125 | U1060 |
| G2456 | G2356 | G2277 | G2168 | C2105 | G1992 | C1852 | G1765 | U1515  | U1406 | C1302 | G1219 | G1125 | U     |
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| G2459 | A2361 | C2283 | A2171 | C2108 | U1995 | A1854 | C1767 | U1519  | G1411 | U1313 | G1223 | G1125 | U1064 |
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| G2487 | G2364 | A2286 | C2174 | C2111 | G1997 | C1866 | A1773 | U1519  | C1416 | C1316 | G1223 | G1125 | U1067 |
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| G2489 | G2372 | A2288 | C2176 | G2116 | G2002 | A1877 | U1779 | G1527  | C1418 | C1318 | G1223 | G1125 | U1069 |
| G2490 | G2373 | G2290 | C2177 | G2117 | G2003 | G1878 | U1780 | A1528  | A1418 | C1320 | G1235 | G1131 | U1070 |
| U2491 | G2374 | U2291 | C2178 | U2118 | A2012 | C1781 | G1781 | C1531  | A1419 | C1320 | G1235 | G1131 | G1071 |
| A2497 | G2375 | C2292 | C2178 | U2119 | A2013 | C1782 | G1782 | C1532  | U1420 | G1324 | G1238 | G1143 | C1072 |
| C2498 | A2377 | U2296 | G2181 | G2120 | A2014 | C1783 | A1783 | G      | G1421 | U1329 | G1238 | G1143 | A1073 |
| C2499 | G2378 | C2297 | G2182 | G2121 | G2018 | A1784 | A1784 | U      | G1422 | C1330 | U1240 | G1149 | G1074 |
| G2502 | G2383 | A2298 | G2183 | U2122 | G2019 | A1785 | A1785 | C      | G1423 | C1331 | U1240 | G1149 | G1075 |
| A2503 | G2384 | G2299 | G2184 | G2123 | U2022 | A1786 | A1786 | U      | G1424 | C1332 | G1244 | G1153 | C1076 |
| U2504 | C2385 | A2305 | G2187 | G2124 | G2023 | C1790 | C1790 | G1537  | C1428 | A1331 | G1252 | G1154 | C1077 |
| G2505 | G2386 | C2306 | C2188 | G2125 | U2028 | A1791 | A1791 | U1540  | A1429 | C1332 | G1252 | G1154 | C1078 |
| U2506 | U2387 | G2307 | G2189 | A2126 | G2029 | G1792 | G1792 | G1541  | U1430 | A1333 | G1252 | G1155 | C1079 |
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| G2513 | U2407 | A2309 | G2192 | C2129 | A2031 | C1795 | G1678 | C1547  | U1433 | U1341 | G1257 | G1161 | U1081 |
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| A2531 | G2413 | A2314 | G2207 | A2135 | G1921 | C1800 | U1688 | A1558  | G1448 | A1356 | A1262 | G1169 | A1087 |
| G2532 | G2414 | C2315 | G2207 | C2136 | G1921 | A1801 | U1688 | A1558  | G1449 | G1357 | G1263 | G1170 | A1088 |
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| G2537 | G2420 | G2319 | G2220 | C2138 | A1927 | A1803 | U1688 | A1558  | G1451 | G1358 | G1266 | G1172 | G1091 |
| G2538 | G2421 | A2320 | G2221 | C2139 | A1928 | A1810 | G1696 | A1569  | A1452 | A1359 | U1267 | G1173 | C1092 |
| G2539 | A2428 | G2321 | G2222 | C2140 | G1929 | G1811 | G1697 | U1578  | U1453 | A1360 | U1267 | G1174 | G1093 |
| A2534 | U2419 | A2322 | G2223 | G2141 | G1930 | A1815 | G1698 | A1579  | G1455 | G1364 | U1267 | G1175 | U1094 |
| G2540 | G2425 | G2323 | G2224 | C2142 | A2054 | A1816 | G1699 | A1580  | G1456 | G1365 | G1270 | G1176 | A1095 |
| G2541 | G2426 | C2324 | A2225 | C2143 | G2056 | G1817 | G1701 | G1581  | G1461 | G1366 | G1270 | G1177 | A1096 |
| G2542 | G2427 | G2325 | U2233 | U2144 | A1937 | G1817 | G1702 | G1581  | G1462 | A1365 | G1271 | G1178 | U1097 |
| G2543 | G2428 | C2326 | U2234 | C2145 | A1938 | G1817 | G1703 | C1584  | G1463 | A1366 | A1272 | G1179 | A1098 |
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| G2546 | A2432 | G2329 | G2236 | A1825 | C1710 | A1825 | C1710 | C1588  | C1468 | G1373 | A1275 | G1185 | U1101 |
| G2547 | G2433 | G2330 | G2237 | G2148 | A1932 | A1826 | U1713 | C1589  | A1471 | A1379 | G1276 | G1186 | C1102 |
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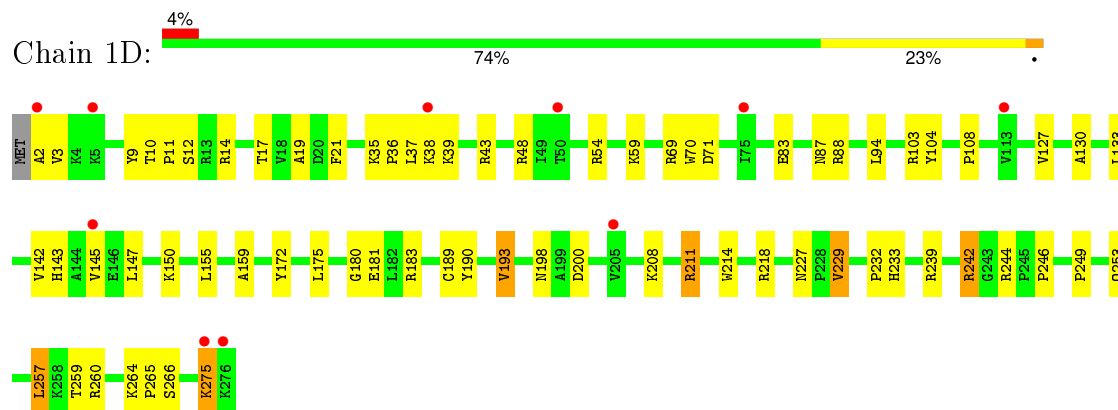
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| U1955 | G1835 | G1756 | C1636 | A1545  | A1469 | G1389  | G1309 | G1225  | A1148 | A | G1024 | C951 | A878 | C866 |
| U1963 | G1839 | U1767 | A1637 | C1546  | A1471 | U1394  | G1310 | A1226  | G1149 | A | G1025 | C951 | A879 | U807 |
|       |       | G1758 | C1638 | C1547  |       | A1395  | G1311 | G1227  | C1150 | A | U1026 | A953 | A880 | U808 |
|       | A1847 | A1762 | C1639 | C1557  | C1474 | U1396  | U1312 | G1228  |       | G | A1027 | A953 | A881 | G809 |
| A1848 | G1763 | G1640 | C1640 | C1558  | G1475 | G1400  | U1313 | G1229  | G1153 | G | A1028 |      | A882 | U810 |
| A1853 | G1764 | A1641 | A1641 | A1558  |       | G1401  | C1314 | C1230  | G1154 | U | A1029 |      | A883 | U811 |
|       |       | G1642 | G1642 | G1559  | G1479 |        | C1315 | G1231  | A1155 | C | G1030 |      | A884 | C812 |
|       |       |       |       | G1560  |       |        | C1318 | G1232  |       | C | A1031 |      | A885 | U813 |
|       | G1877 | G1772 | G1645 | A1566  |       |        | G1319 | C1233  | G1160 | G | A1032 |      | A886 |      |
| G1857 | A1773 | A1773 | C1646 | A1561  | G1482 | C1404  | G1320 | U1234  | G1161 | U | U1033 |      | A887 | C817 |
| G1858 | C1774 | G1484 | G1646 | A1562  | G1485 | U1405  | G1321 | G1235  | G1162 | A |       |      | A888 | C818 |
|       | U1775 | G1485 | G1647 | G1563  | U1406 | U1407  | G1324 | G1236  |       | U |       |      | A889 | A819 |
| A1877 | G1776 | A1486 | G1648 |        |       |        |       | A1237  | C1166 | A |       |      | A890 | A820 |
| G1878 | U1777 | G1487 | G1649 | A1566  |       |        |       | G1238  | U1167 | A |       |      | A891 | A821 |
|       | U1778 |       | G1650 |        |       |        | C1327 | G1239  | G1168 |   |       |      | A892 |      |
| C1882 | U1779 | A1490 | G1651 | A1569  | G1411 | G1411  | G1328 | U1240  | G1169 | G |       |      | A893 | A824 |
| G1883 | A1780 | A1491 | A1652 |        | A1412 | A1412  | U1329 | U1241  | G1170 | C | G1040 |      | A894 |      |
|       | G1781 | C1493 | G1653 | A1572  | G1413 | G1413  | C1330 | A1242  | C1171 | U | G1041 |      | A895 | U827 |
| A1889 | C1782 | A1494 | A1654 |        |       |        | A1331 | G1243  | A     | A | C1043 |      | A896 | U828 |
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| A1900 |       |       | C1579 | U1579  | U1420 | U1420  | G1339 | A1253  | C1178 | U |       |      | A901 | U833 |
|       |       |       | A1580 | C1501  | G1421 | G1421  |       | A1254  |       | C |       |      | A902 | C834 |
| C2002 |       |       | G1581 | C1502  | G1422 | G1422  |       | U1255  |       | G |       |      | A903 | A835 |
|       |       |       | A1582 | U1503  |       |        | A1342 | G1256  |       | A |       |      | A904 |      |
| C2006 |       |       | C1583 |        | A1427 | A1427  | G1343 | G1257  | G1181 | A |       |      |      |      |
|       |       |       | A1584 | A1507  | C1428 | C1428  | G1344 | A1264  | G1182 | C |       |      |      | U839 |
| G2010 | G1912 | C1795 | C1585 | A1508  | G1429 | G1429  | C1345 | A1265  | G1186 | C |       |      | A910 | C840 |
| U2011 | U1913 | U1796 | A1587 | C1509  | C1430 | C1430  | G1346 | G1266  | G1187 | A |       |      | A911 | A841 |
| G2012 | C1914 |       | C1588 | A1509A | U1431 | U1431  | U1352 | U1267  | U1188 | G |       |      | A912 |      |
| A2013 | U1798 |       | C1589 | A1509B | C1432 | C1432  | A1353 | A1268  | A1189 | A |       |      | A913 | G845 |
| A2014 | G1799 |       | U1590 | G1510  | A1434 | A1434  | A1354 | A1269  | G1190 | G |       |      | A917 | C846 |
|       |       |       | G1591 | C1511  | G1355 | G1355  | G1356 | G1271  | G1191 | U |       |      | A918 | U847 |
| A2019 | C1800 |       | C1592 | U1512  | G1436 | G1436  | U1357 | A1272  | G1197 | U |       |      | A919 | A849 |
| G1921 | G1801 |       | C1593 | C1513  | C1437 | C1437  | G1358 | U1273  | U1198 | G |       |      | A920 |      |
| G1922 | A1802 |       | G1594 | G1514  |       |        | A1359 | U1278  | U1199 | G |       |      | A921 | G852 |
| U1923 | A1803 |       |       | G1515  | G1441 | G1441  | A1360 | A1278  | C1200 | C |       |      | A922 | G853 |
|       |       |       | C1600 | C1516  | G1442 | G1442  |       |        | C1201 | A |       |      | A923 | G854 |
| A1927 | U1805 |       | A1603 | U1517  | A1445 | A1445  | G1364 | A1284  | C1202 | U |       |      | A924 | G855 |
| G1928 | A1810 |       | C1607 | G1519  |       |        | A1365 | G1285  | G1203 | U |       |      | A925 | C856 |
| G1929 | A1811 |       | A1608 |        | G1525 |        | A1366 | A1286  | A1204 | A |       |      | A926 | C857 |
| U1931 | A1812 |       | A1609 |        |       |        | A1367 | A1287  | U1205 | G |       |      | A927 | U858 |
| A1932 | G1813 |       | G1703 |        |       |        | G1368 | U1288  | G1206 | A |       |      | A928 | G859 |
| G1933 | G1814 |       |       |        |       |        | G1369 |        | C1207 | A |       |      |      |      |
|       | A1815 |       |       |        |       |        | C1370 | U1292  | C1208 | G |       |      | A932 | A861 |
| A1936 | G1816 |       | C1711 | C1611  | C1530 | C1450A | G1371 | C1293  | G1136 | C |       |      | A933 | G862 |
| A1937 | G1817 |       | U1712 | A1616  | C1531 | C1451  | U1372 | C1294  | G1137 | A |       |      | A938 | G863 |
| A1938 | U1818 |       | G1713 |        | C1532 | A1452  | U1373 |        | G1138 | G |       |      | A939 | G864 |
|       |       |       | G1714 |        | G1533 | U1453  |       | C1297  | U1211 | C |       |      | A940 | C865 |
|       |       |       |       |        | U     |        | A1379 | U1300  | G1212 | C |       |      | A941 | A866 |
| G1941 | G1824 |       | G1721 | A1622  | A     | G1455  | G1380 | A1213  | A1213 | U |       |      | A942 | U868 |
| C1942 |       |       | A1722 | C1625  | C1536 | G1459  | A1381 |        | U1141 | A |       |      | A943 | G869 |
| U1946 | C1827 |       | G1626 | G1537  | A1460 |        | G1382 | G1219  | U1142 | C |       |      | A944 | A870 |
| C1947 | A1828 |       | G1627 | G1538  | G1461 |        | A1384 | A1220  | A1143 | U |       |      | A945 |      |
|       | G1740 |       | G1628 | G1539  | C1462 |        | G1385 | G1221  | G1144 | C |       |      | A946 |      |
| G2045 | C1830 |       | U1629 | U1540  | C1467 |        | C1386 | C1221A |       | U |       |      | A947 |      |
| G2046 |       |       |       | G1541  | C1467 |        | C1387 |        |       | U |       |      | A948 |      |
|       |       |       |       | A1632  | C1468 |        | G1388 | A1308  |       | A |       |      |      |      |
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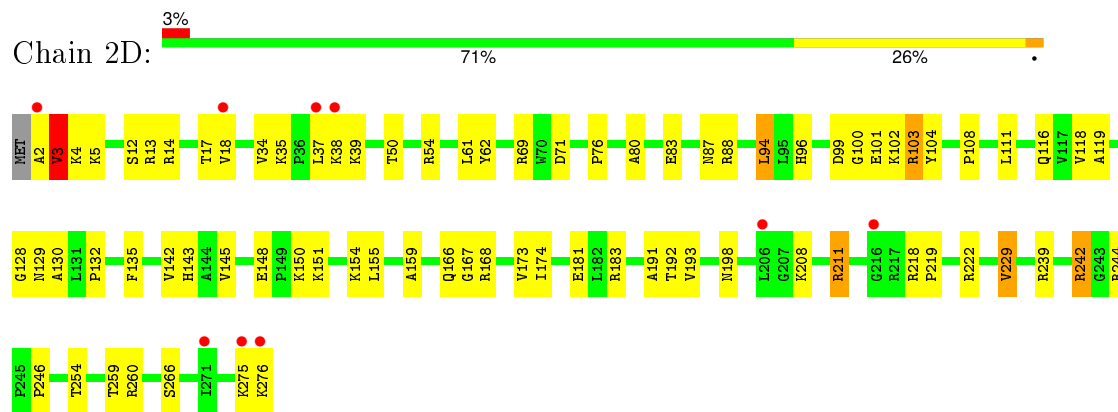




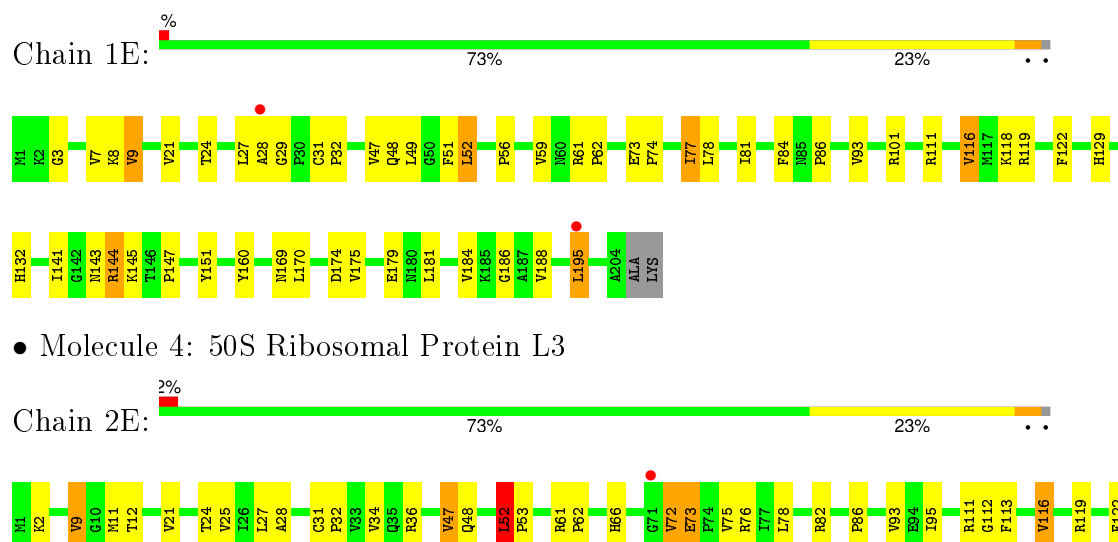
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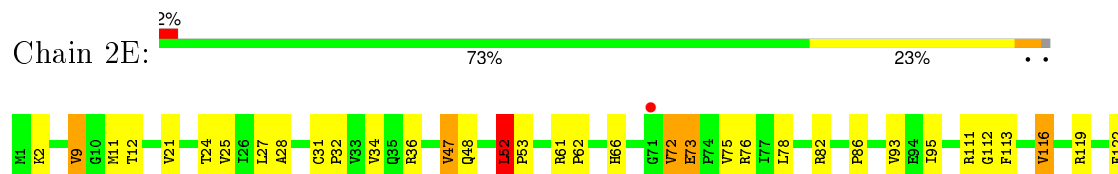
• Molecule 3: 50S Ribosomal Protein L2



• Molecule 4: 50S Ribosomal Protein L3

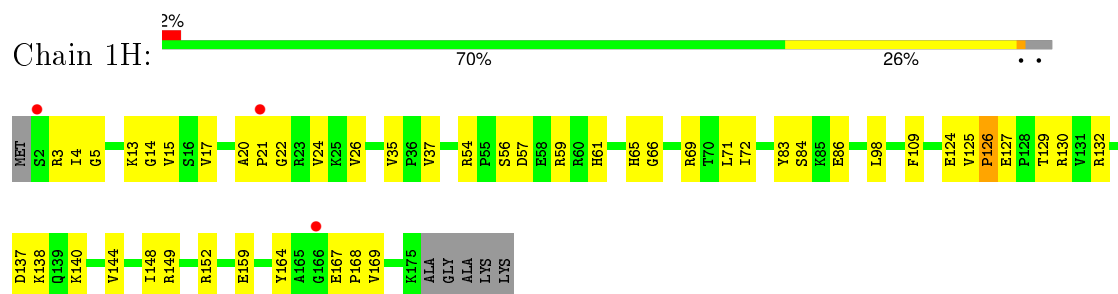


• Molecule 4: 50S Ribosomal Protein L3

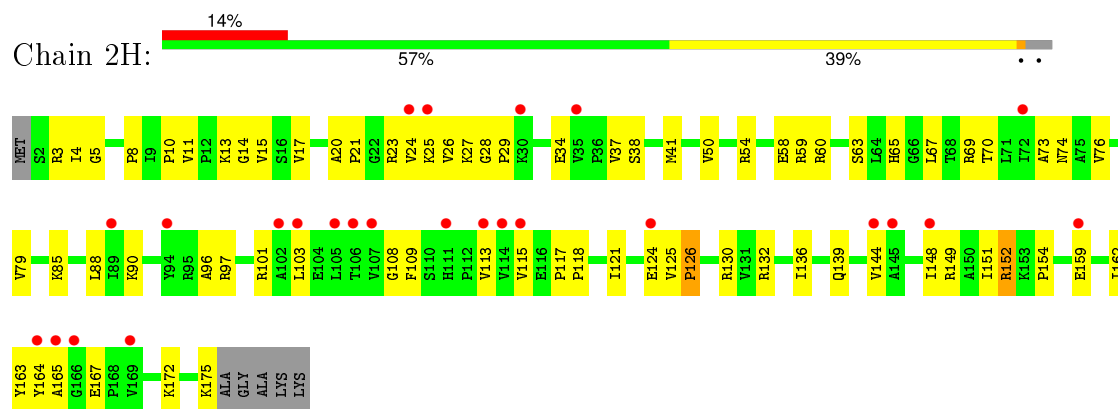




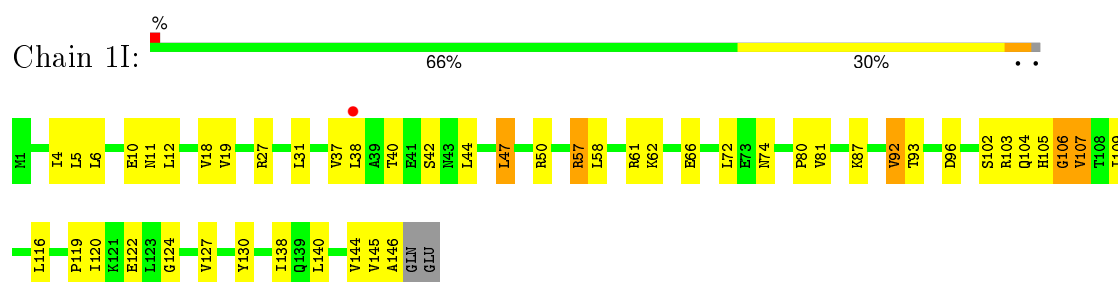
- Molecule 7: 50S Ribosomal Protein L6



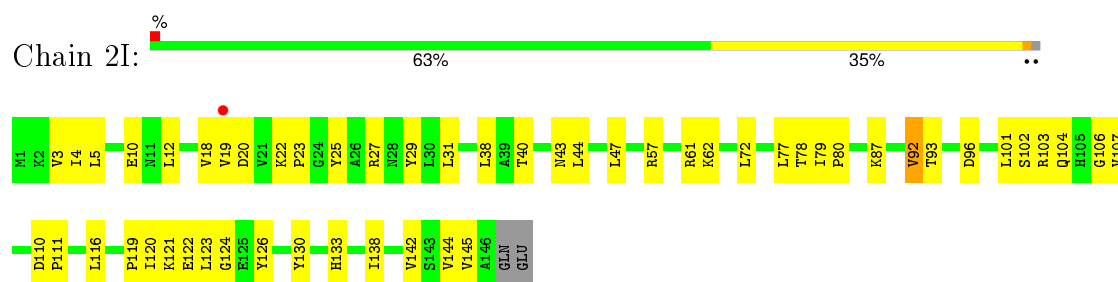
- Molecule 7: 50S Ribosomal Protein L6



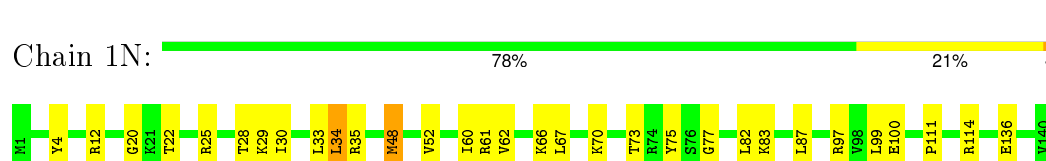
- Molecule 8: 50S Ribosomal Protein L9



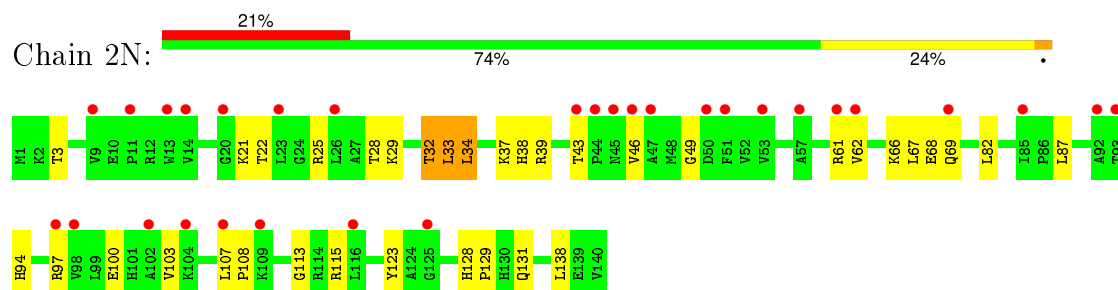
- Molecule 8: 50S Ribosomal Protein L9



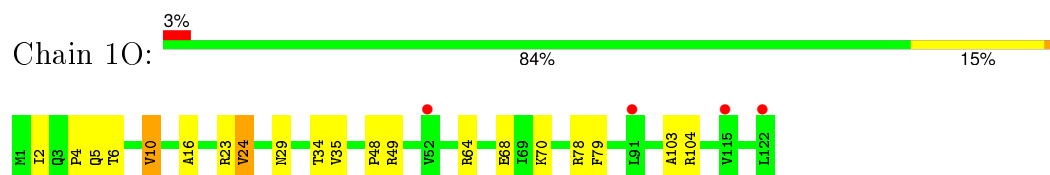
- Molecule 9: 50S Ribosomal Protein L13



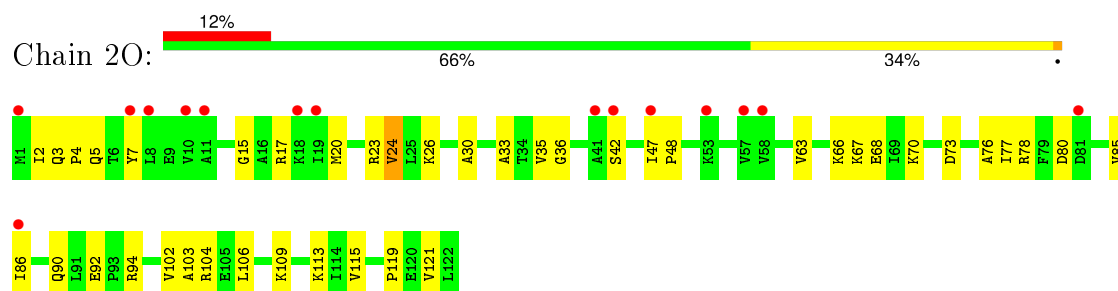
- Molecule 9: 50S Ribosomal Protein L13



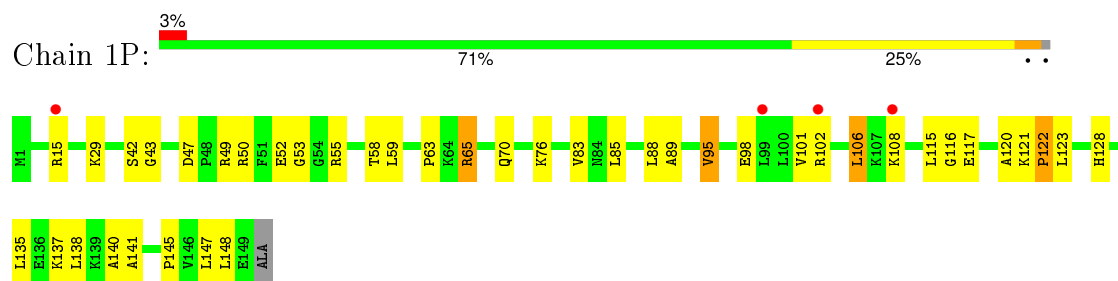
- Molecule 10: 50S Ribosomal Protein L14



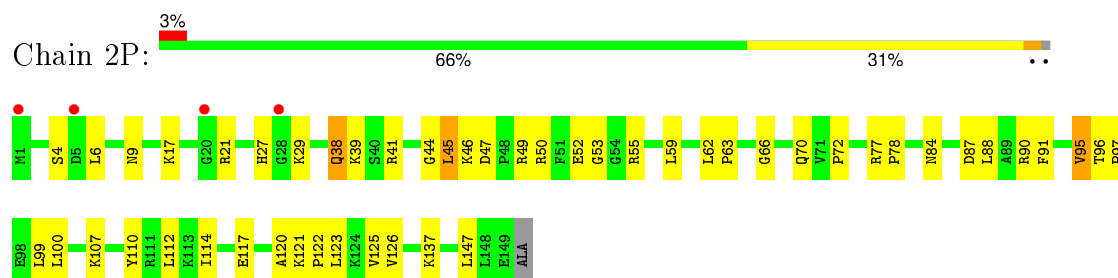
- Molecule 10: 50S Ribosomal Protein L14



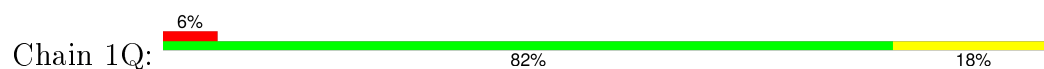
- Molecule 11: 50S Ribosomal Protein L15



- Molecule 11: 50S Ribosomal Protein L15

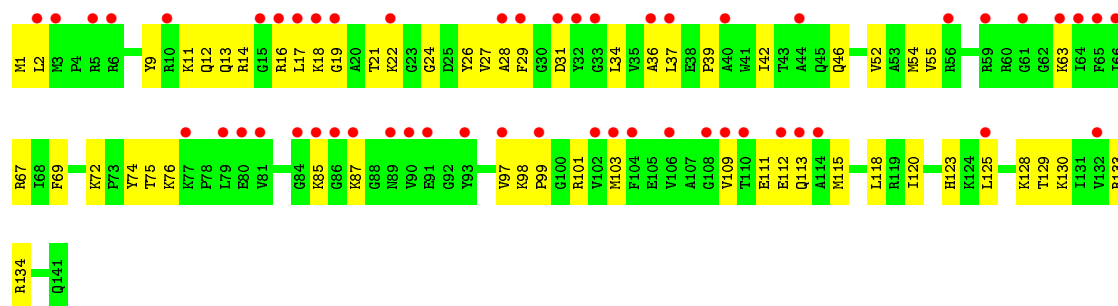
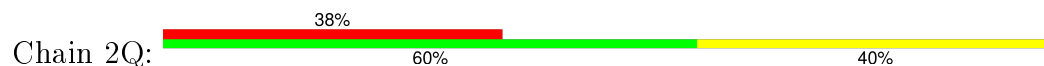


- Molecule 12: 50S Ribosomal Protein L16

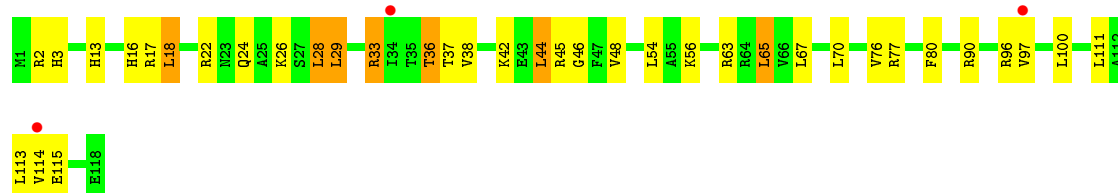




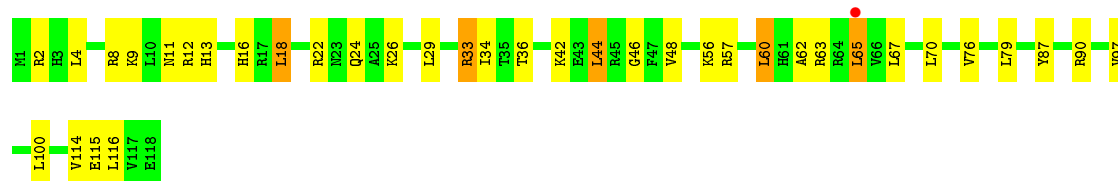
• Molecule 12: 50S Ribosomal Protein L16



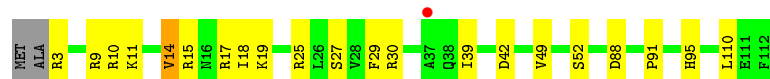
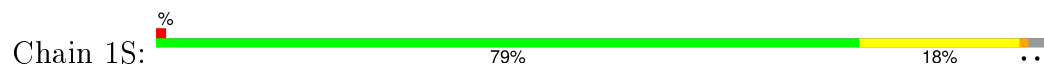
• Molecule 13: 50S Ribosomal Protein L17



• Molecule 13: 50S Ribosomal Protein L17

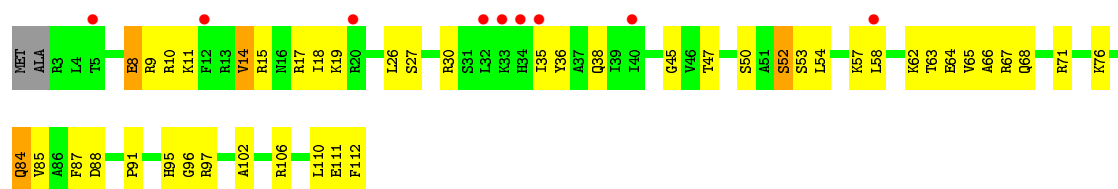


• Molecule 14: 50S Ribosomal Protein L18

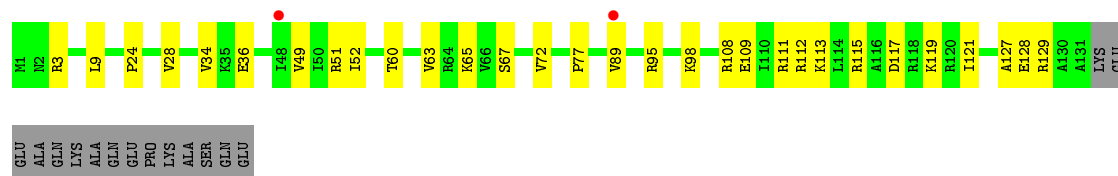


• Molecule 14: 50S Ribosomal Protein L18

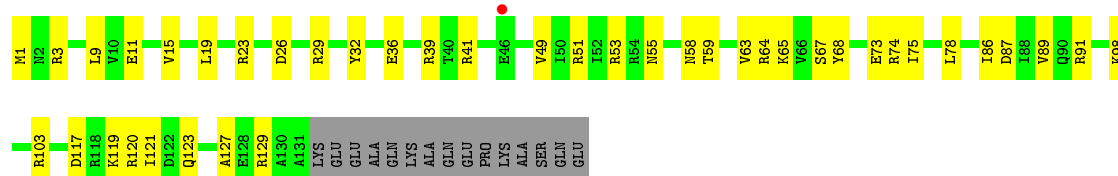




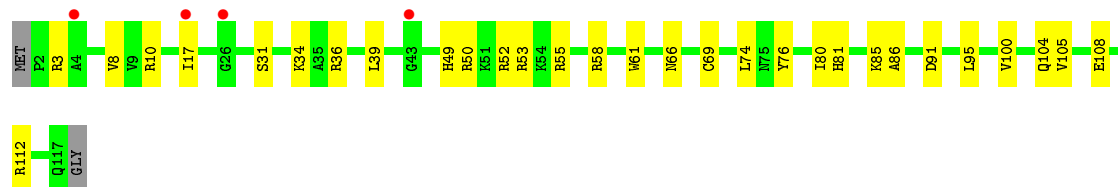
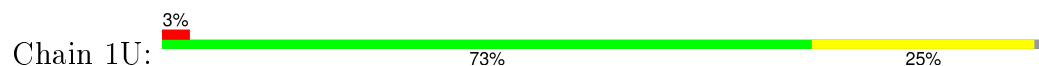
• Molecule 15: 50S Ribosomal Protein L19



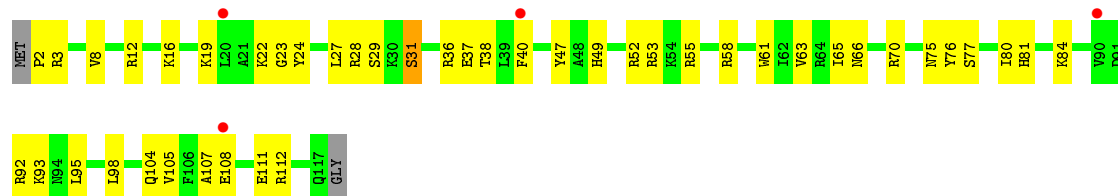
• Molecule 15: 50S Ribosomal Protein L19



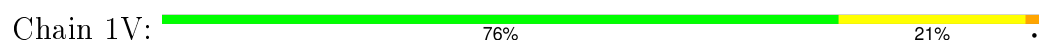
• Molecule 16: 50S Ribosomal Protein L20



• Molecule 16: 50S Ribosomal Protein L20

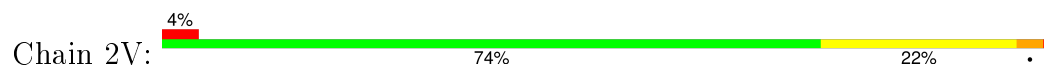


• Molecule 17: 50S Ribosomal Protein L21

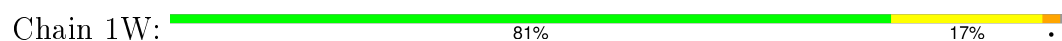




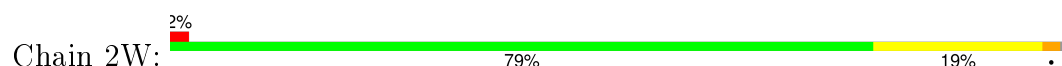
- Molecule 17: 50S Ribosomal Protein L21



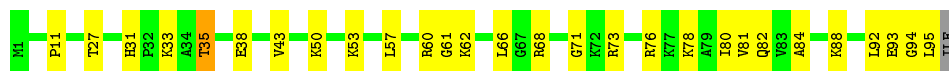
- Molecule 18: 50S Ribosomal Protein L22



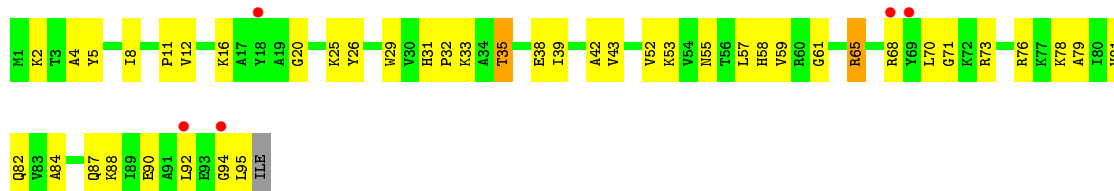
- Molecule 18: 50S Ribosomal Protein L22



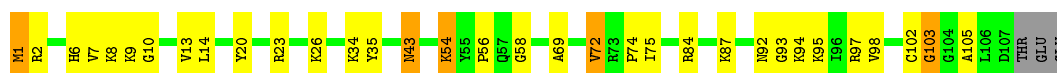
- Molecule 19: 50S Ribosomal Protein L23



- Molecule 19: 50S Ribosomal Protein L23

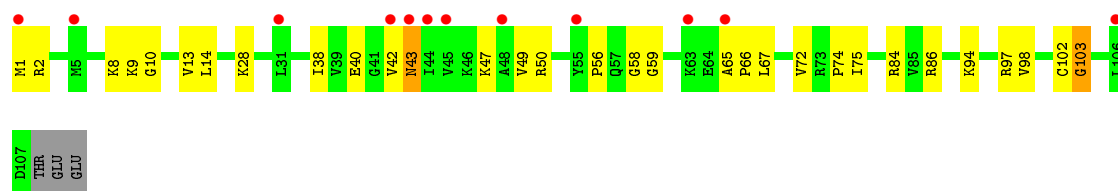


- Molecule 20: 50S Ribosomal Protein L24

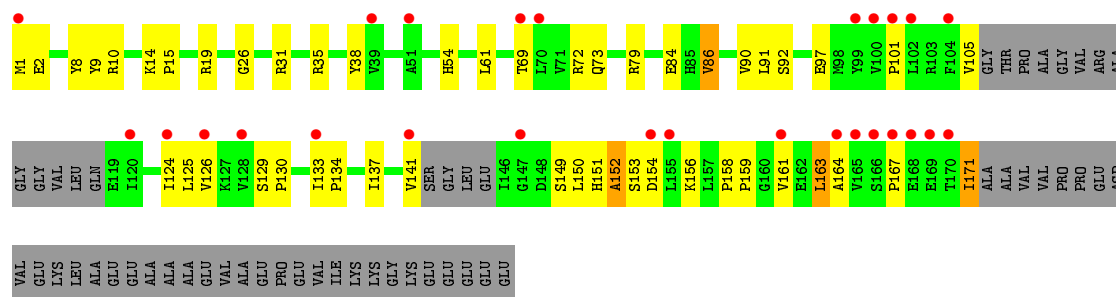


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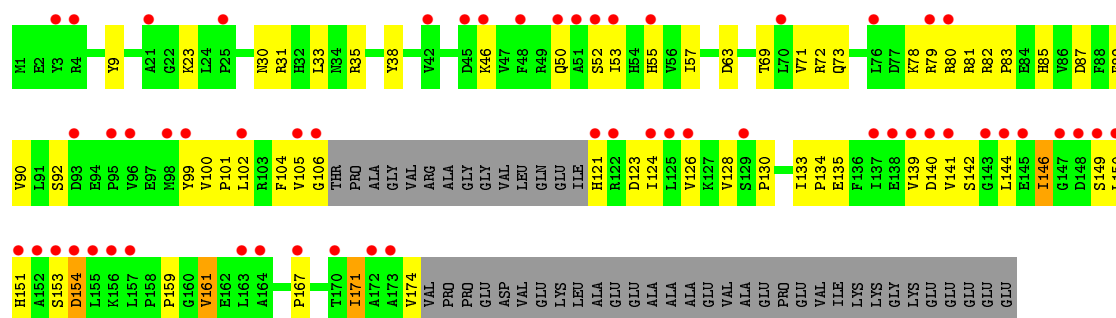




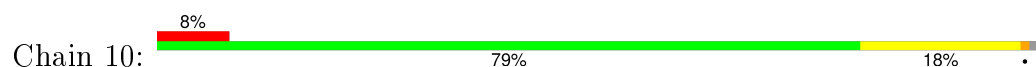
• Molecule 21: 50S Ribosomal Protein L25



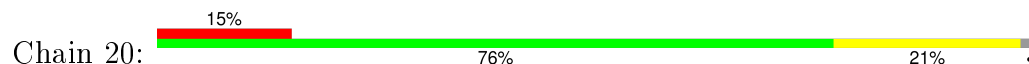
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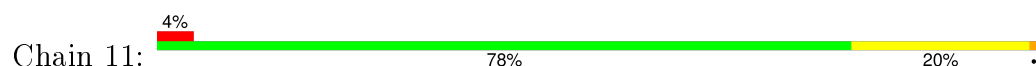
• Molecule 22: 50S Ribosomal Protein L27



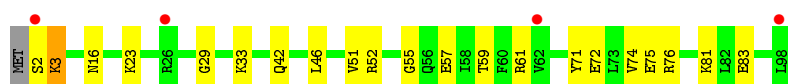
• Molecule 22: 50S Ribosomal Protein L27



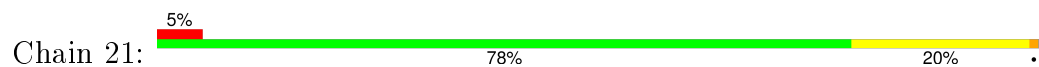
• Molecule 23: 50S Ribosomal Protein L28



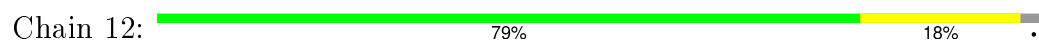




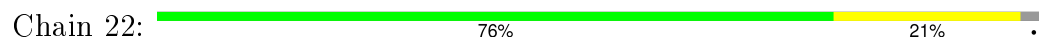
• Molecule 23: 50S Ribosomal Protein L28



• Molecule 24: 50S Ribosomal Protein L29



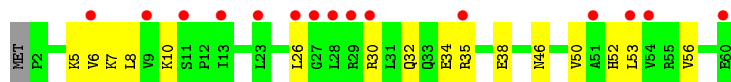
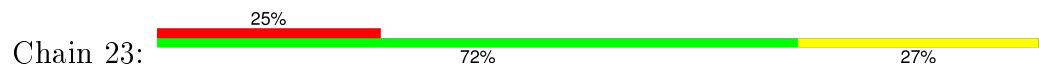
• Molecule 24: 50S Ribosomal Protein L29



• Molecule 25: 50S Ribosomal Protein L30



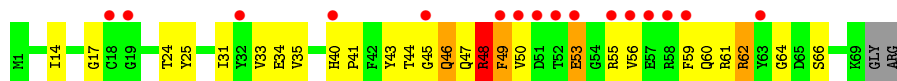
• Molecule 25: 50S Ribosomal Protein L30



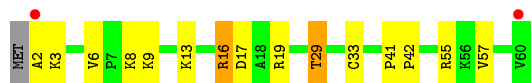
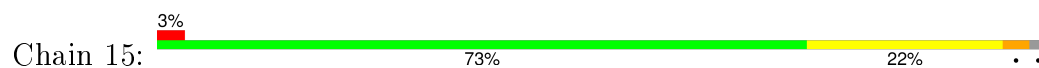
• Molecule 26: 50S Ribosomal Protein L31



• Molecule 26: 50S Ribosomal Protein L31



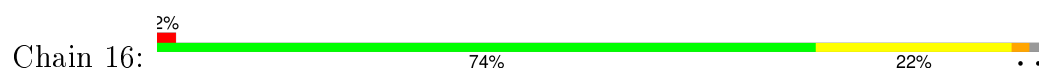
- Molecule 27: 50S Ribosomal Protein L32



- Molecule 27: 50S Ribosomal Protein L32



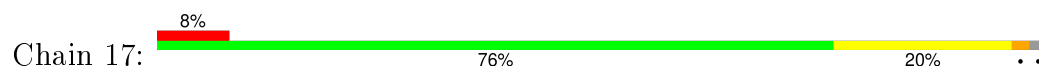
- Molecule 28: 50S Ribosomal Protein L33



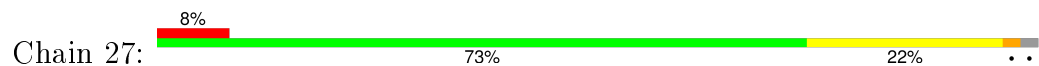
- Molecule 28: 50S Ribosomal Protein L33



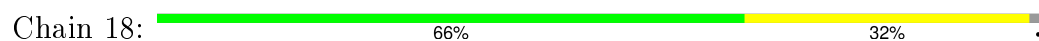
- Molecule 29: 50S Ribosomal Protein L34



- Molecule 29: 50S Ribosomal Protein L34

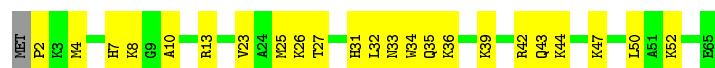


- Molecule 30: 50S Ribosomal Protein L35




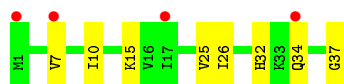
- Molecule 30: 50S Ribosomal Protein L35

Chain 28:  63% 35%



- Molecule 31: 50S Ribosomal Protein L36

Chain 19:  11% 78% 22%




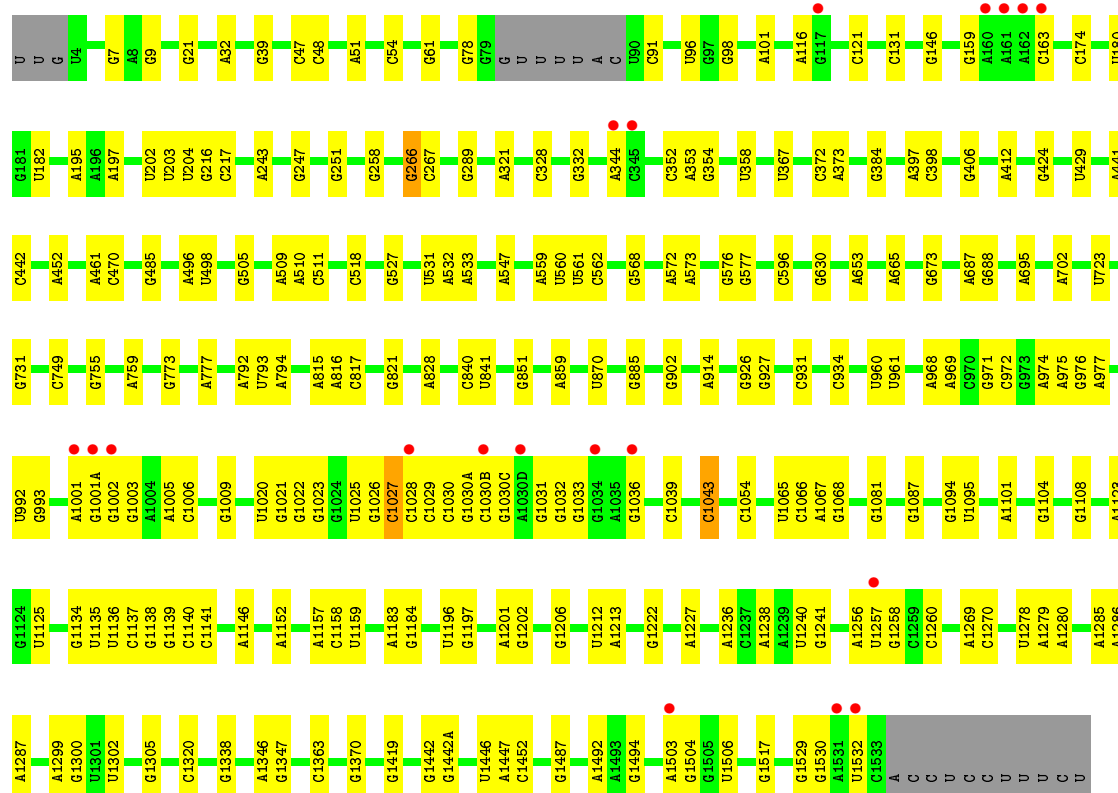
- Molecule 31: 50S Ribosomal Protein L36

Chain 29:  30% 57% 41%




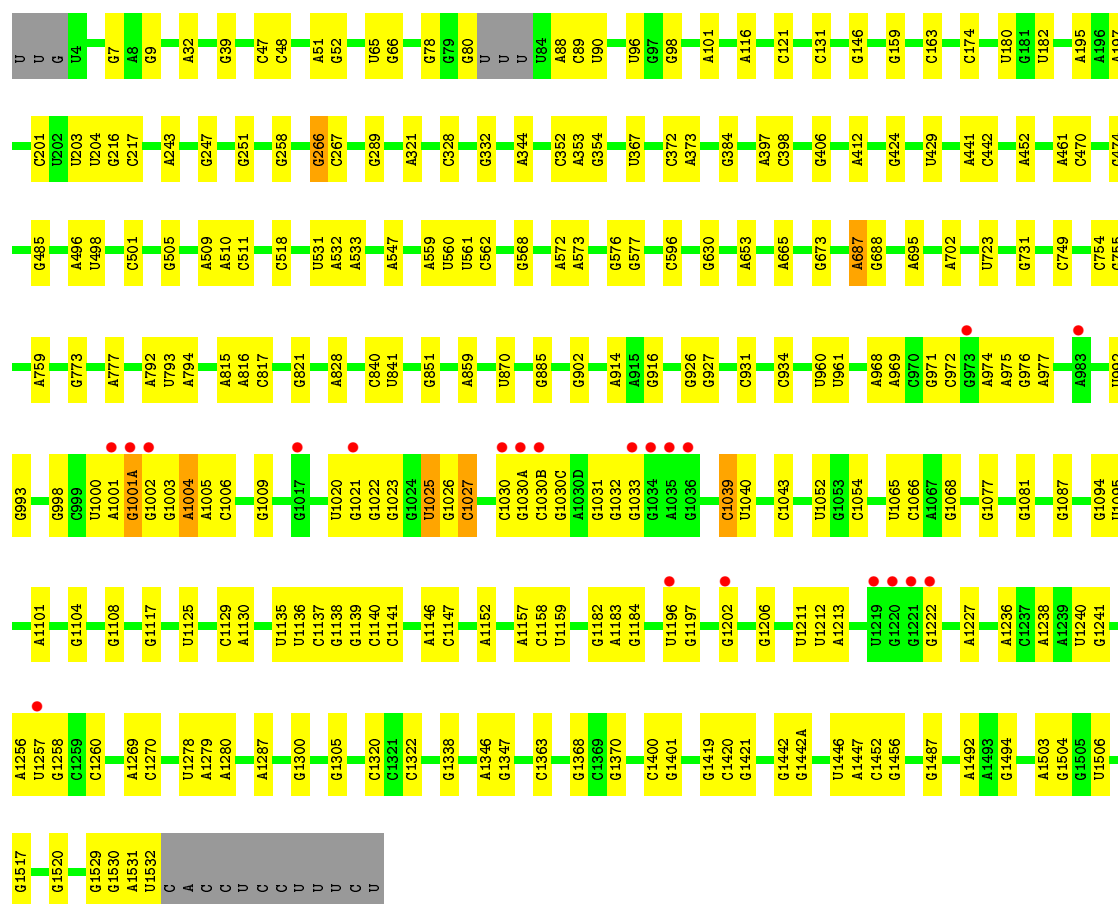
- Molecule 32: 16S Ribosomal RNA

Chain 1a:  %



- Molecule 32: 16S Ribosomal RNA

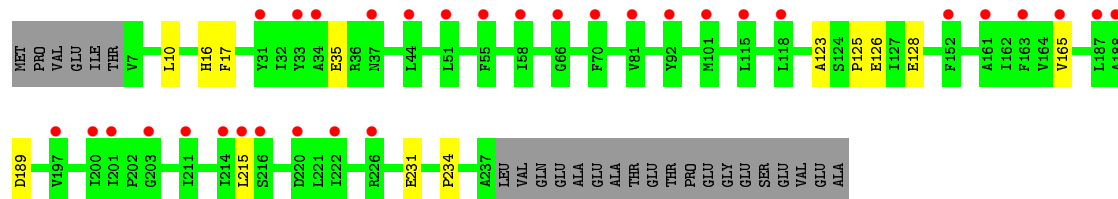
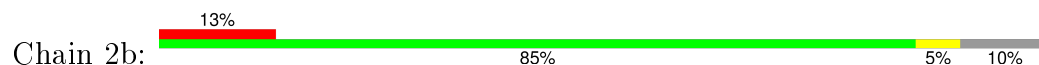
Chain 2a:  82% 16%



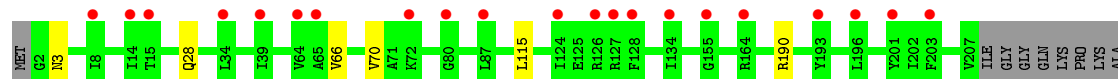
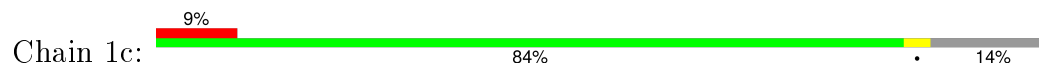
• Molecule 33: 30S Ribosomal Protein S2



• Molecule 33: 30S Ribosomal Protein S2

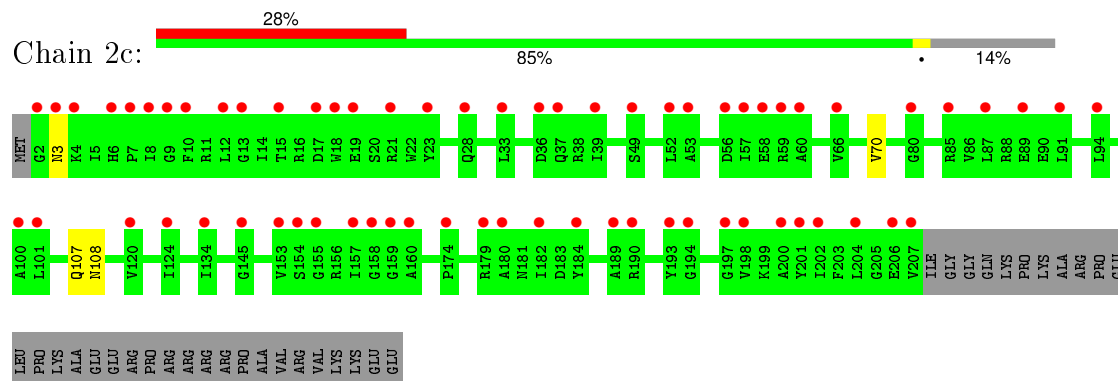


• Molecule 34: 30S Ribosomal Protein S3

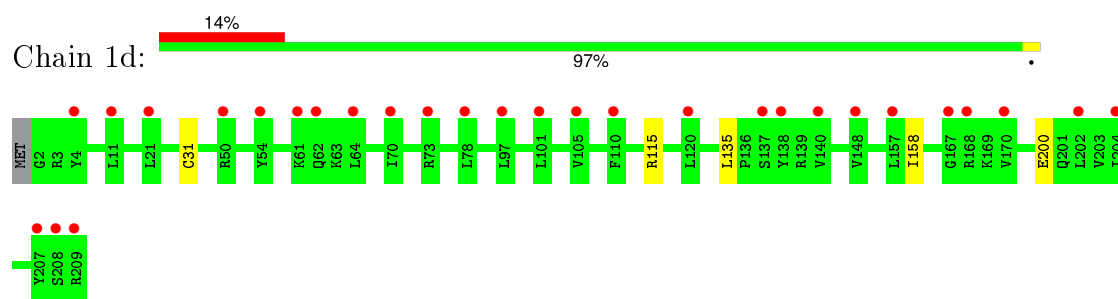


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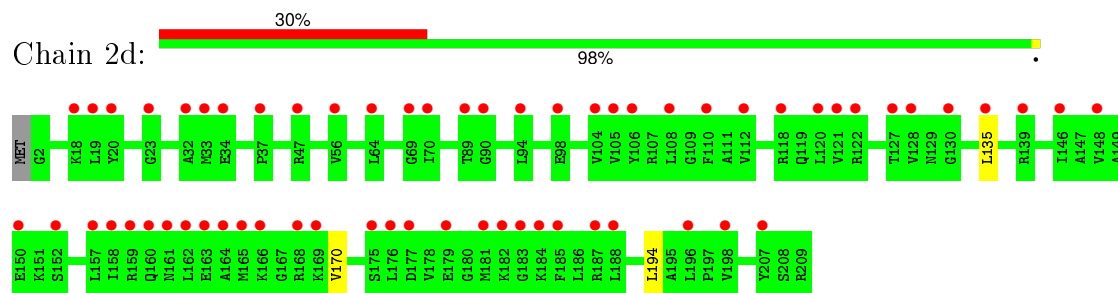
• Molecule 34: 30S Ribosomal Protein S3



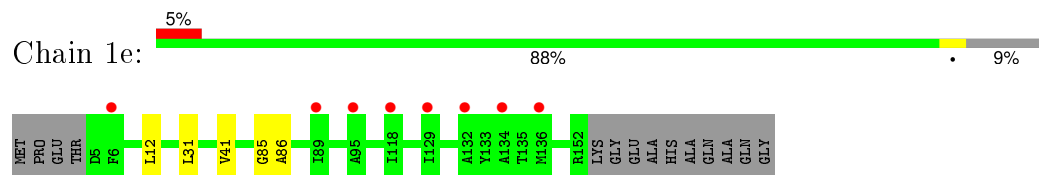
• Molecule 35: 30S Ribosomal Protein S4



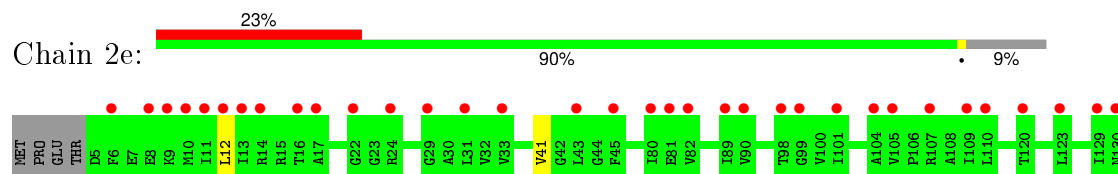
• Molecule 35: 30S Ribosomal Protein S4

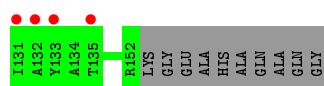


• Molecule 36: 30S Ribosomal Protein S5

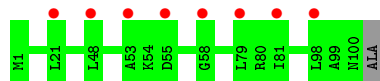


• Molecule 36: 30S Ribosomal Protein S5

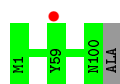




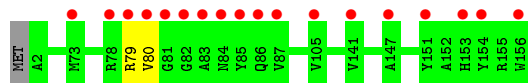
• Molecule 37: 30S Ribosomal Protein S6



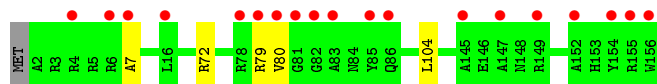
• Molecule 37: 30S Ribosomal Protein S6



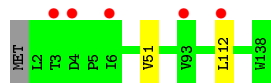
• Molecule 38: 30S Ribosomal Protein S7



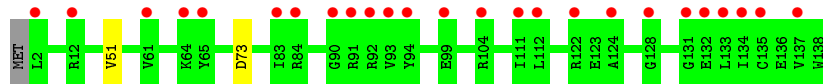
• Molecule 38: 30S Ribosomal Protein S7



• Molecule 39: 30S Ribosomal Protein S8

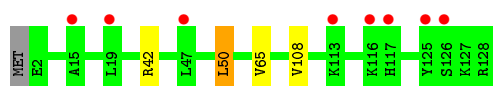


• Molecule 39: 30S Ribosomal Protein S8



• Molecule 40: 30S Ribosomal Protein S9

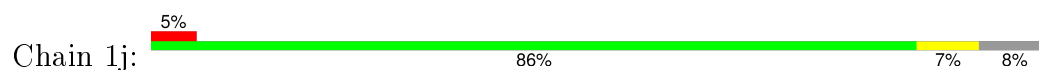




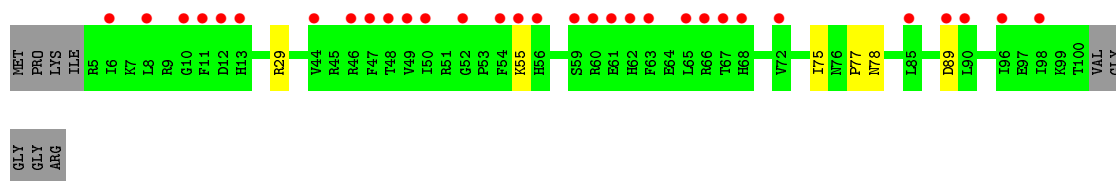
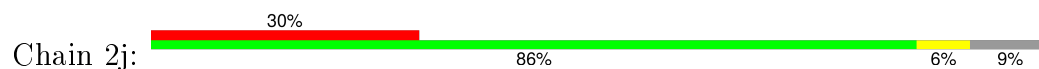
- Molecule 40: 30S Ribosomal Protein S9



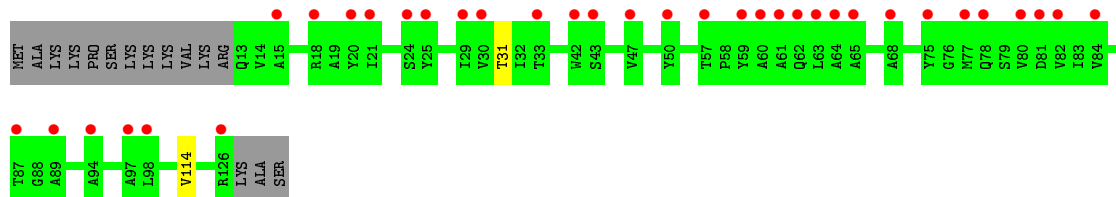
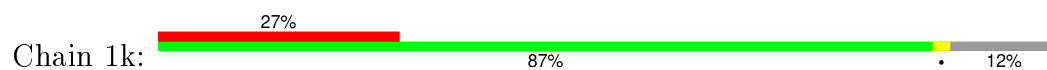
- Molecule 41: 30S Ribosomal Protein S10



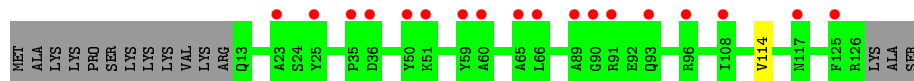
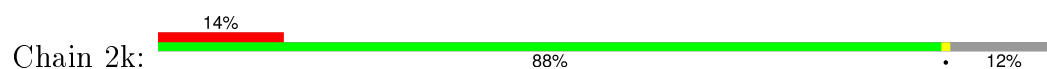
- Molecule 41: 30S Ribosomal Protein S10



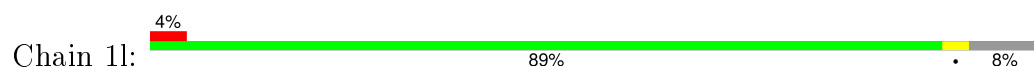
- Molecule 42: 30S Ribosomal Protein S11

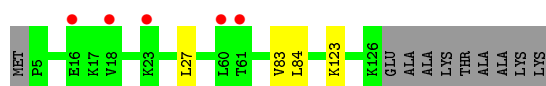


- Molecule 42: 30S Ribosomal Protein S11

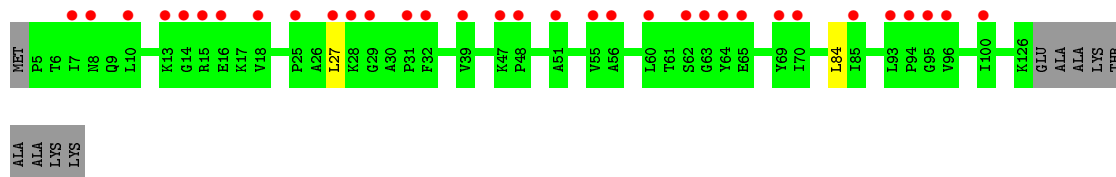
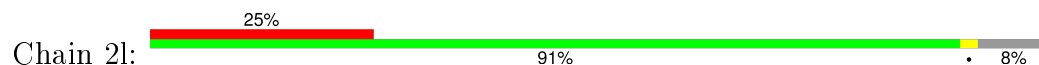


- Molecule 43: 30S Ribosomal Protein S12

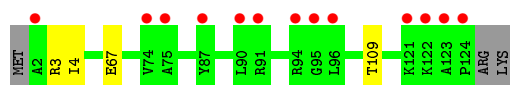




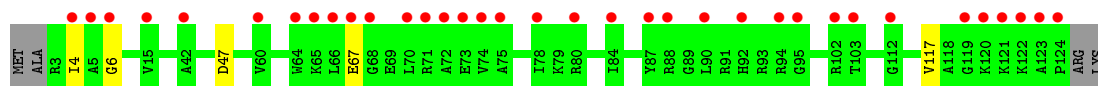
- Molecule 43: 30S Ribosomal Protein S12



- Molecule 44: 30S Ribosomal Protein S13



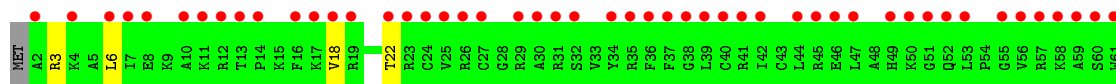
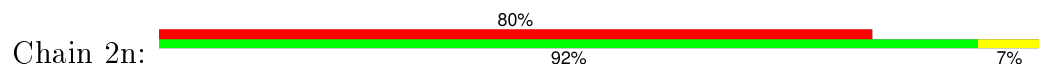
- Molecule 44: 30S Ribosomal Protein S13



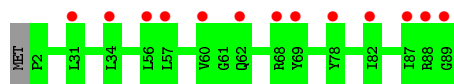
- Molecule 45: 30S Ribosomal Protein S14



- Molecule 45: 30S Ribosomal Protein S14

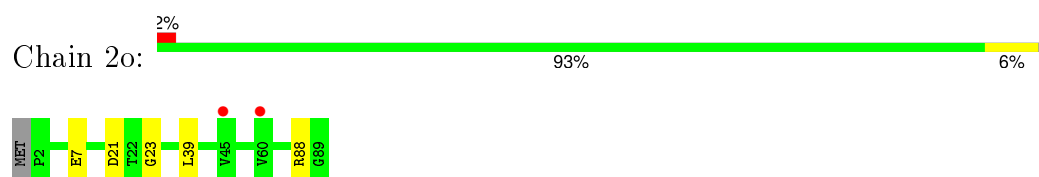


- Molecule 46: 30S Ribosomal Protein S15

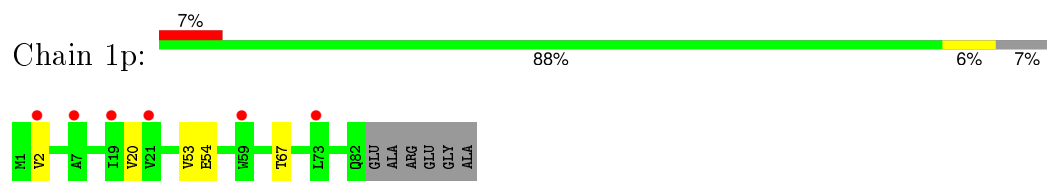


- Molecule 46: 30S Ribosomal Protein S15

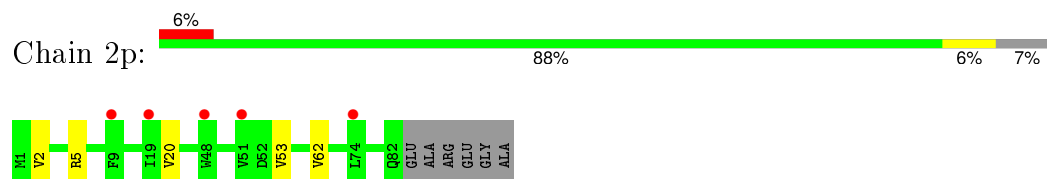




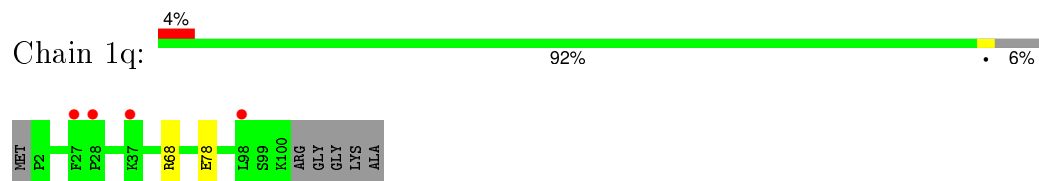
- Molecule 47: 30S Ribosomal Protein S16



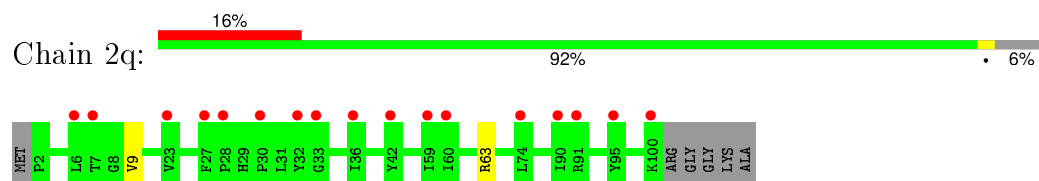
- Molecule 47: 30S Ribosomal Protein S16



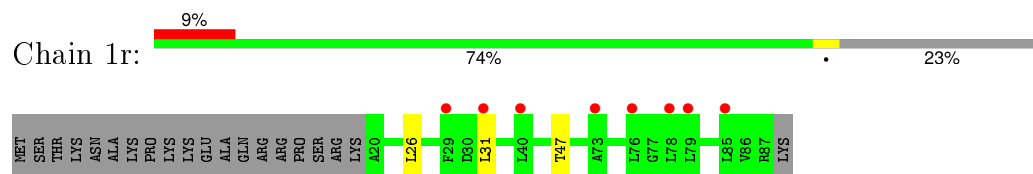
- Molecule 48: 30S Ribosomal Protein S17



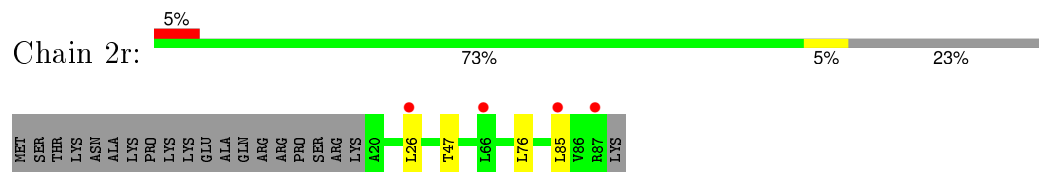
- Molecule 48: 30S Ribosomal Protein S17



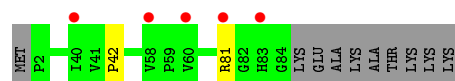
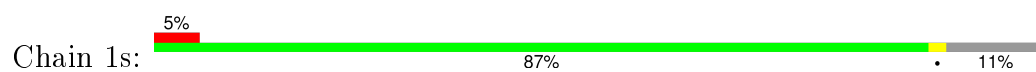
- Molecule 49: 30S Ribosomal Protein S18



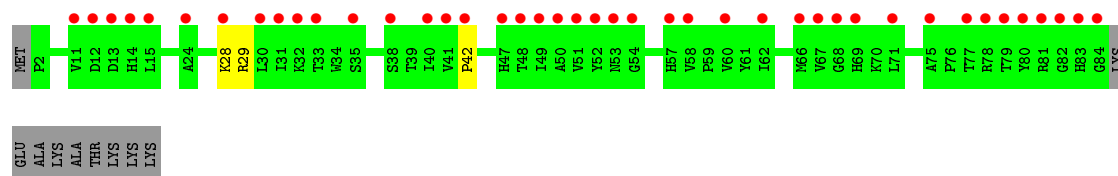
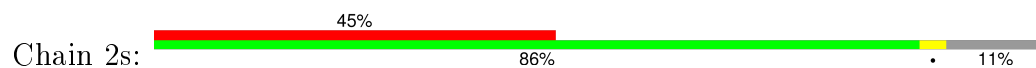
- Molecule 49: 30S Ribosomal Protein S18



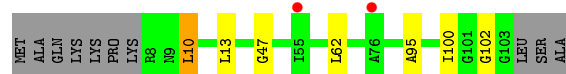
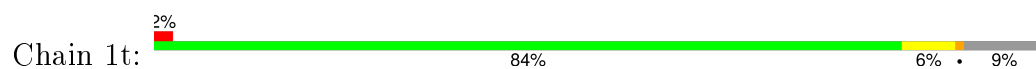
- Molecule 50: 30S Ribosomal Protein S19



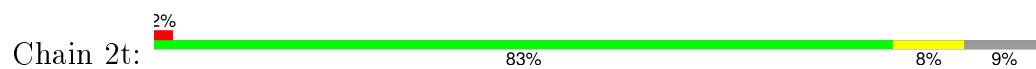
• Molecule 50: 30S Ribosomal Protein S19



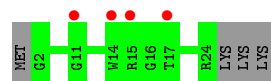
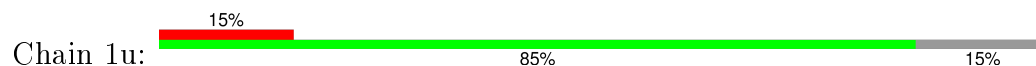
• Molecule 51: 30S Ribosomal Protein S20



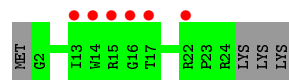
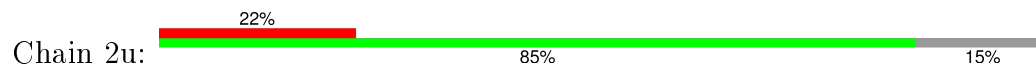
• Molecule 51: 30S Ribosomal Protein S20



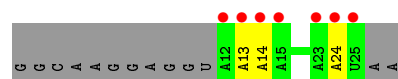
• Molecule 52: 30S Ribosomal Protein THX



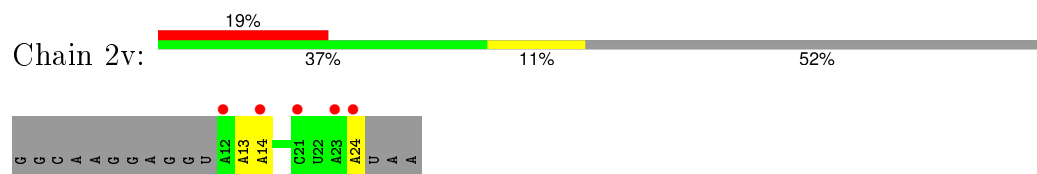
• Molecule 52: 30S Ribosomal Protein THX



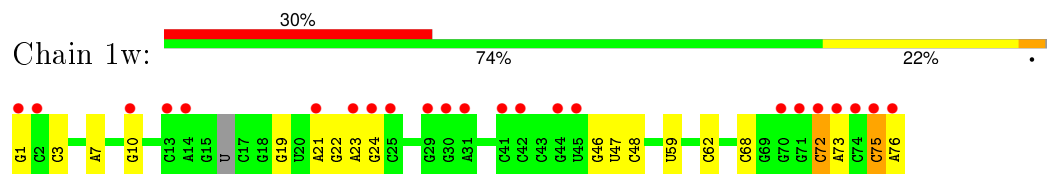
• Molecule 53: mRNA



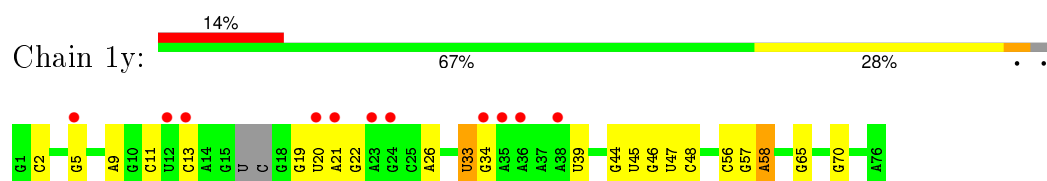
- Molecule 53: mRNA



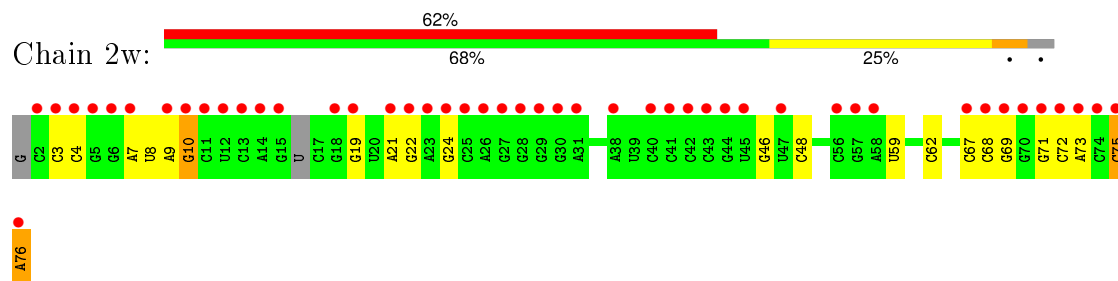
- Molecule 54: A-site and E-site tRNAs



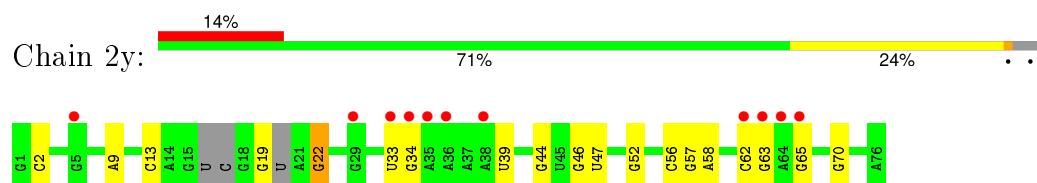
- Molecule 54: A-site and E-site tRNAs



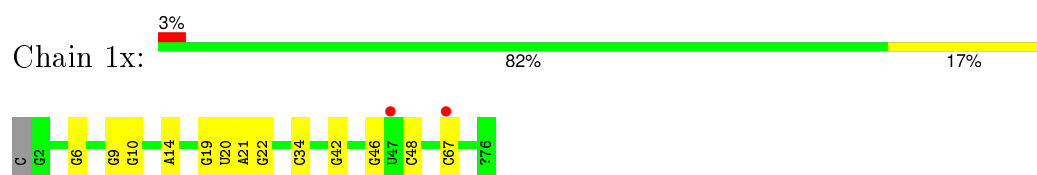
- Molecule 54: A-site and E-site tRNAs



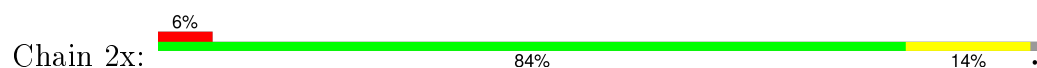
- Molecule 54: A-site and E-site tRNAs



- Molecule 55: P-site tRNA



- Molecule 55: P-site tRNA





## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 21 21 21  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 208.39Å 444.58Å 619.20Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)  | 361.14 – 2.60<br>361.14 – 2.60                              | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.3 (361.14-2.60)<br>99.3 (361.14-2.60)                    | Depositor<br>EDS |
| $R_{merge}$   | 0.19  | Depositor        |
| $R_{sym}$   | (Not available)   | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.29 (at 2.62Å)   | Xtriage          |
| Refinement program  | PHENIX  | Depositor        |
| R, $R_{free}$   | 0.233 , 0.283<br>0.244 , 0.291                              | Depositor<br>DCC |
| $R_{free}$ test set   | 86608 reflections (5.29%)                                   | DCC              |
| Wilson B-factor (Å <sup>2</sup> )                                       | 51.7  | Xtriage          |
| Anisotropy  | 0.120   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.28 , 61.4   | EDS              |
| Estimated twinning fraction   | No twinning to report.                                      | Xtriage          |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.37$ , $\langle L^2 \rangle = 0.19$ | Xtriage          |
| Outliers  | 0 of 1724935 reflections                                    | Xtriage          |
| $F_o, F_c$ correlation  | 0.89  | EDS              |
| Total number of atoms   | 298925  | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 58.0  | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.63% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: 5MU, ZN, 4SU, OMG, 2MU, MIA, SF4, 0TD, HGR, MG, M3O, 2MA, 2MG, 5MC, UR3, MA6, 4OC, M2G, 7MG, K, PSU

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

| Mol | Chain | Bond lengths |               | Bond angles |                  |
|-----|-------|--------------|---------------|-------------|------------------|
|     |       | RMSZ         | # Z  >5       | RMSZ        | # Z  >5          |
| 1   | 1A    | 0.52         | 0/69009       | 0.95        | 67/107712 (0.1%) |
| 1   | 2A    | 0.43         | 0/67293       | 0.93        | 46/105034 (0.0%) |
| 2   | 1B    | 0.46         | 1/2882 (0.0%) | 0.85        | 0/4494           |
| 2   | 2B    | 0.49         | 1/2879 (0.0%) | 0.93        | 2/4487 (0.0%)    |
| 3   | 1D    | 0.38         | 0/2186        | 0.59        | 0/2944           |
| 3   | 2D    | 0.34         | 0/2186        | 0.59        | 0/2944           |
| 4   | 1E    | 0.37         | 0/1592        | 0.57        | 0/2149           |
| 4   | 2E    | 0.33         | 0/1592        | 0.56        | 1/2149 (0.0%)    |
| 5   | 1F    | 0.36         | 0/1619        | 0.55        | 0/2193           |
| 5   | 2F    | 0.33         | 0/1615        | 0.56        | 0/2188           |
| 6   | 1G    | 0.32         | 0/1454        | 0.53        | 0/1964           |
| 6   | 2G    | 0.31         | 0/1453        | 0.56        | 0/1963           |
| 7   | 1H    | 0.33         | 0/1356        | 0.52        | 0/1834           |
| 7   | 2H    | 0.29         | 0/1356        | 0.52        | 0/1834           |
| 8   | 1I    | 0.29         | 0/1112        | 0.54        | 0/1514           |
| 8   | 2I    | 0.28         | 0/1079        | 0.54        | 0/1475           |
| 9   | 1N    | 0.34         | 0/1144        | 0.55        | 0/1543           |
| 9   | 2N    | 0.28         | 0/1144        | 0.53        | 0/1543           |
| 10  | 1O    | 0.37         | 0/943         | 0.55        | 0/1269           |
| 10  | 2O    | 0.33         | 0/943         | 0.52        | 0/1269           |
| 11  | 1P    | 0.35         | 0/1152        | 0.55        | 0/1533           |
| 11  | 2P    | 0.32         | 0/1152        | 0.60        | 0/1533           |
| 12  | 1Q    | 0.39         | 0/1143        | 0.54        | 0/1527           |
| 12  | 2Q    | 0.33         | 0/1143        | 0.58        | 0/1527           |
| 13  | 1R    | 0.37         | 0/982         | 0.59        | 0/1312           |
| 13  | 2R    | 0.33         | 0/982         | 0.56        | 0/1312           |
| 14  | 1S    | 0.32         | 0/883         | 0.53        | 0/1176           |
| 14  | 2S    | 0.32         | 0/880         | 0.57        | 0/1172           |
| 15  | 1T    | 0.34         | 0/1105        | 0.52        | 0/1477           |
| 15  | 2T    | 0.31         | 0/1097        | 0.53        | 0/1468           |
| 16  | 1U    | 0.41         | 0/977         | 0.55        | 0/1301           |

| Mol | Chain | Bond lengths |         | Bond angles |                 |
|-----|-------|--------------|---------|-------------|-----------------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5         |
| 16  | 2U    | 0.34         | 0/977   | 0.53        | 0/1301          |
| 17  | 1V    | 0.39         | 0/782   | 0.54        | 0/1049          |
| 17  | 2V    | 0.33         | 0/782   | 0.53        | 0/1049          |
| 18  | 1W    | 0.40         | 0/897   | 0.56        | 0/1205          |
| 18  | 2W    | 0.34         | 0/897   | 0.52        | 0/1205          |
| 19  | 1X    | 0.41         | 0/764   | 0.59        | 0/1025          |
| 19  | 2X    | 0.34         | 0/764   | 0.53        | 0/1025          |
| 20  | 1Y    | 0.35         | 0/819   | 0.55        | 0/1095          |
| 20  | 2Y    | 0.32         | 0/819   | 0.55        | 0/1095          |
| 21  | 1Z    | 0.32         | 0/1267  | 0.54        | 0/1717          |
| 21  | 2Z    | 0.28         | 0/1299  | 0.53        | 0/1763          |
| 22  | 10    | 0.38         | 0/662   | 0.57        | 0/881           |
| 22  | 20    | 0.31         | 0/662   | 0.54        | 0/881           |
| 23  | 11    | 0.35         | 0/762   | 0.54        | 0/1014          |
| 23  | 21    | 0.32         | 0/762   | 0.53        | 0/1014          |
| 24  | 12    | 0.31         | 0/590   | 0.53        | 0/781           |
| 24  | 22    | 0.29         | 0/590   | 0.45        | 0/781           |
| 25  | 13    | 0.34         | 0/474   | 0.53        | 0/635           |
| 25  | 23    | 0.30         | 0/469   | 0.52        | 0/630           |
| 26  | 14    | 0.34         | 0/565   | 0.66        | 0/761           |
| 26  | 24    | 0.31         | 0/545   | 0.66        | 0/737           |
| 27  | 15    | 0.39         | 0/469   | 0.62        | 0/635           |
| 27  | 25    | 0.31         | 0/469   | 0.57        | 1/635 (0.2%)    |
| 28  | 16    | 0.38         | 0/460   | 0.54        | 0/613           |
| 28  | 26    | 0.31         | 0/456   | 0.51        | 0/608           |
| 29  | 17    | 0.39         | 0/426   | 0.54        | 0/561           |
| 29  | 27    | 0.32         | 0/426   | 0.54        | 0/561           |
| 30  | 18    | 0.38         | 0/525   | 0.56        | 0/691           |
| 30  | 28    | 0.33         | 0/525   | 0.53        | 0/691           |
| 31  | 19    | 0.36         | 0/310   | 0.50        | 0/407           |
| 31  | 29    | 0.32         | 0/310   | 0.58        | 0/407           |
| 32  | 1a    | 0.38         | 0/35795 | 0.88        | 27/55864 (0.0%) |
| 32  | 2a    | 0.37         | 0/35886 | 0.91        | 33/56005 (0.1%) |
| 33  | 1b    | 0.29         | 0/1881  | 0.59        | 0/2542          |
| 33  | 2b    | 0.31         | 0/1860  | 0.57        | 0/2518          |
| 34  | 1c    | 0.28         | 0/1572  | 0.52        | 2/2126 (0.1%)   |
| 34  | 2c    | 0.29         | 0/1566  | 0.55        | 0/2119          |
| 35  | 1d    | 0.28         | 0/1685  | 0.51        | 0/2262          |
| 35  | 2d    | 0.28         | 0/1704  | 0.49        | 0/2284          |
| 36  | 1e    | 0.31         | 0/1145  | 0.54        | 0/1543          |
| 36  | 2e    | 0.29         | 0/1149  | 0.57        | 0/1548          |
| 37  | 1f    | 0.30         | 0/823   | 0.50        | 0/1115          |
| 37  | 2f    | 0.30         | 0/829   | 0.48        | 0/1123          |

| Mol | Chain | Bond lengths |                 | Bond angles |                   |
|-----|-------|--------------|-----------------|-------------|-------------------|
|     |       | RMSZ         | # Z  >5         | RMSZ        | # Z  >5           |
| 38  | 1g    | 0.29         | 0/1250          | 0.53        | 0/1679            |
| 38  | 2g    | 0.29         | 0/1254          | 0.55        | 0/1683            |
| 39  | 1h    | 0.27         | 0/1108          | 0.54        | 0/1494            |
| 39  | 2h    | 0.27         | 0/1108          | 0.54        | 0/1494            |
| 40  | 1i    | 0.28         | 0/1002          | 0.57        | 1/1346 (0.1%)     |
| 40  | 2i    | 0.28         | 0/997           | 0.56        | 0/1343            |
| 41  | 1j    | 0.27         | 0/722           | 0.53        | 0/982             |
| 41  | 2j    | 0.29         | 0/727           | 0.56        | 0/988             |
| 42  | 1k    | 0.28         | 0/844           | 0.52        | 0/1145            |
| 42  | 2k    | 0.27         | 0/848           | 0.48        | 0/1149            |
| 43  | 1l    | 0.32         | 0/937           | 0.53        | 0/1260            |
| 43  | 2l    | 0.30         | 0/937           | 0.56        | 0/1260            |
| 44  | 1m    | 0.29         | 0/969           | 0.54        | 0/1302            |
| 44  | 2m    | 0.30         | 0/961           | 0.56        | 0/1291            |
| 45  | 1n    | 0.31         | 0/501           | 0.48        | 0/664             |
| 45  | 2n    | 0.29         | 0/501           | 0.48        | 0/664             |
| 46  | 1o    | 0.29         | 0/739           | 0.52        | 0/985             |
| 46  | 2o    | 0.27         | 0/739           | 0.54        | 0/985             |
| 47  | 1p    | 0.28         | 0/697           | 0.52        | 0/939             |
| 47  | 2p    | 0.29         | 0/693           | 0.52        | 0/935             |
| 48  | 1q    | 0.29         | 0/836           | 0.51        | 0/1117            |
| 48  | 2q    | 0.28         | 0/836           | 0.52        | 0/1117            |
| 49  | 1r    | 0.29         | 0/560           | 0.49        | 0/746             |
| 49  | 2r    | 0.28         | 0/560           | 0.52        | 0/746             |
| 50  | 1s    | 0.28         | 0/667           | 0.56        | 0/900             |
| 50  | 2s    | 0.32         | 0/661           | 0.62        | 0/893             |
| 51  | 1t    | 0.27         | 0/730           | 0.52        | 0/965             |
| 51  | 2t    | 0.27         | 0/729           | 0.53        | 0/965             |
| 52  | 1u    | 0.27         | 0/203           | 0.47        | 0/266             |
| 52  | 2u    | 0.30         | 0/203           | 0.50        | 0/266             |
| 53  | 1v    | 0.40         | 0/314           | 0.90        | 0/487             |
| 53  | 2v    | 0.40         | 0/310           | 0.87        | 0/480             |
| 54  | 1w    | 0.45         | 0/1585          | 1.14        | 11/2468 (0.4%)    |
| 54  | 1y    | 0.39         | 0/1602          | 1.02        | 3/2493 (0.1%)     |
| 54  | 2w    | 0.52         | 0/1562          | 1.21        | 5/2431 (0.2%)     |
| 54  | 2y    | 0.46         | 0/1579          | 1.10        | 4/2455 (0.2%)     |
| 55  | 1x    | 0.53         | 2/1700 (0.1%)   | 1.15        | 22/2650 (0.8%)    |
| 55  | 2x    | 0.45         | 0/1700          | 1.09        | 8/2650 (0.3%)     |
| All | All   | 0.41         | 4/316623 (0.0%) | 0.85        | 233/474025 (0.0%) |

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



of a sidechain that are expected to be planar.

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 26  | 14    | 0                   | 1                   |
| 50  | 2s    | 0                   | 1                   |
| All | All   | 0                   | 2                   |

All (4) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 2   | 2B    | 1   | U    | OP3-P | -10.32 | 1.48        | 1.61     |
| 2   | 1B    | 1   | U    | OP3-P | -10.29 | 1.48        | 1.61     |
| 55  | 1x    | 22  | G    | N7-C5 | 7.16   | 1.43        | 1.39     |
| 55  | 1x    | 46  | G    | C6-N1 | 5.15   | 1.43        | 1.39     |

All (233) bond angle outliers are listed below:

| Mol | Chain | Res     | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|---------|------|------------|--------|-------------|----------|
| 2   | 2B    | 80      | U    | O4'-C1'-N1 | 11.58  | 117.47      | 108.20   |
| 32  | 2a    | 1420    | C    | OP1-P-O3'  | -11.56 | 79.77       | 105.20   |
| 55  | 1x    | 46      | G    | C6-N1-C2   | -10.60 | 118.74      | 125.10   |
| 32  | 1a    | 1027    | C    | C2-N1-C1'  | 10.47  | 130.32      | 118.80   |
| 1   | 1A    | 975     | C    | N1-C2-O2   | -10.11 | 112.83      | 118.90   |
| 1   | 1A    | 1075    | C    | N1-C2-O2   | 9.84   | 124.81      | 118.90   |
| 54  | 1w    | 72      | C    | C2-N1-C1'  | 9.59   | 129.35      | 118.80   |
| 1   | 2A    | 2139    | C    | N1-C2-O2   | 9.40   | 124.54      | 118.90   |
| 32  | 1a    | 1036    | G    | C4-N9-C1'  | 9.17   | 138.42      | 126.50   |
| 32  | 2a    | 1420    | C    | OP2-P-O3'  | -9.07  | 85.23       | 105.20   |
| 1   | 2A    | 2061    | G    | O5'-P-OP2  | -9.01  | 97.59       | 105.70   |
| 1   | 2A    | 277     | C    | N1-C2-O2   | 9.00   | 124.30      | 118.90   |
| 32  | 1a    | 1030(B) | C    | C2-N1-C1'  | 8.99   | 128.69      | 118.80   |
| 32  | 1a    | 1027    | C    | C6-N1-C1'  | -8.86  | 110.17      | 120.80   |
| 1   | 2A    | 801     | G    | O5'-P-OP2  | -8.68  | 97.89       | 105.70   |
| 32  | 1a    | 1036    | G    | C8-N9-C1'  | -8.31  | 116.19      | 127.00   |
| 55  | 1x    | 22      | G    | C4-C5-C6   | -8.30  | 113.82      | 118.80   |
| 55  | 1x    | 22      | G    | N1-C6-O6   | -8.23  | 114.96      | 119.90   |
| 1   | 1A    | 975     | C    | C2-N1-C1'  | -8.13  | 109.86      | 118.80   |
| 1   | 1A    | 1063    | G    | C5-C6-O6   | 7.97   | 133.38      | 128.60   |
| 1   | 2A    | 277     | C    | C2-N1-C1'  | 7.92   | 127.52      | 118.80   |
| 54  | 1w    | 1       | G    | N3-C4-N9   | 7.81   | 130.69      | 126.00   |
| 1   | 1A    | 2167    | U    | C2-N1-C1'  | 7.74   | 126.99      | 117.70   |
| 1   | 2A    | 2167    | U    | N3-C2-O2   | -7.73  | 116.79      | 122.20   |
| 55  | 2x    | 14      | A    | C4-C5-C6   | 7.71   | 120.85      | 117.00   |
| 1   | 1A    | 801     | G    | O5'-P-OP2  | -7.68  | 98.78       | 105.70   |

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| Mol | Chain | Res     | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|---------|------|------------|-------|-------------|----------|
| 1   | 1A    | 512     | G    | O4'-C1'-N9 | 7.61  | 114.29      | 108.20   |
| 1   | 1A    | 2682    | U    | O5'-P-OP2  | -7.59 | 98.87       | 105.70   |
| 1   | 2A    | 2136    | C    | N1-C2-O2   | 7.58  | 123.45      | 118.90   |
| 54  | 1w    | 72      | C    | C6-N1-C1'  | -7.56 | 111.72      | 120.80   |
| 32  | 1a    | 1030(B) | C    | N1-C2-O2   | 7.54  | 123.42      | 118.90   |
| 1   | 1A    | 1639    | U    | O5'-P-OP2  | -7.39 | 99.05       | 105.70   |
| 55  | 1x    | 22      | G    | C5-N7-C8   | -7.38 | 100.61      | 104.30   |
| 32  | 2a    | 1004    | A    | O4'-C1'-N9 | 7.34  | 114.07      | 108.20   |
| 1   | 1A    | 12      | U    | C2-N1-C1'  | 7.32  | 126.48      | 117.70   |
| 32  | 2a    | 1001(A) | G    | N3-C4-N9   | 7.26  | 130.35      | 126.00   |
| 1   | 2A    | 2139    | C    | C2-N1-C1'  | 7.25  | 126.77      | 118.80   |
| 1   | 2A    | 2167    | U    | N1-C2-O2   | 7.24  | 127.87      | 122.80   |
| 32  | 2a    | 1421    | G    | OP1-P-OP2  | 7.13  | 130.29      | 119.60   |
| 1   | 2A    | 277     | C    | N3-C2-O2   | -7.10 | 116.93      | 121.90   |
| 1   | 1A    | 1075    | C    | C2-N3-C4   | 7.09  | 123.45      | 119.90   |
| 1   | 2A    | 2167    | U    | C2-N1-C1'  | 7.05  | 126.16      | 117.70   |
| 1   | 1A    | 1100    | C    | C2-N1-C1'  | 7.02  | 126.52      | 118.80   |
| 54  | 1w    | 72      | C    | N1-C2-O2   | 7.00  | 123.10      | 118.90   |
| 55  | 2x    | 46      | G    | C6-N1-C2   | -7.00 | 120.90      | 125.10   |
| 55  | 1x    | 22      | G    | N3-C4-N9   | -6.99 | 121.81      | 126.00   |
| 32  | 1a    | 1027    | C    | C5-C6-N1   | 6.94  | 124.47      | 121.00   |
| 55  | 1x    | 22      | G    | C6-C5-N7   | 6.90  | 134.54      | 130.40   |
| 55  | 1x    | 14      | A    | C4-C5-C6   | 6.85  | 120.43      | 117.00   |
| 1   | 1A    | 1992    | G    | P-O3'-C3'  | 6.76  | 127.81      | 119.70   |
| 1   | 1A    | 1086    | A    | N1-C6-N6   | -6.72 | 114.57      | 118.60   |
| 1   | 1A    | 793     | A    | O5'-P-OP2  | -6.61 | 99.75       | 105.70   |
| 32  | 1a    | 1002    | G    | N3-C4-N9   | 6.61  | 129.96      | 126.00   |
| 1   | 1A    | 1176    | G    | OP1-P-O3'  | 6.58  | 119.68      | 105.20   |
| 32  | 1a    | 1036    | G    | N3-C4-N9   | 6.55  | 129.93      | 126.00   |
| 1   | 1A    | 1075    | C    | N3-C2-O2   | -6.54 | 117.33      | 121.90   |
| 1   | 2A    | 1022    | G    | N3-C4-N9   | -6.53 | 122.08      | 126.00   |
| 1   | 1A    | 2167    | U    | N1-C2-O2   | 6.46  | 127.32      | 122.80   |
| 1   | 1A    | 847     | U    | C2-N1-C1'  | 6.45  | 125.43      | 117.70   |
| 1   | 2A    | 574     | C    | O5'-P-OP1  | -6.44 | 99.91       | 105.70   |
| 32  | 2a    | 998     | G    | N9-C4-C5   | 6.42  | 107.97      | 105.40   |
| 1   | 1A    | 2848    | G    | O4'-C1'-N9 | 6.38  | 113.31      | 108.20   |
| 55  | 1x    | 14      | A    | C5-N7-C8   | 6.38  | 107.09      | 103.90   |
| 54  | 2y    | 63      | G    | C5-C6-O6   | 6.38  | 132.43      | 128.60   |
| 1   | 1A    | 975     | C    | C5-C6-N1   | -6.31 | 117.84      | 121.00   |
| 1   | 1A    | 1298    | C    | O5'-P-OP2  | -6.29 | 100.04      | 105.70   |
| 32  | 1a    | 1030(B) | C    | C6-N1-C2   | -6.29 | 117.78      | 120.30   |
| 55  | 2x    | 14      | A    | C5-N7-C8   | 6.24  | 107.02      | 103.90   |

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| Mol | Chain | Res     | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|---------|------|-------------|-------|-------------|----------|
| 1   | 1A    | 2167    | U    | N3-C2-O2    | -6.22 | 117.84      | 122.20   |
| 32  | 2a    | 998     | G    | N3-C4-N9    | -6.22 | 122.27      | 126.00   |
| 1   | 2A    | 277     | C    | C6-N1-C2    | -6.17 | 117.83      | 120.30   |
| 1   | 1A    | 624     | C    | O5'-P-OP1   | -6.17 | 100.15      | 105.70   |
| 1   | 1A    | 1063    | G    | C6-N1-C2    | 6.16  | 128.80      | 125.10   |
| 1   | 2A    | 2139    | C    | C6-N1-C1'   | -6.16 | 113.41      | 120.80   |
| 1   | 2A    | 2554    | U    | O5'-P-OP2   | -6.15 | 100.16      | 105.70   |
| 32  | 2a    | 1322    | C    | N1-C2-O2    | -6.15 | 115.21      | 118.90   |
| 32  | 1a    | 1030(B) | C    | C6-N1-C1'   | -6.14 | 113.44      | 120.80   |
| 27  | 25    | 58      | LEU  | CA-CB-CG    | 6.13  | 129.41      | 115.30   |
| 32  | 1a    | 1036    | G    | N3-C4-C5    | -6.10 | 125.55      | 128.60   |
| 1   | 2A    | 2155    | G    | N3-C2-N2    | 6.07  | 124.15      | 119.90   |
| 32  | 1a    | 1002    | G    | C4-N9-C1'   | 6.06  | 134.38      | 126.50   |
| 1   | 1A    | 975     | C    | C6-N1-C1'   | 6.04  | 128.05      | 120.80   |
| 1   | 2A    | 1300    | U    | P-O3'-C3'   | 6.04  | 126.94      | 119.70   |
| 1   | 2A    | 2897    | U    | C2-N1-C1'   | 6.04  | 124.94      | 117.70   |
| 55  | 1x    | 22      | G    | C8-N9-C1'   | 6.03  | 134.84      | 127.00   |
| 1   | 1A    | 1129    | A    | O4'-C1'-N9  | 6.00  | 113.00      | 108.20   |
| 32  | 2a    | 754     | C    | C2-N1-C1'   | 5.98  | 125.38      | 118.80   |
| 1   | 1A    | 31      | C    | O5'-P-OP1   | -5.95 | 100.35      | 105.70   |
| 1   | 2A    | 2206    | G    | C4-N9-C1'   | -5.94 | 118.78      | 126.50   |
| 55  | 2x    | 14      | A    | C5-C6-N1    | -5.92 | 114.74      | 117.70   |
| 1   | 2A    | 2155    | G    | C6-N1-C2    | 5.91  | 128.65      | 125.10   |
| 55  | 1x    | 46      | G    | N3-C2-N2    | -5.91 | 115.77      | 119.90   |
| 55  | 1x    | 46      | G    | N9-C4-C5    | 5.91  | 107.76      | 105.40   |
| 55  | 1x    | 46      | G    | C5-C6-N1    | 5.91  | 114.45      | 111.50   |
| 32  | 1a    | 560     | U    | C2-N1-C1'   | 5.90  | 124.78      | 117.70   |
| 1   | 1A    | 1170    | G    | C8-N9-C4    | -5.89 | 104.04      | 106.40   |
| 1   | 2A    | 1313    | U    | C2-N1-C1'   | 5.88  | 124.75      | 117.70   |
| 1   | 1A    | 845     | G    | O4'-C1'-N9  | 5.87  | 112.90      | 108.20   |
| 32  | 2a    | 1027    | C    | N3-C2-O2    | -5.86 | 117.80      | 121.90   |
| 32  | 1a    | 1002    | G    | C8-N9-C1'   | -5.86 | 119.39      | 127.00   |
| 1   | 1A    | 226     | G    | O4'-C1'-N9  | 5.86  | 112.89      | 108.20   |
| 55  | 1x    | 46      | G    | N1-C2-N3    | 5.85  | 127.41      | 123.90   |
| 1   | 2A    | 2473    | U    | C2-N1-C1'   | 5.84  | 124.71      | 117.70   |
| 1   | 2A    | 2897    | U    | N1-C2-O2    | 5.83  | 126.88      | 122.80   |
| 54  | 1y    | 33      | U    | N1-C2-O2    | 5.82  | 126.87      | 122.80   |
| 54  | 1w    | 1       | G    | N9-C4-C5    | -5.82 | 103.07      | 105.40   |
| 1   | 1A    | 2061    | G    | O5'-P-OP2   | -5.81 | 100.47      | 105.70   |
| 2   | 2B    | 80      | U    | C5'-C4'-O4' | 5.79  | 116.05      | 109.10   |
| 55  | 1x    | 22      | G    | C5-C6-N1    | 5.76  | 114.38      | 111.50   |
| 54  | 1w    | 1       | G    | C8-N9-C1'   | -5.75 | 119.52      | 127.00   |

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| Mol | Chain | Res     | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|---------|------|------------|-------|-------------|----------|
| 54  | 2w    | 76      | A    | O4'-C1'-N9 | 5.74  | 112.80      | 108.20   |
| 32  | 2a    | 1039    | C    | N1-C2-O2   | 5.74  | 122.34      | 118.90   |
| 32  | 2a    | 1052    | U    | N1-C2-O2   | 5.74  | 126.82      | 122.80   |
| 34  | 1c    | 190     | ARG  | NE-CZ-NH1  | -5.74 | 117.43      | 120.30   |
| 32  | 2a    | 65      | U    | P-O3'-C3'  | 5.71  | 126.56      | 119.70   |
| 55  | 2x    | 46      | G    | N3-C2-N2   | -5.70 | 115.91      | 119.90   |
| 32  | 1a    | 1030(B) | C    | N3-C2-O2   | -5.70 | 117.91      | 121.90   |
| 32  | 1a    | 1030(B) | C    | C5-C6-N1   | 5.69  | 123.84      | 121.00   |
| 1   | 2A    | 527     | C    | C2-N1-C1'  | 5.68  | 125.05      | 118.80   |
| 1   | 2A    | 1575    | C    | N1-C2-O2   | 5.68  | 122.31      | 118.90   |
| 32  | 1a    | 266     | G    | P-O3'-C3'  | 5.67  | 126.51      | 119.70   |
| 32  | 2a    | 1206    | G    | N3-C4-N9   | 5.63  | 129.38      | 126.00   |
| 1   | 2A    | 2136    | C    | N3-C2-O2   | -5.62 | 117.97      | 121.90   |
| 1   | 1A    | 2032    | G    | C5-N7-C8   | 5.61  | 107.11      | 104.30   |
| 55  | 1x    | 22      | G    | N3-C4-C5   | 5.55  | 131.38      | 128.60   |
| 32  | 2a    | 1039    | C    | C5-C4-N4   | -5.55 | 116.32      | 120.20   |
| 1   | 1A    | 1074    | G    | C4-N9-C1'  | 5.54  | 133.70      | 126.50   |
| 55  | 1x    | 46      | G    | C5-C6-O6   | -5.54 | 125.28      | 128.60   |
| 1   | 1A    | 1100    | C    | C6-N1-C1'  | -5.53 | 114.16      | 120.80   |
| 1   | 1A    | 1170    | G    | N7-C8-N9   | 5.53  | 115.86      | 113.10   |
| 32  | 2a    | 754     | C    | N1-C2-O2   | 5.53  | 122.22      | 118.90   |
| 1   | 2A    | 746     | A    | O4'-C1'-N9 | 5.53  | 112.62      | 108.20   |
| 54  | 1w    | 1       | G    | C4-N9-C1'  | 5.52  | 133.67      | 126.50   |
| 32  | 2a    | 266     | G    | P-O3'-C3'  | 5.52  | 126.32      | 119.70   |
| 1   | 1A    | 1177    | A    | O5'-P-OP1  | -5.52 | 100.74      | 105.70   |
| 1   | 2A    | 1992    | G    | P-O3'-C3'  | 5.51  | 126.31      | 119.70   |
| 1   | 2A    | 2156    | G    | C8-N9-C4   | -5.51 | 104.20      | 106.40   |
| 32  | 2a    | 266     | G    | N3-C4-C5   | -5.51 | 125.84      | 128.60   |
| 32  | 2a    | 1003    | G    | C4-N9-C1'  | 5.51  | 133.66      | 126.50   |
| 1   | 2A    | 787     | U    | O5'-P-OP1  | -5.49 | 100.76      | 105.70   |
| 32  | 2a    | 1040    | U    | C5-C4-O4   | 5.48  | 129.19      | 125.90   |
| 1   | 1A    | 975     | C    | C2-N3-C4   | -5.48 | 117.16      | 119.90   |
| 1   | 2A    | 2206    | G    | C8-N9-C1'  | 5.48  | 134.12      | 127.00   |
| 55  | 1x    | 14      | A    | C5-C6-N1   | -5.48 | 114.96      | 117.70   |
| 55  | 2x    | 22      | G    | N1-C6-O6   | -5.47 | 116.62      | 119.90   |
| 1   | 1A    | 1372    | U    | N3-C4-O4   | 5.46  | 123.22      | 119.40   |
| 54  | 2y    | 22      | G    | N1-C6-O6   | 5.45  | 123.17      | 119.90   |
| 54  | 1y    | 58      | A    | N1-C6-N6   | 5.44  | 121.86      | 118.60   |
| 54  | 1y    | 33      | U    | C2-N1-C1'  | 5.44  | 124.22      | 117.70   |
| 32  | 2a    | 1001(A) | G    | N3-C4-C5   | -5.42 | 125.89      | 128.60   |
| 1   | 1A    | 2554    | U    | O5'-P-OP1  | -5.42 | 100.82      | 105.70   |
| 1   | 2A    | 1530    | C    | P-O3'-C3'  | 5.42  | 126.20      | 119.70   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | 2A    | 265  | A    | O4'-C1'-N9 | 5.42  | 112.53      | 108.20   |
| 54  | 2w    | 69   | G    | C5-C6-O6   | -5.41 | 125.35      | 128.60   |
| 1   | 1A    | 1313 | U    | C2-N1-C1'  | 5.40  | 124.18      | 117.70   |
| 1   | 1A    | 1131 | G    | O4'-C1'-N9 | 5.38  | 112.50      | 108.20   |
| 1   | 2A    | 2139 | C    | N3-C2-O2   | -5.37 | 118.14      | 121.90   |
| 1   | 1A    | 889  | C    | N1-C2-O2   | 5.36  | 122.12      | 118.90   |
| 1   | 2A    | 1313 | U    | O4'-C1'-N1 | 5.36  | 112.49      | 108.20   |
| 32  | 2a    | 998  | G    | C4-C5-N7   | -5.35 | 108.66      | 110.80   |
| 32  | 2a    | 1040 | U    | O4'-C1'-N1 | 5.34  | 112.47      | 108.20   |
| 55  | 1x    | 22   | G    | C4-N9-C1'  | -5.34 | 119.56      | 126.50   |
| 55  | 1x    | 46   | G    | C4-C5-N7   | -5.33 | 108.67      | 110.80   |
| 1   | 2A    | 512  | G    | O4'-C1'-N9 | 5.33  | 112.47      | 108.20   |
| 32  | 1a    | 1067 | A    | P-O3'-C3'  | 5.33  | 126.09      | 119.70   |
| 55  | 1x    | 10   | G    | N3-C2-N2   | -5.33 | 116.17      | 119.90   |
| 1   | 2A    | 2473 | U    | N1-C2-O2   | 5.31  | 126.52      | 122.80   |
| 54  | 2w    | 67   | C    | C2-N3-C4   | 5.30  | 122.55      | 119.90   |
| 55  | 2x    | 22   | G    | C8-N9-C1'  | 5.30  | 133.89      | 127.00   |
| 1   | 2A    | 527  | C    | C6-N1-C1'  | -5.30 | 114.44      | 120.80   |
| 32  | 2a    | 1025 | U    | O4'-C1'-N1 | 5.28  | 112.42      | 108.20   |
| 1   | 1A    | 748  | G    | N1-C6-O6   | -5.27 | 116.74      | 119.90   |
| 55  | 2x    | 22   | G    | C4-C5-C6   | -5.27 | 115.64      | 118.80   |
| 1   | 1A    | 999  | U    | O5'-P-OP2  | -5.26 | 100.96      | 105.70   |
| 1   | 1A    | 975  | C    | N3-C2-O2   | 5.26  | 125.58      | 121.90   |
| 32  | 2a    | 1004 | A    | N1-C6-N6   | -5.26 | 115.44      | 118.60   |
| 32  | 2a    | 1158 | C    | N1-C2-O2   | 5.25  | 122.05      | 118.90   |
| 55  | 1x    | 14   | A    | C4-N9-C1'  | 5.25  | 135.75      | 126.30   |
| 54  | 2w    | 10   | G    | N3-C2-N2   | -5.25 | 116.23      | 119.90   |
| 54  | 2y    | 62   | C    | C2-N3-C4   | 5.24  | 122.52      | 119.90   |
| 32  | 1a    | 1201 | A    | P-O3'-C3'  | 5.23  | 125.98      | 119.70   |
| 40  | 1i    | 50   | LEU  | CA-CB-CG   | 5.23  | 127.32      | 115.30   |
| 54  | 1w    | 72   | C    | C5-C6-N1   | 5.23  | 123.61      | 121.00   |
| 1   | 1A    | 1076 | C    | O4'-C1'-N1 | 5.22  | 112.38      | 108.20   |
| 1   | 1A    | 1100 | C    | N1-C2-O2   | 5.21  | 122.02      | 118.90   |
| 55  | 1x    | 14   | A    | C8-N9-C1'  | -5.21 | 118.33      | 127.70   |
| 1   | 1A    | 2028 | U    | N3-C4-O4   | -5.20 | 115.76      | 119.40   |
| 1   | 1A    | 889  | C    | C2-N1-C1'  | 5.20  | 124.52      | 118.80   |
| 1   | 1A    | 944  | G    | C4-N9-C1'  | 5.20  | 133.26      | 126.50   |
| 1   | 2A    | 845  | G    | C4-N9-C1'  | 5.20  | 133.26      | 126.50   |
| 1   | 1A    | 1352 | U    | O5'-P-OP1  | -5.19 | 101.03      | 105.70   |
| 1   | 1A    | 1074 | G    | C8-N9-C1'  | -5.18 | 120.26      | 127.00   |
| 4   | 2E    | 72   | VAL  | C-N-CA     | 5.18  | 134.65      | 121.70   |
| 1   | 1A    | 1063 | G    | N1-C6-O6   | -5.18 | 116.79      | 119.90   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | 1A    | 1175 | U    | P-O3'-C3'  | 5.17  | 125.91      | 119.70   |
| 54  | 1w    | 1    | G    | C6-C5-N7   | -5.17 | 127.30      | 130.40   |
| 32  | 1a    | 1206 | G    | C5-C6-O6   | -5.16 | 125.50      | 128.60   |
| 32  | 2a    | 1206 | G    | N3-C4-C5   | -5.16 | 126.02      | 128.60   |
| 1   | 1A    | 12   | U    | C6-N1-C1'  | -5.15 | 113.99      | 121.20   |
| 1   | 1A    | 1313 | U    | N3-C2-O2   | -5.15 | 118.59      | 122.20   |
| 32  | 2a    | 1039 | C    | C2-N1-C1'  | 5.15  | 124.47      | 118.80   |
| 1   | 1A    | 1075 | C    | C6-N1-C2   | -5.15 | 118.24      | 120.30   |
| 54  | 1w    | 72   | C    | C5-C4-N4   | -5.14 | 116.60      | 120.20   |
| 1   | 1A    | 34   | C    | N1-C2-O2   | 5.14  | 121.98      | 118.90   |
| 32  | 1a    | 1158 | C    | C2-N1-C1'  | 5.14  | 124.45      | 118.80   |
| 32  | 2a    | 687  | A    | P-O3'-C3'  | 5.14  | 125.86      | 119.70   |
| 32  | 2a    | 1025 | U    | C2-N1-C1'  | -5.14 | 111.54      | 117.70   |
| 1   | 2A    | 614  | U    | N3-C2-O2   | -5.13 | 118.61      | 122.20   |
| 32  | 1a    | 1043 | C    | C2-N1-C1'  | 5.12  | 124.44      | 118.80   |
| 1   | 2A    | 277  | C    | C6-N1-C1'  | -5.12 | 114.65      | 120.80   |
| 32  | 2a    | 1027 | C    | N1-C2-O2   | 5.11  | 121.97      | 118.90   |
| 1   | 2A    | 1129 | A    | O4'-C1'-N9 | 5.11  | 112.29      | 108.20   |
| 1   | 2A    | 1022 | G    | C6-C5-N7   | 5.10  | 133.46      | 130.40   |
| 1   | 1A    | 1086 | A    | C2-N3-C4   | 5.10  | 113.15      | 110.60   |
| 32  | 1a    | 1002 | G    | N3-C4-C5   | -5.09 | 126.05      | 128.60   |
| 32  | 2a    | 501  | C    | C6-N1-C2   | -5.09 | 118.26      | 120.30   |
| 1   | 1A    | 12   | U    | N1-C2-O2   | 5.08  | 126.36      | 122.80   |
| 1   | 1A    | 1617 | C    | C2-N1-C1'  | -5.08 | 113.22      | 118.80   |
| 54  | 2y    | 63   | G    | C6-N1-C2   | 5.07  | 128.14      | 125.10   |
| 1   | 2A    | 228  | A    | P-O3'-C3'  | 5.07  | 125.78      | 119.70   |
| 32  | 1a    | 1285 | A    | P-O3'-C3'  | 5.07  | 125.78      | 119.70   |
| 32  | 2a    | 1206 | G    | C5-C6-O6   | -5.06 | 125.56      | 128.60   |
| 1   | 1A    | 1074 | G    | N3-C4-N9   | 5.05  | 129.03      | 126.00   |
| 34  | 1c    | 190  | ARG  | NE-CZ-NH2  | 5.04  | 122.82      | 120.30   |
| 54  | 1w    | 75   | C    | P-O3'-C3'  | 5.04  | 125.75      | 119.70   |
| 1   | 1A    | 944  | G    | C8-N9-C1'  | -5.03 | 120.46      | 127.00   |
| 54  | 2w    | 75   | C    | P-O3'-C3'  | 5.03  | 125.74      | 119.70   |
| 32  | 1a    | 266  | G    | O4'-C1'-N9 | -5.03 | 104.18      | 108.20   |
| 32  | 1a    | 21   | G    | O5'-P-OP1  | -5.03 | 101.17      | 105.70   |
| 1   | 2A    | 1022 | G    | N3-C2-N2   | -5.02 | 116.39      | 119.90   |
| 1   | 1A    | 1075 | C    | C5-C6-N1   | 5.01  | 123.51      | 121.00   |
| 1   | 1A    | 1068 | G    | O4'-C1'-N9 | 5.01  | 112.21      | 108.20   |
| 1   | 1A    | 1372 | U    | C5-C4-O4   | -5.01 | 122.89      | 125.90   |

There are no chirality outliers.

All (2) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 26  | 14    | 67  | TYR  | Peptide |
| 50  | 2s    | 28  | LYS  | Peptide |

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | 1A    | 61852 | 0        | 31191    | 833     | 0            |
| 1   | 2A    | 60322 | 0        | 30426    | 1115    | 0            |
| 2   | 1B    | 2577  | 0        | 1305     | 34      | 0            |
| 2   | 2B    | 2575  | 0        | 1303     | 76      | 0            |
| 3   | 1D    | 2136  | 0        | 2218     | 59      | 0            |
| 3   | 2D    | 2136  | 0        | 2218     | 63      | 0            |
| 4   | 1E    | 1559  | 0        | 1618     | 40      | 0            |
| 4   | 2E    | 1559  | 0        | 1618     | 39      | 0            |
| 5   | 1F    | 1584  | 0        | 1625     | 39      | 0            |
| 5   | 2F    | 1580  | 0        | 1619     | 50      | 0            |
| 6   | 1G    | 1429  | 0        | 1447     | 39      | 0            |
| 6   | 2G    | 1428  | 0        | 1438     | 70      | 0            |
| 7   | 1H    | 1330  | 0        | 1407     | 35      | 0            |
| 7   | 2H    | 1330  | 0        | 1407     | 48      | 0            |
| 8   | 1I    | 1097  | 0        | 1140     | 33      | 0            |
| 8   | 2I    | 1064  | 0        | 1082     | 33      | 1            |
| 9   | 1N    | 1117  | 0        | 1184     | 23      | 0            |
| 9   | 2N    | 1117  | 0        | 1184     | 28      | 0            |
| 10  | 1O    | 933   | 0        | 996      | 20      | 0            |
| 10  | 2O    | 933   | 0        | 996      | 34      | 0            |
| 11  | 1P    | 1135  | 0        | 1212     | 33      | 0            |
| 11  | 2P    | 1135  | 0        | 1212     | 48      | 0            |
| 12  | 1Q    | 1122  | 0        | 1179     | 22      | 0            |
| 12  | 2Q    | 1122  | 0        | 1179     | 44      | 0            |
| 13  | 1R    | 968   | 0        | 1033     | 29      | 0            |
| 13  | 2R    | 968   | 0        | 1033     | 31      | 0            |
| 14  | 1S    | 873   | 0        | 927      | 19      | 0            |
| 14  | 2S    | 870   | 0        | 923      | 42      | 0            |
| 15  | 1T    | 1091  | 0        | 1151     | 21      | 0            |
| 15  | 2T    | 1083  | 0        | 1136     | 33      | 0            |
| 16  | 1U    | 959   | 0        | 1019     | 28      | 0            |
| 16  | 2U    | 959   | 0        | 1019     | 37      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 17  | 1V    | 771   | 0        | 830      | 15      | 0            |
| 17  | 2V    | 771   | 0        | 829      | 24      | 0            |
| 18  | 1W    | 886   | 0        | 940      | 14      | 0            |
| 18  | 2W    | 886   | 0        | 940      | 15      | 0            |
| 19  | 1X    | 750   | 0        | 814      | 21      | 0            |
| 19  | 2X    | 750   | 0        | 814      | 31      | 0            |
| 20  | 1Y    | 806   | 0        | 881      | 24      | 0            |
| 20  | 2Y    | 806   | 0        | 881      | 25      | 0            |
| 21  | 1Z    | 1240  | 0        | 1240     | 32      | 0            |
| 21  | 2Z    | 1271  | 0        | 1273     | 49      | 0            |
| 22  | 10    | 653   | 0        | 674      | 18      | 0            |
| 22  | 20    | 653   | 0        | 674      | 15      | 0            |
| 23  | 11    | 755   | 0        | 826      | 18      | 0            |
| 23  | 21    | 755   | 0        | 826      | 17      | 0            |
| 24  | 12    | 588   | 0        | 643      | 7       | 0            |
| 24  | 22    | 588   | 0        | 643      | 12      | 0            |
| 25  | 13    | 469   | 0        | 518      | 8       | 0            |
| 25  | 23    | 464   | 0        | 514      | 13      | 0            |
| 26  | 14    | 552   | 0        | 533      | 23      | 0            |
| 26  | 24    | 532   | 0        | 503      | 19      | 0            |
| 27  | 15    | 455   | 0        | 465      | 13      | 0            |
| 27  | 25    | 455   | 0        | 465      | 17      | 0            |
| 28  | 16    | 453   | 0        | 472      | 8       | 0            |
| 28  | 26    | 449   | 0        | 469      | 12      | 0            |
| 29  | 17    | 418   | 0        | 467      | 8       | 0            |
| 29  | 27    | 418   | 0        | 467      | 9       | 0            |
| 30  | 18    | 517   | 0        | 582      | 18      | 0            |
| 30  | 28    | 517   | 0        | 582      | 19      | 0            |
| 31  | 19    | 307   | 0        | 335      | 6       | 0            |
| 31  | 29    | 307   | 0        | 335      | 15      | 0            |
| 32  | 1a    | 32246 | 0        | 16296    | 0       | 1            |
| 32  | 2a    | 32327 | 0        | 16340    | 0       | 0            |
| 33  | 1b    | 1846  | 0        | 1867     | 0       | 0            |
| 33  | 2b    | 1825  | 0        | 1828     | 0       | 0            |
| 34  | 1c    | 1548  | 0        | 1535     | 0       | 0            |
| 34  | 2c    | 1542  | 0        | 1517     | 0       | 0            |
| 35  | 1d    | 1655  | 0        | 1671     | 0       | 0            |
| 35  | 2d    | 1674  | 0        | 1714     | 0       | 0            |
| 36  | 1e    | 1129  | 0        | 1185     | 0       | 0            |
| 36  | 2e    | 1133  | 0        | 1191     | 0       | 0            |
| 37  | 1f    | 810   | 0        | 804      | 0       | 0            |
| 37  | 2f    | 816   | 0        | 808      | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 38  | 1g    | 1231  | 0        | 1238     | 0       | 0            |
| 38  | 2g    | 1235  | 0        | 1249     | 0       | 0            |
| 39  | 1h    | 1088  | 0        | 1126     | 0       | 0            |
| 39  | 2h    | 1088  | 0        | 1126     | 0       | 0            |
| 40  | 1i    | 983   | 0        | 986      | 0       | 0            |
| 40  | 2i    | 978   | 0        | 966      | 0       | 0            |
| 41  | 1j    | 709   | 0        | 650      | 0       | 0            |
| 41  | 2j    | 714   | 0        | 672      | 0       | 0            |
| 42  | 1k    | 829   | 0        | 825      | 0       | 0            |
| 42  | 2k    | 833   | 0        | 836      | 0       | 0            |
| 43  | 1l    | 932   | 0        | 981      | 0       | 0            |
| 43  | 2l    | 932   | 0        | 980      | 0       | 0            |
| 44  | 1m    | 958   | 0        | 1002     | 0       | 0            |
| 44  | 2m    | 950   | 0        | 988      | 0       | 0            |
| 45  | 1n    | 492   | 0        | 529      | 0       | 0            |
| 45  | 2n    | 492   | 0        | 529      | 0       | 0            |
| 46  | 1o    | 728   | 0        | 760      | 0       | 0            |
| 46  | 2o    | 728   | 0        | 760      | 0       | 0            |
| 47  | 1p    | 681   | 0        | 697      | 0       | 0            |
| 47  | 2p    | 677   | 0        | 686      | 0       | 0            |
| 48  | 1q    | 823   | 0        | 891      | 0       | 0            |
| 48  | 2q    | 823   | 0        | 891      | 0       | 0            |
| 49  | 1r    | 555   | 0        | 618      | 0       | 0            |
| 49  | 2r    | 555   | 0        | 618      | 0       | 0            |
| 50  | 1s    | 652   | 0        | 662      | 0       | 0            |
| 50  | 2s    | 646   | 0        | 644      | 0       | 0            |
| 51  | 1t    | 728   | 0        | 798      | 0       | 0            |
| 51  | 2t    | 727   | 0        | 796      | 0       | 0            |
| 52  | 1u    | 199   | 0        | 208      | 0       | 0            |
| 52  | 2u    | 199   | 0        | 208      | 0       | 0            |
| 53  | 1v    | 281   | 0        | 139      | 0       | 0            |
| 53  | 2v    | 277   | 0        | 140      | 0       | 0            |
| 54  | 1w    | 1574  | 0        | 810      | 0       | 0            |
| 54  | 1y    | 1581  | 0        | 805      | 0       | 0            |
| 54  | 2w    | 1547  | 0        | 783      | 0       | 0            |
| 54  | 2y    | 1561  | 0        | 796      | 0       | 0            |
| 55  | 1x    | 1635  | 0        | 838      | 0       | 0            |
| 55  | 2x    | 1635  | 0        | 838      | 0       | 0            |
| 56  | 10    | 4     | 0        | 0        | 0       | 0            |
| 56  | 11    | 3     | 0        | 0        | 0       | 0            |
| 56  | 12    | 1     | 0        | 0        | 0       | 0            |
| 56  | 13    | 3     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 56  | 15    | 2     | 0        | 0        | 0       | 0            |
| 56  | 16    | 1     | 0        | 0        | 0       | 0            |
| 56  | 17    | 2     | 0        | 0        | 0       | 0            |
| 56  | 18    | 2     | 0        | 0        | 0       | 0            |
| 56  | 19    | 2     | 0        | 0        | 0       | 0            |
| 56  | 1A    | 963   | 0        | 0        | 1       | 0            |
| 56  | 1B    | 29    | 0        | 0        | 0       | 0            |
| 56  | 1D    | 5     | 0        | 0        | 0       | 0            |
| 56  | 1E    | 6     | 0        | 0        | 0       | 0            |
| 56  | 1F    | 7     | 0        | 0        | 0       | 0            |
| 56  | 1G    | 4     | 0        | 0        | 0       | 0            |
| 56  | 1I    | 1     | 0        | 0        | 0       | 0            |
| 56  | 1N    | 7     | 0        | 0        | 0       | 0            |
| 56  | 1O    | 6     | 0        | 0        | 0       | 0            |
| 56  | 1P    | 4     | 0        | 0        | 0       | 0            |
| 56  | 1Q    | 6     | 0        | 0        | 0       | 0            |
| 56  | 1R    | 3     | 0        | 0        | 0       | 0            |
| 56  | 1S    | 2     | 0        | 0        | 0       | 0            |
| 56  | 1T    | 3     | 0        | 0        | 0       | 0            |
| 56  | 1U    | 5     | 0        | 0        | 0       | 0            |
| 56  | 1V    | 2     | 0        | 0        | 0       | 0            |
| 56  | 1W    | 6     | 0        | 0        | 0       | 0            |
| 56  | 1X    | 4     | 0        | 0        | 0       | 0            |
| 56  | 1Y    | 1     | 0        | 0        | 0       | 0            |
| 56  | 1Z    | 5     | 0        | 0        | 0       | 0            |
| 56  | 1a    | 239   | 0        | 0        | 0       | 0            |
| 56  | 1b    | 2     | 0        | 0        | 0       | 0            |
| 56  | 1d    | 2     | 0        | 0        | 0       | 0            |
| 56  | 1e    | 1     | 0        | 0        | 0       | 0            |
| 56  | 1f    | 2     | 0        | 0        | 0       | 0            |
| 56  | 1l    | 3     | 0        | 0        | 0       | 0            |
| 56  | 1t    | 1     | 0        | 0        | 0       | 0            |
| 56  | 1v    | 1     | 0        | 0        | 0       | 0            |
| 56  | 1w    | 6     | 0        | 0        | 0       | 0            |
| 56  | 1x    | 10    | 0        | 0        | 0       | 0            |
| 56  | 1y    | 2     | 0        | 0        | 0       | 0            |
| 56  | 20    | 3     | 0        | 0        | 0       | 0            |
| 56  | 23    | 1     | 0        | 0        | 0       | 0            |
| 56  | 26    | 1     | 0        | 0        | 0       | 0            |
| 56  | 28    | 1     | 0        | 0        | 0       | 0            |
| 56  | 2A    | 673   | 0        | 0        | 0       | 0            |
| 56  | 2B    | 18    | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 56  | 2D    | 4     | 0        | 0        | 0       | 0            |
| 56  | 2E    | 5     | 0        | 0        | 0       | 0            |
| 56  | 2F    | 4     | 0        | 0        | 0       | 0            |
| 56  | 2G    | 1     | 0        | 0        | 0       | 0            |
| 56  | 2O    | 2     | 0        | 0        | 0       | 0            |
| 56  | 2P    | 1     | 0        | 0        | 0       | 0            |
| 56  | 2Q    | 4     | 0        | 0        | 0       | 0            |
| 56  | 2R    | 1     | 0        | 0        | 0       | 0            |
| 56  | 2T    | 1     | 0        | 0        | 0       | 0            |
| 56  | 2U    | 4     | 0        | 0        | 0       | 0            |
| 56  | 2V    | 1     | 0        | 0        | 0       | 0            |
| 56  | 2X    | 1     | 0        | 0        | 0       | 0            |
| 56  | 2Z    | 1     | 0        | 0        | 0       | 0            |
| 56  | 2a    | 196   | 0        | 0        | 0       | 0            |
| 56  | 2d    | 1     | 0        | 0        | 0       | 0            |
| 56  | 2e    | 1     | 0        | 0        | 0       | 0            |
| 56  | 2f    | 2     | 0        | 0        | 0       | 0            |
| 56  | 2g    | 1     | 0        | 0        | 0       | 0            |
| 56  | 2j    | 2     | 0        | 0        | 0       | 0            |
| 56  | 2l    | 2     | 0        | 0        | 0       | 0            |
| 56  | 2p    | 1     | 0        | 0        | 0       | 0            |
| 56  | 2q    | 2     | 0        | 0        | 0       | 0            |
| 56  | 2r    | 1     | 0        | 0        | 0       | 0            |
| 56  | 2t    | 1     | 0        | 0        | 0       | 0            |
| 56  | 2v    | 1     | 0        | 0        | 0       | 0            |
| 56  | 2w    | 3     | 0        | 0        | 0       | 0            |
| 56  | 2x    | 2     | 0        | 0        | 0       | 0            |
| 57  | 1A    | 1     | 0        | 0        | 0       | 0            |
| 57  | 2A    | 1     | 0        | 0        | 0       | 0            |
| 58  | 1A    | 36    | 0        | 29       | 2       | 0            |
| 58  | 2A    | 36    | 0        | 29       | 4       | 0            |
| 59  | 14    | 1     | 0        | 0        | 0       | 0            |
| 59  | 15    | 1     | 0        | 0        | 0       | 0            |
| 59  | 16    | 1     | 0        | 0        | 0       | 0            |
| 59  | 19    | 1     | 0        | 0        | 0       | 0            |
| 59  | 1Y    | 1     | 0        | 0        | 0       | 0            |
| 59  | 1n    | 1     | 0        | 0        | 0       | 0            |
| 59  | 24    | 1     | 0        | 0        | 0       | 0            |
| 59  | 25    | 1     | 0        | 0        | 0       | 0            |
| 59  | 26    | 1     | 0        | 0        | 0       | 0            |
| 59  | 29    | 1     | 0        | 0        | 0       | 0            |
| 59  | 2Y    | 1     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 59  | 2n    | 1     | 0        | 0        | 0       | 0            |
| 60  | 1d    | 8     | 0        | 0        | 0       | 0            |
| 60  | 2d    | 8     | 0        | 0        | 0       | 0            |
| 61  | 10    | 9     | 0        | 0        | 2       | 0            |
| 61  | 11    | 3     | 0        | 0        | 0       | 0            |
| 61  | 12    | 4     | 0        | 0        | 0       | 0            |
| 61  | 13    | 3     | 0        | 0        | 0       | 0            |
| 61  | 14    | 1     | 0        | 0        | 0       | 0            |
| 61  | 15    | 4     | 0        | 0        | 0       | 0            |
| 61  | 16    | 2     | 0        | 0        | 0       | 0            |
| 61  | 17    | 5     | 0        | 0        | 0       | 0            |
| 61  | 18    | 10    | 0        | 0        | 0       | 0            |
| 61  | 19    | 1     | 0        | 0        | 0       | 0            |
| 61  | 1A    | 1577  | 0        | 0        | 94      | 0            |
| 61  | 1B    | 43    | 0        | 0        | 2       | 0            |
| 61  | 1D    | 23    | 0        | 0        | 0       | 0            |
| 61  | 1E    | 25    | 0        | 0        | 2       | 0            |
| 61  | 1F    | 17    | 0        | 0        | 0       | 0            |
| 61  | 1G    | 3     | 0        | 0        | 1       | 0            |
| 61  | 1H    | 1     | 0        | 0        | 0       | 0            |
| 61  | 1N    | 3     | 0        | 0        | 1       | 0            |
| 61  | 1O    | 4     | 0        | 0        | 1       | 0            |
| 61  | 1P    | 20    | 0        | 0        | 3       | 0            |
| 61  | 1Q    | 4     | 0        | 0        | 0       | 0            |
| 61  | 1R    | 5     | 0        | 0        | 0       | 0            |
| 61  | 1S    | 3     | 0        | 0        | 0       | 0            |
| 61  | 1T    | 4     | 0        | 0        | 0       | 0            |
| 61  | 1U    | 9     | 0        | 0        | 0       | 0            |
| 61  | 1V    | 5     | 0        | 0        | 0       | 0            |
| 61  | 1W    | 8     | 0        | 0        | 2       | 0            |
| 61  | 1X    | 7     | 0        | 0        | 0       | 0            |
| 61  | 1Y    | 2     | 0        | 0        | 1       | 0            |
| 61  | 1Z    | 1     | 0        | 0        | 0       | 0            |
| 61  | 1a    | 287   | 0        | 0        | 0       | 0            |
| 61  | 1e    | 1     | 0        | 0        | 0       | 0            |
| 61  | 1h    | 1     | 0        | 0        | 0       | 0            |
| 61  | 1i    | 1     | 0        | 0        | 0       | 0            |
| 61  | 1l    | 4     | 0        | 0        | 0       | 0            |
| 61  | 1m    | 1     | 0        | 0        | 0       | 0            |
| 61  | 1n    | 1     | 0        | 0        | 0       | 0            |
| 61  | 1o    | 1     | 0        | 0        | 0       | 0            |
| 61  | 1p    | 1     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 6l  | 1q    | 1     | 0        | 0        | 0       | 0            |
| 6l  | 1s    | 1     | 0        | 0        | 0       | 0            |
| 6l  | 1v    | 3     | 0        | 0        | 0       | 0            |
| 6l  | 1w    | 8     | 0        | 0        | 0       | 0            |
| 6l  | 1x    | 6     | 0        | 0        | 0       | 0            |
| 6l  | 1y    | 1     | 0        | 0        | 0       | 0            |
| 6l  | 20    | 4     | 0        | 0        | 0       | 0            |
| 6l  | 21    | 3     | 0        | 0        | 0       | 0            |
| 6l  | 23    | 1     | 0        | 0        | 0       | 0            |
| 6l  | 25    | 2     | 0        | 0        | 0       | 0            |
| 6l  | 26    | 2     | 0        | 0        | 1       | 0            |
| 6l  | 28    | 5     | 0        | 0        | 0       | 0            |
| 6l  | 29    | 1     | 0        | 0        | 0       | 0            |
| 6l  | 2A    | 1063  | 0        | 0        | 90      | 0            |
| 6l  | 2B    | 10    | 0        | 0        | 1       | 0            |
| 6l  | 2D    | 20    | 0        | 0        | 0       | 0            |
| 6l  | 2E    | 9     | 0        | 0        | 1       | 0            |
| 6l  | 2F    | 7     | 0        | 0        | 0       | 0            |
| 6l  | 2I    | 1     | 0        | 0        | 0       | 0            |
| 6l  | 2N    | 2     | 0        | 0        | 1       | 0            |
| 6l  | 2O    | 1     | 0        | 0        | 0       | 0            |
| 6l  | 2P    | 14    | 0        | 0        | 1       | 0            |
| 6l  | 2Q    | 1     | 0        | 0        | 0       | 0            |
| 6l  | 2R    | 3     | 0        | 0        | 0       | 0            |
| 6l  | 2T    | 2     | 0        | 0        | 0       | 0            |
| 6l  | 2U    | 1     | 0        | 0        | 0       | 0            |
| 6l  | 2V    | 2     | 0        | 0        | 0       | 0            |
| 6l  | 2W    | 2     | 0        | 0        | 0       | 0            |
| 6l  | 2X    | 3     | 0        | 0        | 0       | 0            |
| 6l  | 2Y    | 1     | 0        | 0        | 1       | 0            |
| 6l  | 2Z    | 1     | 0        | 0        | 0       | 0            |
| 6l  | 2a    | 213   | 0        | 0        | 0       | 0            |
| 6l  | 2d    | 3     | 0        | 0        | 0       | 0            |
| 6l  | 2g    | 2     | 0        | 0        | 0       | 0            |
| 6l  | 2i    | 2     | 0        | 0        | 0       | 0            |
| 6l  | 2j    | 5     | 0        | 0        | 0       | 0            |
| 6l  | 2l    | 3     | 0        | 0        | 0       | 0            |
| 6l  | 2n    | 1     | 0        | 0        | 0       | 0            |
| 6l  | 2o    | 1     | 0        | 0        | 0       | 0            |
| 6l  | 2p    | 3     | 0        | 0        | 0       | 0            |
| 6l  | 2r    | 1     | 0        | 0        | 0       | 0            |
| 6l  | 2t    | 2     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 61  | 2v    | 1      | 0        | 0        | 0       | 0            |
| 61  | 2w    | 2      | 0        | 0        | 0       | 0            |
| 61  | 2x    | 6      | 0        | 0        | 0       | 0            |
| All | All   | 298925 | 0        | 196763   | 3133    | 1            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (3133) 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    | 1.44                     | 1.14              |
| 1:2A:79:G:H1      | 1:2A:90:U:H3      | 28.99                    | 1.03              |
| 1:1A:1059:G:H1    | 1:1A:1079:C:N4    | 1.61                     | 0.97              |
| 1:1A:2499:C:OP1   | 61:1A:4001:HOH:O  | 1.82                     | 0.97              |
| 1:1A:631:A:OP1    | 11:1P:65:ARG:NH1  | 1.98                     | 0.97              |
| 1:2A:2104:G:H1    | 1:2A:2185:C:N4    | 1.62                     | 0.94              |
| 1:1A:1082:U:O4    | 1:1A:1086:A:N1    | 1.99                     | 0.94              |
| 12:2Q:21:THR:HG21 | 12:2Q:101:ARG:HG2 | 1.50                     | 0.93              |
| 1:2A:1422:G:H5''  | 10:2O:48:PRO:HB3  | 99.11                    | 0.93              |
| 22:10:10:THR:HG22 | 22:10:12:ASN:H    | 1.32                     | 0.93              |
| 1:1A:2099:U:H3    | 1:1A:2190:G:H1    | 1.15                     | 0.92              |
| 20:1Y:92:ASN:HB3  | 20:1Y:94:LYS:H    | 1.36                     | 0.91              |
| 12:2Q:85:LYS:HG2  | 22:20:7:LEU:HB3   | 1.51                     | 0.90              |
| 1:2A:76:C:H42     | 1:2A:93:G:H1      | 26.76                    | 0.89              |
| 1:1A:1082:U:H3    | 1:1A:1086:A:H61   | 0.90                     | 0.89              |
| 21:1Z:153:SER:HB3 | 21:1Z:167:PRO:HB3 | 1.54                     | 0.88              |
| 1:2A:2121:G:H1    | 1:2A:2177:C:H42   | 1.21                     | 0.88              |
| 1:2A:2736:G:N2    | 1:2A:2768:C:O2    | 2.05                     | 0.88              |
| 1:2A:300:A:OP1    | 20:2Y:86:ARG:NH2  | 2.08                     | 0.87              |
| 1:2A:1204:A:H2    | 1:2A:1241:A:H62   | 1.24                     | 0.86              |
| 1:2A:2139:C:N4    | 1:2A:2152:G:N1    | 2.22                     | 0.86              |
| 3:2D:242:ARG:HH11 | 3:2D:242:ARG:HG3  | 1.40                     | 0.86              |
| 1:2A:198:C:OP2    | 61:2A:3701:HOH:O  | 1.94                     | 0.86              |
| 1:1A:1065:U:O2    | 1:1A:1073:A:N6    | 2.07                     | 0.86              |
| 22:20:10:THR:HG22 | 22:20:12:ASN:H    | 1.39                     | 0.86              |
| 1:1A:2136:C:H42   | 1:1A:2155:G:H1    | 1.20                     | 0.86              |
| 1:2A:2138:C:H42   | 1:2A:2153:G:H1    | 1.24                     | 0.85              |
| 1:2A:2839:G:H5'   | 13:2R:46:GLY:HA2  | 1.58                     | 0.85              |
| 8:1I:130:TYR:HB3  | 8:1I:138:ILE:HB   | 1.58                     | 0.85              |
| 1:1A:2239:G:OP2   | 61:1A:4002:HOH:O  | 1.92                     | 0.85              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:1D:242:ARG:HG3   | 3:1D:242:ARG:HH11  | 1.41                     | 0.85              |
| 1:2A:1689:A:H62    | 1:2A:1698:A:H2     | 1.20                     | 0.84              |
| 1:2A:2637:U:H5''   | 4:2E:82:ARG:HH12   | 1.41                     | 0.84              |
| 1:2A:1532:C:H42    | 1:2A:1537:G:H1     | 1.24                     | 0.83              |
| 1:2A:1310:G:H1     | 1:2A:1327:C:H42    | 25.99                    | 0.83              |
| 1:2A:792:G:O6      | 61:2A:3702:HOH:O   | 1.94                     | 0.83              |
| 10:1O:35:VAL:HG11  | 10:1O:103:ALA:HB3  | 1.61                     | 0.83              |
| 1:2A:2104:G:H1     | 1:2A:2185:C:H42    | 0.88                     | 0.83              |
| 6:2G:38:VAL:HG22   | 6:2G:93:THR:HG23   | 1.61                     | 0.82              |
| 1:1A:266:G:H5''    | 1:1A:268:C:H41     | 11.64                    | 0.82              |
| 1:1A:1602:U:O4     | 61:1A:4003:HOH:O   | 1.95                     | 0.82              |
| 1:2A:2139:C:N3     | 1:2A:2152:G:N2     | 2.26                     | 0.82              |
| 19:2X:53:LYS:HB3   | 19:2X:82:GLN:HB3   | 1.62                     | 0.81              |
| 12:1Q:111:GLU:OE2  | 12:1Q:133:ARG:NH2  | 2.13                     | 0.81              |
| 7:2H:24:VAL:HG13   | 7:2H:37:VAL:HG21   | 1.62                     | 0.81              |
| 17:2V:24:LYS:HG3   | 17:2V:64:HIS:HD2   | 1.45                     | 0.81              |
| 1:2A:878:A:N6      | 1:2A:899:A:O2'     | 2.13                     | 0.81              |
| 5:2F:53:THR:HG23   | 5:2F:55:GLY:H      | 1.45                     | 0.81              |
| 1:2A:740:U:OP2     | 61:2A:3703:HOH:O   | 1.98                     | 0.81              |
| 1:1A:1059:G:H1     | 1:1A:1079:C:H42    | 1.27                     | 0.81              |
| 1:1A:1784:A:OP2    | 61:1A:4005:HOH:O   | 1.98                     | 0.81              |
| 10:2O:35:VAL:HG11  | 10:2O:103:ALA:HB3  | 1.64                     | 0.80              |
| 1:1A:1013:C:OP2    | 61:1A:4006:HOH:O   | 1.98                     | 0.80              |
| 1:1A:2723:C:OP1    | 13:1R:3:HIS:ND1    | 2.13                     | 0.80              |
| 1:1A:568:U:O4      | 61:1A:4007:HOH:O   | 2.00                     | 0.80              |
| 1:1A:792:G:O6      | 61:1A:4004:HOH:O   | 1.98                     | 0.80              |
| 1:2A:64:A:N6       | 1:2A:90:U:O4       | 2.14                     | 0.80              |
| 1:2A:2099:U:H3     | 1:2A:2190:G:H1     | 1.30                     | 0.79              |
| 1:1A:2100:G:H1     | 1:1A:2189:U:H3     | 1.29                     | 0.79              |
| 11:2P:100:LEU:HD12 | 11:2P:112:LEU:HD11 | 1.64                     | 0.79              |
| 1:1A:2384:G:OP2    | 22:10:55:ARG:NH1   | 2.15                     | 0.79              |
| 1:1A:2136:C:N3     | 1:1A:2155:G:N2     | 2.30                     | 0.79              |
| 1:1A:1053:C:H42    | 1:1A:1106:G:H1     | 1.30                     | 0.79              |
| 1:2A:76:C:N4       | 1:2A:93:G:H1       | 25.93                    | 0.79              |
| 1:1A:1817:G:OP1    | 3:1D:88:ARG:NH2    | 2.15                     | 0.79              |
| 1:1A:998:C:OP1     | 61:1A:4011:HOH:O   | 2.01                     | 0.78              |
| 6:2G:64:THR:HB     | 6:2G:94:LEU:HD21   | 1.64                     | 0.78              |
| 1:2A:987:G:O2'     | 1:2A:1000:A:N3     | 2.14                     | 0.78              |
| 1:1A:1647:G:OP1    | 61:1A:4012:HOH:O   | 2.02                     | 0.78              |
| 20:2Y:94:LYS:NZ    | 61:2Y:601:HOH:O    | 2.17                     | 0.78              |
| 1:2A:1973:G:OP1    | 61:2A:3704:HOH:O   | 2.01                     | 0.78              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1A:1264:G:OP1   | 27:15:19:ARG:NH2  | 2.16                     | 0.78              |
| 1:1A:2447:G:OP2   | 61:1A:4009:HOH:O  | 2.01                     | 0.78              |
| 1:2A:958:U:OP2    | 12:2Q:14:ARG:NH1  | 2.17                     | 0.77              |
| 23:11:52:ARG:HH21 | 23:11:57:GLU:HG3  | 1.48                     | 0.77              |
| 1:2A:1772:G:OP1   | 61:2A:3705:HOH:O  | 2.02                     | 0.77              |
| 1:1A:1985:G:OP2   | 61:1A:4008:HOH:O  | 2.00                     | 0.77              |
| 1:2A:2615:U:OP1   | 61:2A:3706:HOH:O  | 2.02                     | 0.77              |
| 2:2B:83:G:H1      | 2:2B:94:C:H42     | 1.29                     | 0.77              |
| 3:2D:38:LYS:NZ    | 3:2D:39:LYS:O     | 2.18                     | 0.77              |
| 1:1A:1779:U:OP2   | 61:1A:4010:HOH:O  | 2.01                     | 0.77              |
| 11:1P:52:GLU:OE1  | 11:1P:55:ARG:NH1  | 2.18                     | 0.77              |
| 20:1Y:102:CYS:SG  | 20:1Y:103:GLY:N   | 2.58                     | 0.77              |
| 1:2A:971:C:OP2    | 61:2A:3707:HOH:O  | 2.03                     | 0.77              |
| 1:2A:1434:A:H61   | 1:2A:1558:A:H62   | 1.31                     | 0.77              |
| 1:1A:2448:A:OP1   | 61:1A:4001:HOH:O  | 2.02                     | 0.77              |
| 1:2A:2819:G:N7    | 61:2A:3740:HOH:O  | 2.18                     | 0.77              |
| 1:1A:2139:C:N4    | 1:1A:2152:G:H1    | 1.83                     | 0.77              |
| 1:2A:1300:U:H4'   | 1:2A:1301:A:H5'   | 1.67                     | 0.77              |
| 1:2A:527:C:N4     | 1:2A:2779:U:OP2   | 2.17                     | 0.77              |
| 1:1A:1054:A:H61   | 1:1A:1105:U:H3    | 1.34                     | 0.76              |
| 1:1A:517:C:OP1    | 27:15:16:ARG:NH2  | 2.17                     | 0.76              |
| 1:1A:2139:C:N3    | 1:1A:2152:G:N2    | 2.33                     | 0.76              |
| 11:2P:52:GLU:OE1  | 11:2P:55:ARG:NH1  | 2.19                     | 0.76              |
| 1:1A:248:G:OP1    | 61:1A:4015:HOH:O  | 2.03                     | 0.76              |
| 1:1A:1059:G:N2    | 1:1A:1079:C:N3    | 2.33                     | 0.76              |
| 23:21:51:VAL:HG11 | 23:21:74:VAL:HG21 | 1.67                     | 0.76              |
| 1:2A:1022:G:H22   | 1:2A:1142(A):A:H2 | 1.34                     | 0.76              |
| 1:1A:2574:G:OP1   | 61:1A:4014:HOH:O  | 2.03                     | 0.76              |
| 12:2Q:26:TYR:O    | 12:2Q:67:ARG:NH1  | 2.19                     | 0.75              |
| 1:2A:1007:C:N3    | 1:2A:1022:G:O6    | 16.72                    | 0.75              |
| 1:2A:1801:G:OP2   | 3:2D:154:LYS:NZ   | 2.19                     | 0.75              |
| 1:2A:1171:G:H1    | 1:2A:1178:C:H42   | 1.32                     | 0.75              |
| 1:2A:2139:C:N4    | 1:2A:2152:G:H1    | 1.82                     | 0.75              |
| 19:2X:8:ILE:O     | 24:22:36:ARG:NH2  | 2.19                     | 0.75              |
| 1:2A:1830:C:OP2   | 61:2A:3709:HOH:O  | 2.05                     | 0.75              |
| 1:1A:1815:A:N1    | 61:1A:4058:HOH:O  | 2.20                     | 0.75              |
| 9:2N:128:HIS:O    | 9:2N:131:GLN:NE2  | 2.19                     | 0.75              |
| 7:1H:159:GLU:HG2  | 7:1H:169:VAL:HG11 | 1.67                     | 0.75              |
| 21:2Z:106:GLY:HA3 | 21:2Z:141:VAL:H   | 1.50                     | 0.75              |
| 1:1A:2136:C:N4    | 1:1A:2155:G:H1    | 1.83                     | 0.75              |
| 1:2A:1652:A:OP1   | 13:2R:8:ARG:NH1   | 2.20                     | 0.75              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:2A:143:G:H4'    | 19:2X:35:THR:HG21  | 1.69                     | 0.75              |
| 12:2Q:67:ARG:O    | 12:2Q:101:ARG:NH2  | 2.20                     | 0.75              |
| 1:2A:195:A:N7     | 61:2A:3701:HOH:O   | 2.19                     | 0.75              |
| 1:2A:2134:A:O2'   | 1:2A:2159:G:N2     | 2.15                     | 0.75              |
| 1:1A:1105:U:H2'   | 1:1A:1106:G:H8     | 1.52                     | 0.74              |
| 1:1A:1986:A:OP1   | 61:1A:4013:HOH:O   | 2.03                     | 0.74              |
| 29:17:24:THR:HG22 | 29:17:27:GLY:H     | 1.52                     | 0.74              |
| 1:2A:2364:C:OP1   | 22:20:55:ARG:NH1   | 2.20                     | 0.74              |
| 1:2A:301:G:OP2    | 20:2Y:84:ARG:NH2   | 2.20                     | 0.74              |
| 1:2A:2063:C:OP1   | 61:2A:3708:HOH:O   | 2.04                     | 0.74              |
| 1:2A:1264:G:OP1   | 27:25:19:ARG:NH2   | 2.20                     | 0.74              |
| 1:2A:833:U:O2     | 11:2P:55:ARG:NH2   | 2.20                     | 0.74              |
| 1:1A:1798:U:H5'   | 3:1D:259:THR:HG22  | 1.70                     | 0.74              |
| 1:1A:72:U:OP1     | 61:1A:4017:HOH:O   | 2.06                     | 0.74              |
| 1:2A:2807:G:N1    | 1:2A:2893:G:O6     | 2.20                     | 0.74              |
| 14:2S:38:GLN:NE2  | 14:2S:47:THR:OG1   | 2.20                     | 0.74              |
| 1:2A:765:G:H1     | 1:2A:812:C:HO2'    | 84.31                    | 0.74              |
| 1:2A:2012:G:OP1   | 18:2W:11:ARG:NH2   | 2.19                     | 0.74              |
| 2:1B:105:A:OP1    | 21:1Z:72:ARG:NH1   | 2.21                     | 0.74              |
| 1:2A:1155:A:H5''  | 16:2U:55:ARG:HH11  | 1.52                     | 0.74              |
| 1:1A:2124:G:H1    | 1:1A:2174:C:H42    | 1.33                     | 0.73              |
| 1:2A:2127:G:O6    | 1:2A:2161:C:N3     | 2.21                     | 0.73              |
| 21:2Z:150:LEU:HB3 | 21:2Z:171:ILE:HD11 | 1.70                     | 0.73              |
| 3:1D:38:LYS:NZ    | 3:1D:39:LYS:O      | 2.20                     | 0.73              |
| 1:1A:981:A:OP1    | 61:1A:4018:HOH:O   | 2.06                     | 0.73              |
| 1:2A:253:C:O2'    | 61:2A:3710:HOH:O   | 2.05                     | 0.73              |
| 1:2A:2042:A:OP1   | 61:2A:3712:HOH:O   | 2.07                     | 0.73              |
| 1:1A:301:G:OP2    | 20:1Y:84:ARG:NH2   | 2.21                     | 0.73              |
| 1:1A:400:G:N7     | 61:1A:4067:HOH:O   | 2.21                     | 0.73              |
| 1:1A:279:C:H42    | 1:1A:361:G:H1      | 1.37                     | 0.73              |
| 1:2A:1530:C:O2'   | 1:2A:1531:C:O5'    | 2.06                     | 0.73              |
| 1:2A:83:G:H1      | 1:2A:102:G:HO2'    | 1.34                     | 0.73              |
| 1:1A:2196:C:OP2   | 61:1A:4016:HOH:O   | 2.05                     | 0.73              |
| 8:2I:43:ASN:ND2   | 23:21:75:GLU:OE2   | 2.22                     | 0.73              |
| 1:1A:1324:G:O6    | 61:1A:4019:HOH:O   | 2.07                     | 0.73              |
| 2:2B:55:U:H1'     | 6:2G:29:TRP:HE1    | 1.54                     | 0.73              |
| 1:2A:527:C:OP1    | 61:2A:3711:HOH:O   | 2.06                     | 0.73              |
| 1:1A:2749:A:OP1   | 7:1H:3:ARG:NH1     | 2.22                     | 0.73              |
| 1:2A:1031:G:N3    | 31:29:36:GLN:NE2   | 2.37                     | 0.72              |
| 13:1R:67:LEU:HD13 | 13:1R:76:VAL:HG21  | 1.71                     | 0.72              |
| 15:2T:119:LYS:HG2 | 15:2T:123:GLN:HE21 | 1.53                     | 0.72              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:1A:1070:A:N7    | 1:1A:1096:A:O2'    | 2.18                     | 0.72              |
| 1:1A:1783:A:OP1   | 61:1A:4005:HOH:O   | 2.07                     | 0.72              |
| 1:2A:307:G:N1     | 1:2A:310:A:OP2     | 2.22                     | 0.72              |
| 1:1A:1041:C:H42   | 1:1A:1114:G:H1     | 1.34                     | 0.72              |
| 1:2A:2129:C:H42   | 1:2A:2159:G:H1     | 1.37                     | 0.72              |
| 1:2A:2206:G:H5''  | 1:2A:2207:G:C6     | 2.25                     | 0.72              |
| 12:2Q:34:LEU:HB2  | 12:2Q:118:LEU:HD22 | 1.71                     | 0.72              |
| 1:1A:1173:G:O2'   | 1:1A:1174:A:O4'    | 2.07                     | 0.72              |
| 1:1A:1422:G:H5''  | 10:1O:48:PRO:HB3   | 99.43                    | 0.72              |
| 1:1A:973:A:OP2    | 61:1A:4007:HOH:O   | 2.07                     | 0.72              |
| 31:29:25:VAL:HB   | 31:29:34:GLN:HB2   | 1.70                     | 0.72              |
| 1:2A:2141:G:O6    | 1:2A:2150:U:O2     | 2.07                     | 0.72              |
| 1:1A:1169:G:H2'   | 1:1A:1170:G:H5''   | 1.72                     | 0.72              |
| 1:2A:1798:U:H5'   | 3:2D:259:THR:HG22  | 1.72                     | 0.71              |
| 3:1D:180:GLY:HA3  | 3:1D:275:LYS:HG3   | 1.70                     | 0.71              |
| 1:1A:2807:G:N1    | 1:1A:2893:G:O6     | 2.18                     | 0.71              |
| 1:1A:1315:C:OP2   | 61:1A:4022:HOH:O   | 2.08                     | 0.71              |
| 1:1A:400:G:O6     | 61:1A:4021:HOH:O   | 2.08                     | 0.71              |
| 3:2D:71:ASP:OD2   | 3:2D:103:ARG:NH2   | 2.22                     | 0.71              |
| 1:2A:1324:G:O6    | 61:2A:3715:HOH:O   | 2.09                     | 0.71              |
| 1:1A:271(R):G:OP1 | 23:11:76:ARG:NH1   | 2.22                     | 0.71              |
| 1:2A:2234:G:N7    | 61:2A:3767:HOH:O   | 2.22                     | 0.71              |
| 4:2E:34:VAL:HG21  | 4:2E:78:LEU:HD23   | 1.71                     | 0.71              |
| 2:2B:41:U:H5      | 6:2G:70:VAL:H      | 1.36                     | 0.71              |
| 1:2A:399:G:OP2    | 61:2A:3713:HOH:O   | 2.07                     | 0.71              |
| 1:2A:2595:G:N7    | 61:2A:3776:HOH:O   | 2.24                     | 0.71              |
| 1:2A:197:A:OP1    | 61:2A:3701:HOH:O   | 2.09                     | 0.71              |
| 1:2A:2753:A:N3    | 31:29:15:LYS:NZ    | 2.38                     | 0.71              |
| 3:1D:17:THR:O     | 3:1D:211:ARG:NH2   | 2.23                     | 0.70              |
| 1:1A:740:U:OP2    | 61:1A:4005:HOH:O   | 2.08                     | 0.70              |
| 1:2A:1645:G:H5''  | 1:2A:1646:C:H5'    | 1.72                     | 0.70              |
| 1:1A:563:G:OP2    | 61:1A:4020:HOH:O   | 2.07                     | 0.70              |
| 1:1A:2144:U:O2    | 1:1A:2147:G:N1     | 2.20                     | 0.70              |
| 1:1A:1630:G:O2'   | 61:1A:4023:HOH:O   | 2.09                     | 0.70              |
| 1:1A:1354:A:H4'   | 3:1D:38:LYS:HE2    | 1.73                     | 0.70              |
| 1:2A:1297:C:OP2   | 61:2A:3716:HOH:O   | 2.10                     | 0.70              |
| 1:2A:1189:A:OP2   | 61:2A:3714:HOH:O   | 2.08                     | 0.70              |
| 2:2B:93:G:OP1     | 21:2Z:79:ARG:NH2   | 2.18                     | 0.70              |
| 1:2A:1028:A:N6    | 1:2A:1125:G:H2'    | 2.07                     | 0.69              |
| 1:2A:1315:C:OP2   | 61:2A:3719:HOH:O   | 2.10                     | 0.69              |
| 11:2P:39:LYS:HB2  | 11:2P:45:LEU:HG    | 1.72                     | 0.69              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1A:2469:A:O2'   | 12:1Q:56:ARG:NH1  | 2.25                     | 0.69              |
| 1:1A:847:U:OP2    | 61:1A:4024:HOH:O  | 2.10                     | 0.69              |
| 1:1A:2612:C:OP2   | 27:15:2:ALA:N     | 2.25                     | 0.69              |
| 1:2A:994:C:OP1    | 16:2U:53:ARG:NH2  | 2.25                     | 0.69              |
| 1:1A:1332:G:OP1   | 61:1A:4022:HOH:O  | 2.10                     | 0.69              |
| 2:2B:106:G:H5'    | 21:2Z:31:ARG:HG2  | 1.74                     | 0.69              |
| 1:1A:2049:G:N7    | 61:1A:4080:HOH:O  | 2.24                     | 0.69              |
| 5:2F:101:LEU:O    | 5:2F:106:ARG:NH1  | 2.25                     | 0.69              |
| 1:2A:2857:G:N2    | 1:2A:2860:A:OP2   | 2.26                     | 0.69              |
| 1:2A:821:A:N1     | 61:2A:3781:HOH:O  | 2.25                     | 0.69              |
| 1:1A:880:G:H2'    | 1:1A:881:G:H8     | 1.58                     | 0.69              |
| 23:21:50:ARG:HG2  | 23:21:59:THR:HG22 | 1.74                     | 0.69              |
| 14:2S:67:ARG:HG2  | 14:2S:71:ARG:HD2  | 1.74                     | 0.69              |
| 1:2A:2624:G:N7    | 61:2A:3785:HOH:O  | 2.26                     | 0.69              |
| 20:2Y:102:CYS:SG  | 20:2Y:103:GLY:N   | 2.64                     | 0.69              |
| 2:1B:48:A:H4'     | 14:1S:95:HIS:HD2  | 1.56                     | 0.69              |
| 1:2A:1021:A:H62   | 1:2A:1141:U:H3    | 1.40                     | 0.69              |
| 1:2A:854:G:H2'    | 1:2A:855:G:H8     | 1.58                     | 0.69              |
| 15:2T:65:LYS:HE3  | 15:2T:67:SER:HB2  | 1.74                     | 0.68              |
| 1:1A:2139:C:N4    | 1:1A:2152:G:N1    | 2.41                     | 0.68              |
| 1:2A:2127:G:N1    | 1:2A:2161:C:O2    | 2.27                     | 0.68              |
| 1:1A:2312:U:H5'   | 6:1G:88:ILE:HD11  | 1.75                     | 0.68              |
| 1:1A:392:C:OP1    | 61:1A:4028:HOH:O  | 2.11                     | 0.68              |
| 1:2A:1036:G:OP2   | 7:2H:59:ARG:NH2   | 2.26                     | 0.68              |
| 1:2A:946:G:OP1    | 61:2A:3717:HOH:O  | 2.10                     | 0.68              |
| 1:2A:2637:U:H5''  | 4:2E:82:ARG:NH1   | 2.08                     | 0.68              |
| 21:2Z:153:SER:HB3 | 21:2Z:167:PRO:HB3 | 1.75                     | 0.68              |
| 5:2F:143:ALA:HB1  | 5:2F:148:LEU:HB2  | 1.76                     | 0.68              |
| 18:2W:88:ARG:NH1  | 18:2W:94:ASP:OD2  | 2.25                     | 0.68              |
| 1:1A:1014:U:OP2   | 61:1A:4006:HOH:O  | 2.11                     | 0.68              |
| 1:1A:2124:G:H1    | 1:1A:2174:C:N4    | 1.91                     | 0.68              |
| 6:1G:3:LEU:O      | 6:1G:8:LYS:NZ     | 2.21                     | 0.68              |
| 1:1A:1664:A:OP1   | 61:1A:4026:HOH:O  | 2.10                     | 0.68              |
| 1:1A:1968:G:OP1   | 61:1A:4030:HOH:O  | 2.12                     | 0.68              |
| 1:2A:1622:G:OP2   | 61:2A:3723:HOH:O  | 2.12                     | 0.68              |
| 1:1A:2719:G:OP2   | 61:1A:4029:HOH:O  | 2.11                     | 0.68              |
| 1:2A:2836:U:H2'   | 1:2A:2837:G:C8    | 2.29                     | 0.68              |
| 1:1A:2589:A:N7    | 61:1A:4096:HOH:O  | 2.26                     | 0.68              |
| 1:2A:568:U:H5'    | 1:2A:945:A:N1     | 2.09                     | 0.68              |
| 1:2A:1019:U:HO2'  | 1:2A:1021:A:H2    | 1.42                     | 0.68              |
| 1:2A:900:A:O2'    | 1:2A:901:A:OP1    | 2.11                     | 0.68              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 15:1T:112:ARG:HG3 | 15:1T:115:ARG:HH21 | 1.58                     | 0.68              |
| 1:1A:1701:A:OP2   | 61:1A:4027:HOH:O   | 2.10                     | 0.68              |
| 1:1A:2014:A:N1    | 61:1A:4086:HOH:O   | 2.25                     | 0.68              |
| 1:2A:1592:C:H2'   | 1:2A:1593:G:H8     | 1.58                     | 0.68              |
| 1:2A:886:C:O2'    | 1:2A:889:C:N4      | 2.25                     | 0.67              |
| 1:2A:643:A:N1     | 1:2A:2369:A:O2'    | 2.25                     | 0.67              |
| 1:1A:1385:G:O2'   | 1:1A:1396:U:O2     | 2.11                     | 0.67              |
| 1:2A:1796:U:H2'   | 1:2A:1797:C:C6     | 2.29                     | 0.67              |
| 1:2A:624:C:OP1    | 61:2A:3720:HOH:O   | 2.11                     | 0.67              |
| 5:2F:53:THR:HG22  | 5:2F:56:GLU:HG3    | 1.77                     | 0.67              |
| 5:2F:20:LEU:HD23  | 5:2F:22:ALA:HB2    | 1.76                     | 0.67              |
| 1:2A:1314:C:OP1   | 61:2A:3719:HOH:O   | 2.11                     | 0.67              |
| 4:2E:116:VAL:HG13 | 4:2E:122:PHE:HB2   | 1.75                     | 0.67              |
| 2:1B:33:G:H5'     | 6:1G:2:PRO:HD3     | 1.77                     | 0.67              |
| 1:2A:921:G:O6     | 61:2A:3718:HOH:O   | 2.10                     | 0.67              |
| 10:2O:68:GLU:HB3  | 10:2O:78:ARG:HG3   | 1.76                     | 0.67              |
| 1:2A:1912:A:OP1   | 61:2A:3722:HOH:O   | 2.12                     | 0.67              |
| 25:13:5:LYS:NZ    | 25:13:34:GLU:OE2   | 2.25                     | 0.67              |
| 4:1E:47:VAL:HG21  | 4:1E:86:PRO:HD2    | 1.76                     | 0.67              |
| 1:1A:1054:A:N6    | 1:1A:1105:U:H3     | 1.92                     | 0.67              |
| 1:1A:2592:G:OP1   | 61:1A:4033:HOH:O   | 2.13                     | 0.67              |
| 16:1U:52:ARG:HH11 | 16:1U:55:ARG:HH21  | 1.42                     | 0.67              |
| 1:2A:2640:G:N7    | 61:2A:3753:HOH:O   | 2.26                     | 0.67              |
| 18:1W:31:GLU:OE1  | 61:1W:3101:HOH:O   | 2.12                     | 0.67              |
| 1:2A:2632:A:HO2'  | 1:2A:2811:G:HO2'   | 1.36                     | 0.67              |
| 11:2P:87:ASP:O    | 11:2P:90:ARG:NH1   | 2.29                     | 0.66              |
| 1:2A:1031:G:H5''  | 31:29:8:LYS:HE3    | 1.76                     | 0.66              |
| 1:2A:882:G:H2'    | 1:2A:883:G:C8      | 2.30                     | 0.66              |
| 1:2A:2630:G:N2    | 1:2A:2788:C:O2     | 2.19                     | 0.66              |
| 1:2A:881:G:H1     | 1:2A:895:U:H3      | 1.41                     | 0.66              |
| 1:1A:1053:C:N4    | 1:1A:1106:G:H1     | 1.93                     | 0.66              |
| 19:2X:35:THR:HG22 | 19:2X:38:GLU:H     | 1.59                     | 0.66              |
| 1:1A:1452:A:OP2   | 61:1A:4036:HOH:O   | 2.13                     | 0.66              |
| 1:2A:2105:C:H2'   | 1:2A:2106:G:H8     | 1.60                     | 0.66              |
| 1:2A:77:C:O2'     | 24:22:14:ARG:NH2   | 2.28                     | 0.66              |
| 1:2A:1005:C:H2'   | 1:2A:1006:C:C6     | 2.31                     | 0.66              |
| 11:1P:59:LEU:HD11 | 30:18:10:ALA:HB2   | 1.77                     | 0.66              |
| 1:1A:2483:C:N3    | 12:1Q:124:LYS:NZ   | 2.39                     | 0.66              |
| 1:1A:607:U:OP1    | 5:1F:102:PRO:HA    | 1.96                     | 0.66              |
| 9:2N:94:HIS:HB3   | 9:2N:97:ARG:HD3    | 1.77                     | 0.66              |
| 1:1A:674:G:H2'    | 1:1A:675:A:H8      | 4.73                     | 0.66              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:1I:93:THR:H     | 8:1I:96:ASP:HB2   | 1.60                     | 0.66              |
| 1:2A:1762:A:N1    | 61:2A:3805:HOH:O  | 2.29                     | 0.66              |
| 1:1A:1642:G:N7    | 61:1A:4101:HOH:O  | 2.27                     | 0.66              |
| 8:1I:104:GLN:O    | 8:1I:106:GLY:N    | 2.28                     | 0.66              |
| 1:2A:2121:G:H1    | 1:2A:2177:C:N4    | 1.92                     | 0.66              |
| 1:2A:2171:A:N3    | 1:2A:2172:U:N3    | 2.44                     | 0.66              |
| 2:1B:48:A:OP2     | 14:1S:30:ARG:NH2  | 2.28                     | 0.66              |
| 1:2A:11:G:H2'     | 1:2A:12:U:H5'     | 1.77                     | 0.66              |
| 1:1A:2059:A:OP2   | 61:1A:4034:HOH:O  | 2.13                     | 0.66              |
| 19:2X:57:LEU:HD11 | 19:2X:78:LYS:HE2  | 1.77                     | 0.66              |
| 8:2I:87:LYS:NZ    | 8:2I:122:GLU:OE2  | 2.25                     | 0.66              |
| 1:2A:2133:G:H22   | 1:2A:2157:G:H1'   | 1.61                     | 0.66              |
| 1:1A:1267:U:OP1   | 61:1A:4037:HOH:O  | 2.14                     | 0.66              |
| 1:2A:992:C:OP1    | 16:2U:47:TYR:OH   | 2.08                     | 0.66              |
| 1:1A:730:C:OP2    | 61:1A:4032:HOH:O  | 2.12                     | 0.66              |
| 1:2A:2136:C:HO2'  | 1:2A:2137:C:P     | 2.18                     | 0.65              |
| 1:1A:583:G:OP2    | 16:1U:10:ARG:NH1  | 2.29                     | 0.65              |
| 1:2A:974:G:N7     | 61:2A:3707:HOH:O  | 2.29                     | 0.65              |
| 21:1Z:69:THR:HG22 | 21:1Z:90:VAL:HA   | 1.78                     | 0.65              |
| 1:1A:1783:A:N7    | 61:1A:4121:HOH:O  | 2.29                     | 0.65              |
| 2:1B:102:A:N7     | 61:1B:3102:HOH:O  | 2.28                     | 0.65              |
| 1:2A:2232:U:P     | 23:21:40:ARG:HH12 | 2.19                     | 0.65              |
| 1:1A:2759:G:N7    | 61:1A:4113:HOH:O  | 2.28                     | 0.65              |
| 7:2H:23:ARG:NH1   | 7:2H:34:GLU:OE1   | 2.30                     | 0.65              |
| 1:1A:2029:G:OP2   | 61:1A:4035:HOH:O  | 2.13                     | 0.65              |
| 1:2A:276:A:H5''   | 1:2A:277:C:H5'    | 1.79                     | 0.65              |
| 1:2A:662:G:OP1    | 61:2A:3726:HOH:O  | 2.14                     | 0.65              |
| 1:1A:2134:A:H62   | 1:1A:2157:G:H1'   | 1.62                     | 0.65              |
| 1:2A:861:A:N3     | 2:2B:79:C:O2'     | 2.29                     | 0.65              |
| 1:1A:2763:G:OP2   | 61:1A:4040:HOH:O  | 2.15                     | 0.65              |
| 1:2A:1671:U:OP2   | 61:2A:3725:HOH:O  | 2.13                     | 0.65              |
| 1:1A:2415:G:OP1   | 61:1A:4042:HOH:O  | 2.15                     | 0.65              |
| 5:1F:185:ASP:HA   | 5:1F:188:ARG:HD3  | 1.79                     | 0.65              |
| 1:1A:18:C:O2'     | 1:1A:554:U:OP1    | 2.15                     | 0.65              |
| 17:2V:72:VAL:HG13 | 17:2V:85:LYS:HB2  | 1.78                     | 0.65              |
| 11:2P:59:LEU:HD11 | 30:28:10:ALA:HB2  | 1.79                     | 0.65              |
| 3:2D:69:ARG:HE    | 3:2D:130:ALA:HB2  | 1.62                     | 0.65              |
| 26:24:33:VAL:HG12 | 26:24:35:VAL:H    | 1.61                     | 0.65              |
| 1:2A:2070:G:OP2   | 61:2A:3727:HOH:O  | 2.14                     | 0.65              |
| 1:1A:2328:A:H2'   | 1:1A:2329:G:C8    | 2.31                     | 0.65              |
| 1:2A:880:G:H2'    | 1:2A:881:G:H8     | 1.62                     | 0.65              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:2A:2116:G:N2    | 1:2A:2162:G:OP1   | 2.30                     | 0.65              |
| 7:1H:86:GLU:OE2   | 7:1H:132:ARG:NH2  | 2.30                     | 0.65              |
| 1:1A:2815:C:H5'   | 27:15:29:THR:HG21 | 1.77                     | 0.65              |
| 1:1A:1155:A:OP1   | 16:1U:55:ARG:HD2  | 1.97                     | 0.64              |
| 1:2A:2547:U:O2    | 10:2O:23:ARG:NH2  | 2.29                     | 0.64              |
| 1:2A:2287:A:H62   | 1:2A:2344:U:H3    | 1.45                     | 0.64              |
| 1:1A:2810:A:N6    | 1:1A:2891:G:O2'   | 2.28                     | 0.64              |
| 1:1A:987:G:O2'    | 1:1A:1000:A:N3    | 2.30                     | 0.64              |
| 1:1A:1173:G:O2'   | 1:1A:1174:A:O5'   | 2.16                     | 0.64              |
| 1:1A:993:G:OP1    | 16:1U:50:ARG:NH2  | 2.29                     | 0.64              |
| 16:1U:50:ARG:HH12 | 17:1V:72:VAL:HA   | 1.60                     | 0.64              |
| 1:1A:2278:A:OP2   | 22:10:12:ASN:ND2  | 2.30                     | 0.64              |
| 1:2A:1015:G:H2'   | 1:2A:1016:G:H8    | 1.61                     | 0.64              |
| 1:1A:1156:A:OP1   | 16:1U:55:ARG:NH1  | 2.29                     | 0.64              |
| 1:2A:2070:G:H2'   | 1:2A:2071:A:H8    | 1.62                     | 0.64              |
| 13:2R:67:LEU:HD13 | 13:2R:76:VAL:HG21 | 1.79                     | 0.64              |
| 1:1A:2871:C:N3    | 61:1A:4123:HOH:O  | 2.30                     | 0.64              |
| 1:1A:2136:C:N4    | 1:1A:2155:G:N1    | 2.35                     | 0.64              |
| 4:1E:56:PRO:HG3   | 4:1E:74:PRO:HG2   | 1.80                     | 0.64              |
| 1:1A:380:U:OP1    | 61:1A:4041:HOH:O  | 2.15                     | 0.64              |
| 1:2A:2849:U:H4'   | 1:2A:2868:A:C2    | 2.33                     | 0.64              |
| 5:2F:184:TYR:CE2  | 5:2F:188:ARG:HD2  | 2.32                     | 0.64              |
| 9:2N:68:GLU:HG3   | 9:2N:69:GLN:HG3   | 1.79                     | 0.64              |
| 1:2A:41:C:H2'     | 1:2A:42:G:H8      | 1.62                     | 0.64              |
| 1:1A:1070:A:H5''  | 1:1A:1072:C:OP1   | 1.97                     | 0.64              |
| 1:1A:1048:A:OP2   | 1:1A:1109:C:N4    | 2.30                     | 0.64              |
| 1:2A:2104:G:N2    | 1:2A:2185:C:N3    | 2.37                     | 0.64              |
| 2:1B:13:A:N1      | 2:1B:69:G:O2'     | 2.27                     | 0.64              |
| 1:2A:2365:G:N7    | 30:28:39:LYS:NZ   | 2.40                     | 0.64              |
| 12:2Q:27:VAL:O    | 12:2Q:29:PHE:N    | 2.30                     | 0.64              |
| 1:1A:2849:U:OP2   | 15:1T:95:ARG:NH1  | 2.30                     | 0.64              |
| 1:1A:1174:A:H4'   | 1:1A:1175:U:OP1   | 1.96                     | 0.64              |
| 1:2A:2126:A:H61   | 1:2A:2162:G:HO2'  | 1.46                     | 0.64              |
| 1:1A:1796:U:H2'   | 1:1A:1797:C:C6    | 2.31                     | 0.64              |
| 1:2A:2727:G:O2'   | 10:2O:70:LYS:NZ   | 2.30                     | 0.64              |
| 1:2A:2138:C:N4    | 1:2A:2153:G:H1    | 1.94                     | 0.64              |
| 30:28:33:ASN:HA   | 30:28:36:LYS:HD2  | 1.79                     | 0.64              |
| 26:14:55:ARG:H    | 26:14:56:VAL:HA   | 1.62                     | 0.64              |
| 1:2A:400:G:N7     | 61:2A:3814:HOH:O  | 2.30                     | 0.64              |
| 1:2A:1670:C:OP1   | 61:2A:3725:HOH:O  | 2.15                     | 0.64              |
| 1:2A:2590:A:O3'   | 3:2D:239:ARG:NH2  | 2.31                     | 0.64              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:2A:2126:A:N6    | 1:2A:2163:C:O4'   | 2.31                     | 0.64              |
| 1:1A:1453:U:OP1   | 13:1R:77:ARG:NH1  | 2.29                     | 0.64              |
| 1:1A:1587:A:H2'   | 1:1A:1588:C:C6    | 2.33                     | 0.64              |
| 1:2A:2454:G:O6    | 61:2A:3730:HOH:O  | 2.15                     | 0.64              |
| 3:1D:108:PRO:HB3  | 3:1D:143:HIS:CE1  | 2.32                     | 0.64              |
| 1:2A:1012:U:H5    | 9:2N:28:THR:HG21  | 1.63                     | 0.63              |
| 8:2I:4:ILE:HD11   | 8:2I:44:LEU:HD12  | 1.80                     | 0.63              |
| 1:1A:1143:A:OP2   | 61:1A:4043:HOH:O  | 2.15                     | 0.63              |
| 1:2A:1147:C:H2'   | 1:2A:1148:A:H8    | 1.62                     | 0.63              |
| 1:2A:2070:G:H2'   | 1:2A:2071:A:C8    | 2.33                     | 0.63              |
| 1:1A:2105:C:H2'   | 1:1A:2106:G:C8    | 2.34                     | 0.63              |
| 1:2A:2385:C:OP1   | 61:2A:3731:HOH:O  | 2.15                     | 0.63              |
| 1:1A:363:G:H2'    | 1:1A:363(A):A:H8  | 1.63                     | 0.63              |
| 1:1A:2687:U:OP2   | 61:1A:4044:HOH:O  | 2.15                     | 0.63              |
| 7:2H:101:ARG:NH2  | 7:2H:121:ILE:O    | 2.31                     | 0.63              |
| 24:12:32:LEU:HD11 | 24:12:54:LYS:HG2  | 1.81                     | 0.63              |
| 1:1A:1889:A:H2'   | 1:1A:1890:A:C8    | 2.34                     | 0.63              |
| 1:2A:84:A:H5'     | 20:2Y:8:LYS:HG2   | 1.80                     | 0.63              |
| 1:2A:1803:A:O2'   | 3:2D:259:THR:HG21 | 1.98                     | 0.63              |
| 1:2A:1713:U:H2'   | 1:2A:1714:G:H8    | 1.64                     | 0.63              |
| 1:1A:516:C:OP1    | 27:15:13:LYS:NZ   | 2.32                     | 0.63              |
| 4:2E:179:GLU:HG3  | 15:2T:9:LEU:HD21  | 1.79                     | 0.63              |
| 5:2F:21:ALA:HB3   | 5:2F:22:ALA:HA    | 1.81                     | 0.63              |
| 1:2A:890:A:H2'    | 1:2A:892:G:H8     | 1.62                     | 0.63              |
| 8:2I:40:THR:O     | 8:2I:44:LEU:HB2   | 1.98                     | 0.63              |
| 1:1A:1113:U:H2'   | 1:1A:1114:G:C8    | 2.33                     | 0.63              |
| 1:1A:1113:U:H2'   | 1:1A:1114:G:H8    | 1.63                     | 0.63              |
| 1:2A:2630:G:H2'   | 1:2A:2631:G:C8    | 2.34                     | 0.63              |
| 26:24:44:THR:O    | 26:24:46:GLN:N    | 2.32                     | 0.63              |
| 1:1A:2336:A:H61   | 22:10:43:THR:HG22 | 1.62                     | 0.63              |
| 1:2A:2608:G:N7    | 61:2A:3811:HOH:O  | 2.30                     | 0.63              |
| 5:1F:178:PRO:HB2  | 5:1F:201:VAL:HG21 | 1.81                     | 0.63              |
| 14:2S:50:SER:O    | 14:2S:76:LYS:NZ   | 2.21                     | 0.63              |
| 6:2G:79:ASN:OD1   | 6:2G:79:ASN:N     | 2.22                     | 0.63              |
| 1:2A:2176:A:H2'   | 1:2A:2177:C:C6    | 2.34                     | 0.63              |
| 1:1A:1357:U:O4    | 61:1A:4025:HOH:O  | 2.10                     | 0.63              |
| 1:2A:247:G:H4'    | 1:2A:386:G:C5     | 2.34                     | 0.63              |
| 1:2A:2693:A:H2'   | 1:2A:2694:G:H8    | 1.63                     | 0.63              |
| 1:2A:2022:U:O2'   | 1:2A:2617:C:H5'   | 1.98                     | 0.62              |
| 1:2A:582:G:H2'    | 1:2A:583:G:C8     | 2.34                     | 0.62              |
| 1:1A:1989:G:O6    | 61:1A:4031:HOH:O  | 2.12                     | 0.62              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:2A:648:G:O2'    | 1:2A:2351:G:OP1    | 2.15                     | 0.62              |
| 8:1I:106:GLY:HA2  | 8:1I:107:VAL:O     | 1.99                     | 0.62              |
| 1:2A:2737:G:O6    | 61:2A:3724:HOH:O   | 2.12                     | 0.62              |
| 17:1V:34:GLU:HB3  | 17:1V:56:SER:HB2   | 1.80                     | 0.62              |
| 1:2A:1012:U:OP1   | 16:2U:75:ASN:ND2   | 2.25                     | 0.62              |
| 1:2A:602:G:O2'    | 1:2A:655:A:N6      | 2.32                     | 0.62              |
| 2:2B:80:U:H2'     | 2:2B:81:G:C8       | 2.34                     | 0.62              |
| 1:1A:1653:G:H3'   | 13:1R:2:ARG:HD3    | 1.81                     | 0.62              |
| 27:25:16:ARG:NH1  | 27:25:17:ASP:OD1   | 2.31                     | 0.62              |
| 1:2A:1310:G:H1    | 1:2A:1327:C:N4     | 26.41                    | 0.62              |
| 13:1R:33:ARG:HB2  | 13:1R:115:GLU:HB3  | 1.80                     | 0.62              |
| 11:2P:88:LEU:HD11 | 11:2P:114:ILE:HD12 | 1.80                     | 0.62              |
| 1:2A:302:C:H42    | 1:2A:315:G:H1      | 1.47                     | 0.62              |
| 1:2A:897:C:H3'    | 1:2A:898:C:C6      | 2.35                     | 0.62              |
| 6:1G:41:GLN:NE2   | 6:1G:154:GLY:O     | 2.32                     | 0.62              |
| 11:1P:50:ARG:HD3  | 30:18:7:HIS:CD2    | 2.34                     | 0.62              |
| 1:2A:2296:U:OP2   | 14:2S:9:ARG:NH2    | 2.30                     | 0.62              |
| 2:1B:23:G:O6      | 61:1B:3101:HOH:O   | 2.11                     | 0.62              |
| 26:14:61:ARG:HG3  | 26:14:62:ARG:N     | 2.15                     | 0.62              |
| 1:2A:1019:U:H3    | 1:2A:1142(A):A:H62 | 1.48                     | 0.62              |
| 1:2A:2365:G:O6    | 30:28:43:GLN:NE2   | 2.28                     | 0.62              |
| 5:1F:116:ASP:OD1  | 5:1F:119:ARG:NH2   | 2.32                     | 0.62              |
| 1:1A:322:A:OP1    | 5:1F:168:ARG:HD2   | 2.00                     | 0.62              |
| 1:2A:674:G:H2'    | 1:2A:675:A:H8      | 4.71                     | 0.62              |
| 1:2A:2674:G:H5''  | 10:2O:26:LYS:HE3   | 1.82                     | 0.62              |
| 1:1A:1238:G:OP2   | 61:1A:4045:HOH:O   | 2.16                     | 0.62              |
| 1:1A:1187:G:H5''  | 17:1V:81:TYR:CE1   | 2.34                     | 0.62              |
| 15:1T:49:VAL:HG12 | 15:1T:63:VAL:HG22  | 1.80                     | 0.62              |
| 5:1F:161:GLU:HG2  | 5:1F:164:ARG:NH2   | 2.15                     | 0.62              |
| 5:2F:197:ASP:OD1  | 5:2F:198:ALA:N     | 2.31                     | 0.62              |
| 1:2A:568:U:O4     | 61:2A:3728:HOH:O   | 2.14                     | 0.62              |
| 30:28:26:LYS:HB3  | 30:28:44:LYS:O     | 2.00                     | 0.62              |
| 6:2G:19:LEU:HD13  | 6:2G:32:PRO:HG2    | 1.80                     | 0.62              |
| 1:1A:2183:C:H2'   | 1:1A:2184:G:H8     | 1.65                     | 0.62              |
| 1:1A:278:A:H2     | 1:1A:362:U:H3      | 1.47                     | 0.62              |
| 3:1D:69:ARG:HE    | 3:1D:130:ALA:HB2   | 1.65                     | 0.62              |
| 1:1A:271(M):G:N2  | 8:1I:50:ARG:HH12   | 1.98                     | 0.62              |
| 1:1A:2629:A:O2'   | 1:1A:2630:G:OP2    | 2.15                     | 0.62              |
| 12:2Q:16:ARG:HD2  | 12:2Q:18:LYS:HG3   | 1.82                     | 0.61              |
| 18:2W:71:VAL:HA   | 18:2W:107:LEU:HD12 | 1.81                     | 0.61              |
| 1:2A:2803:C:H2'   | 1:2A:2804:C:H6     | 1.65                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:2G:125:PHE:CE2  | 6:2G:170:ARG:HB2  | 2.35                     | 0.61              |
| 1:1A:1178:C:H2'   | 1:1A:1179:C:C6    | 2.35                     | 0.61              |
| 17:2V:25:LEU:O    | 17:2V:64:HIS:NE2  | 2.31                     | 0.61              |
| 5:2F:11:VAL:HG22  | 5:2F:125:LEU:HB2  | 1.82                     | 0.61              |
| 1:1A:1087:G:H2'   | 1:1A:1089:G:C8    | 2.35                     | 0.61              |
| 4:2E:72:VAL:HG13  | 4:2E:73:GLU:HB3   | 1.83                     | 0.61              |
| 1:1A:602:G:O2'    | 1:1A:655:A:N6     | 2.33                     | 0.61              |
| 6:1G:27:ASN:HB3   | 6:1G:30:GLU:HG3   | 1.82                     | 0.61              |
| 1:2A:2117:A:O2'   | 1:2A:2118:U:H5''  | 2.01                     | 0.61              |
| 1:2A:2327:A:H2'   | 1:2A:2328:A:C8    | 2.35                     | 0.61              |
| 6:2G:32:PRO:HB2   | 6:2G:172:LEU:HD22 | 1.82                     | 0.61              |
| 1:2A:2769:C:H2'   | 1:2A:2770:G:O4'   | 2.00                     | 0.61              |
| 1:1A:243:U:OP1    | 30:18:6:THR:OG1   | 2.16                     | 0.61              |
| 1:2A:2880:C:O3'   | 13:2R:90:ARG:NH1  | 2.33                     | 0.61              |
| 1:2A:586:A:N1     | 1:2A:809:G:O2'    | 2.25                     | 0.61              |
| 1:1A:2869:G:H2'   | 1:1A:2870:C:O4'   | 2.00                     | 0.61              |
| 2:1B:42:C:N4      | 6:1G:91:ARG:HH12  | 1.99                     | 0.61              |
| 1:1A:882:G:H1     | 1:1A:894:C:H42    | 1.48                     | 0.61              |
| 3:1D:260:ARG:NH2  | 3:1D:266:SER:OG   | 2.33                     | 0.61              |
| 7:2H:113:VAL:HG11 | 7:2H:151:ILE:HD13 | 1.83                     | 0.61              |
| 1:2A:812:C:H2'    | 1:2A:813:U:H6     | 1.66                     | 0.61              |
| 12:1Q:30:GLY:HA2  | 12:1Q:107:ALA:HB2 | 1.80                     | 0.61              |
| 1:2A:1005:C:H2'   | 1:2A:1006:C:H6    | 1.66                     | 0.61              |
| 1:2A:1187:G:H5'   | 17:2V:81:TYR:CE1  | 2.35                     | 0.61              |
| 1:2A:1507:A:O2'   | 1:2A:1508:A:O4'   | 2.18                     | 0.61              |
| 19:1X:35:THR:HG22 | 19:1X:38:GLU:H    | 1.65                     | 0.61              |
| 8:2I:116:LEU:HD11 | 8:2I:120:ILE:HG13 | 1.83                     | 0.61              |
| 23:11:51:VAL:HG11 | 23:11:74:VAL:HG21 | 1.82                     | 0.61              |
| 1:1A:2577:A:OP2   | 27:15:3:LYS:NZ    | 2.28                     | 0.60              |
| 1:1A:1508:A:O2'   | 1:1A:1509:C:OP1   | 2.19                     | 0.60              |
| 11:1P:121:LYS:HG2 | 11:1P:122:PRO:HD2 | 1.83                     | 0.60              |
| 8:2I:31:LEU:HD21  | 8:2I:38:LEU:HG    | 1.82                     | 0.60              |
| 14:2S:30:ARG:HB2  | 14:2S:35:ILE:HD13 | 1.81                     | 0.60              |
| 16:1U:81:HIS:CE1  | 16:1U:85:LYS:HD2  | 2.35                     | 0.60              |
| 1:1A:1165:U:H2'   | 1:1A:1166:C:C6    | 2.37                     | 0.60              |
| 8:2I:78:THR:H     | 8:2I:104:GLN:HE22 | 1.49                     | 0.60              |
| 21:1Z:151:HIS:O   | 21:1Z:153:SER:N   | 2.30                     | 0.60              |
| 2:2B:7:G:H21      | 14:2S:38:GLN:HE22 | 1.48                     | 0.60              |
| 26:14:61:ARG:HG3  | 26:14:62:ARG:H    | 1.65                     | 0.60              |
| 1:1A:2001:A:H2'   | 1:1A:2002:G:C8    | 2.36                     | 0.60              |
| 1:1A:2867:G:OP2   | 15:1T:119:LYS:NZ  | 2.24                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1A:456:C:H4'    | 61:1A:5025:HOH:O  | 2.01                     | 0.60              |
| 8:2I:93:THR:H     | 8:2I:96:ASP:HB2   | 1.66                     | 0.60              |
| 1:1A:493:G:O6     | 61:1A:4039:HOH:O  | 2.15                     | 0.60              |
| 5:2F:185:ASP:HA   | 5:2F:188:ARG:HD3  | 1.84                     | 0.60              |
| 5:2F:140:LEU:HD11 | 5:2F:170:LEU:HD11 | 1.83                     | 0.60              |
| 1:2A:2552:2MU:H2' | 1:2A:2554:U:OP2   | 2.01                     | 0.60              |
| 1:2A:991:C:OP2    | 61:2A:3732:HOH:O  | 2.15                     | 0.60              |
| 1:1A:184:C:H2'    | 1:1A:185:U:C6     | 2.37                     | 0.60              |
| 1:1A:1141:U:OP1   | 9:1N:25:ARG:NH1   | 2.35                     | 0.60              |
| 1:1A:2728:U:H5'   | 10:1O:70:LYS:HZ3  | 1.65                     | 0.60              |
| 14:1S:15:ARG:O    | 14:1S:19:LYS:HG2  | 2.01                     | 0.60              |
| 6:2G:73:ALA:HB3   | 6:2G:85:GLY:H     | 1.66                     | 0.60              |
| 28:16:35:GLU:OE2  | 28:16:50:ARG:NH1  | 2.34                     | 0.60              |
| 11:2P:44:GLY:O    | 61:2P:301:HOH:O   | 2.16                     | 0.60              |
| 1:2A:687:C:H5''   | 29:27:2:LYS:HE2   | 1.82                     | 0.60              |
| 9:2N:38:HIS:CE1   | 9:2N:39:ARG:HG3   | 2.36                     | 0.60              |
| 1:2A:1239:G:H2'   | 1:2A:1240:U:O4'   | 2.01                     | 0.60              |
| 1:2A:1517:G:H1'   | 1:2A:1919:A:O3'   | 102.01                   | 0.60              |
| 19:1X:53:LYS:HB3  | 19:1X:82:GLN:HB3  | 1.83                     | 0.60              |
| 7:2H:25:LYS:HG3   | 7:2H:27:LYS:HE3   | 1.84                     | 0.60              |
| 1:2A:1815:A:P     | 3:2D:54:ARG:HH22  | 2.25                     | 0.60              |
| 1:2A:1507:A:O2'   | 1:2A:1508:A:O5'   | 2.20                     | 0.60              |
| 1:1A:2134:A:OP1   | 1:1A:2156:G:N2    | 2.34                     | 0.60              |
| 1:2A:2387:U:O2'   | 22:20:19:LYS:NZ   | 2.35                     | 0.60              |
| 8:2I:4:ILE:HG12   | 8:2I:18:VAL:HG22  | 1.83                     | 0.60              |
| 1:2A:2127:G:N1    | 1:2A:2161:C:C2    | 2.67                     | 0.60              |
| 1:1A:2646:C:OP2   | 1:1A:2732:G:O2'   | 2.18                     | 0.60              |
| 1:1A:532:A:N6     | 1:1A:1206:G:O2'   | 62.04                    | 0.60              |
| 21:2Z:46:LYS:O    | 21:2Z:50:GLN:NE2  | 2.30                     | 0.60              |
| 3:1D:14:ARG:HG2   | 3:1D:14:ARG:HH11  | 1.67                     | 0.60              |
| 3:2D:14:ARG:HH11  | 3:2D:14:ARG:HG2   | 1.67                     | 0.60              |
| 1:2A:1786:A:H1'   | 1:2A:1938:A:N6    | 2.17                     | 0.60              |
| 22:10:46:LYS:NZ   | 22:10:75:LEU:O    | 2.24                     | 0.60              |
| 1:2A:882:G:H2'    | 1:2A:883:G:H8     | 1.66                     | 0.59              |
| 1:1A:2683:C:O2    | 10:1O:70:LYS:NZ   | 2.28                     | 0.59              |
| 1:1A:2042:A:OP1   | 61:1A:4047:HOH:O  | 2.17                     | 0.59              |
| 1:2A:203:C:OP2    | 61:2A:3736:HOH:O  | 2.17                     | 0.59              |
| 1:2A:1799:G:O2'   | 3:2D:181:GLU:OE2  | 2.16                     | 0.59              |
| 1:2A:2334:G:O6    | 22:20:74:ARG:NH2  | 2.35                     | 0.59              |
| 1:2A:1653:G:H3'   | 13:2R:2:ARG:HD3   | 1.84                     | 0.59              |
| 1:2A:848:G:H2'    | 1:2A:849:A:C8     | 2.36                     | 0.59              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:1A:880:G:H2'     | 1:1A:881:G:C8      | 2.37                     | 0.59              |
| 1:2A:2693:A:H2'    | 1:2A:2694:G:C8     | 2.37                     | 0.59              |
| 2:2B:50:G:OP1      | 14:2S:63:THR:N     | 2.34                     | 0.59              |
| 6:2G:15:VAL:HG22   | 6:2G:175:LEU:HB3   | 1.84                     | 0.59              |
| 1:2A:8:A:H2'       | 1:2A:9:U:H6        | 1.67                     | 0.59              |
| 20:2Y:86:ARG:HB2   | 20:2Y:98:VAL:HG23  | 1.84                     | 0.59              |
| 1:2A:1783:A:OP1    | 61:2A:3703:HOH:O   | 2.16                     | 0.59              |
| 9:1N:22:THR:HB     | 9:1N:25:ARG:HB2    | 1.83                     | 0.59              |
| 1:1A:278:A:H2'     | 1:1A:279:C:C6      | 2.37                     | 0.59              |
| 11:1P:63:PRO:HD3   | 30:18:27:THR:HG22  | 1.82                     | 0.59              |
| 1:1A:10:G:N2       | 1:1A:2802:G:OP1    | 2.35                     | 0.59              |
| 1:2A:2379:G:O2'    | 14:2S:17:ARG:NH2   | 2.35                     | 0.59              |
| 1:2A:468:G:N7      | 29:27:39:ARG:NH2   | 2.51                     | 0.59              |
| 1:1A:671:C:N4      | 61:1A:4155:HOH:O   | 2.35                     | 0.59              |
| 1:2A:2218:U:H1'    | 23:21:52:ARG:HH12  | 1.67                     | 0.59              |
| 21:1Z:92:SER:O     | 21:1Z:130:PRO:HG2  | 2.02                     | 0.59              |
| 21:2Z:141:VAL:HG12 | 21:2Z:144:LEU:HD13 | 1.83                     | 0.59              |
| 1:2A:854:G:H2'     | 1:2A:855:G:C8      | 2.36                     | 0.59              |
| 2:2B:48:A:H4'      | 14:2S:95:HIS:HD2   | 1.67                     | 0.59              |
| 3:2D:76:PRO:HB2    | 3:2D:116:GLN:HE21  | 1.67                     | 0.59              |
| 17:2V:43:GLU:OE1   | 17:2V:43:GLU:N     | 2.36                     | 0.59              |
| 1:1A:323:G:C8      | 5:1F:171:PRO:HG3   | 2.38                     | 0.59              |
| 1:1A:2296:U:OP2    | 14:1S:9:ARG:NH2    | 2.35                     | 0.59              |
| 1:1A:2567:G:H2'    | 1:1A:2568:C:C6     | 2.37                     | 0.59              |
| 1:2A:1951:U:O4     | 61:2A:3721:HOH:O   | 2.11                     | 0.59              |
| 1:1A:1059:G:N2     | 1:1A:1079:C:C2     | 2.70                     | 0.59              |
| 1:1A:882:G:N2      | 1:1A:894:C:N3      | 2.45                     | 0.59              |
| 1:1A:271(E):U:H2'  | 1:1A:271(F):C:C6   | 2.37                     | 0.59              |
| 1:2A:1355:G:O6     | 61:2A:3734:HOH:O   | 2.16                     | 0.59              |
| 1:1A:1405:U:H2'    | 1:1A:1406:U:C6     | 2.38                     | 0.59              |
| 1:1A:1062:G:P      | 1:1A:1070:A:H1'    | 2.43                     | 0.59              |
| 14:1S:25:ARG:NH1   | 14:1S:42:ASP:OD1   | 2.36                     | 0.59              |
| 10:2O:76:ALA:HB3   | 15:2T:75:ILE:HB    | 1.85                     | 0.59              |
| 1:1A:2887:U:H2'    | 1:1A:2888:C:C6     | 2.38                     | 0.59              |
| 1:2A:2377:A:H2'    | 1:2A:2378:A:C8     | 2.38                     | 0.59              |
| 26:24:24:THR:OG1   | 26:24:25:TYR:N     | 2.36                     | 0.59              |
| 1:2A:1557:C:OP2    | 1:2A:1558:A:O2'    | 2.16                     | 0.59              |
| 5:1F:158:THR:O     | 5:1F:164:ARG:NH1   | 2.33                     | 0.59              |
| 1:1A:2379:G:O2'    | 14:1S:17:ARG:NH2   | 2.36                     | 0.59              |
| 1:2A:2305:A:H5''   | 6:2G:134:GLY:HA3   | 1.84                     | 0.59              |
| 1:1A:1786:A:H1'    | 1:1A:1938:A:N6     | 2.17                     | 0.59              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:2A:658:C:H2'     | 1:2A:659:C:C6      | 2.38                     | 0.58              |
| 19:1X:57:LEU:HD11  | 19:1X:78:LYS:HE2   | 1.85                     | 0.58              |
| 1:2A:1688:U:O2     | 1:2A:1700:A:H5'    | 2.03                     | 0.58              |
| 3:2D:148:GLU:HB2   | 3:2D:151:LYS:HD2   | 1.85                     | 0.58              |
| 1:2A:362:U:O2'     | 1:2A:363:G:H5''    | 2.02                     | 0.58              |
| 1:1A:1039:G:H1     | 1:1A:1116:C:H42    | 1.51                     | 0.58              |
| 1:2A:1342:A:H2     | 1:2A:1396:U:HO2'   | 1.51                     | 0.58              |
| 1:1A:729:G:C6      | 3:1D:208:LYS:HB2   | 2.38                     | 0.58              |
| 1:2A:184:C:H2'     | 1:2A:185:U:C6      | 2.37                     | 0.58              |
| 1:2A:2060:A:N3     | 61:2A:3825:HOH:O   | 2.32                     | 0.58              |
| 21:2Z:146:ILE:HG12 | 21:2Z:174:VAL:HG12 | 1.83                     | 0.58              |
| 19:2X:88:LYS:NZ    | 19:2X:90:GLU:OE1   | 2.36                     | 0.58              |
| 1:2A:2705:A:O2'    | 1:2A:2852:G:OP1    | 2.17                     | 0.58              |
| 1:1A:2319:G:H22    | 14:1S:3:ARG:HD3    | 1.67                     | 0.58              |
| 15:2T:26:ASP:OD1   | 15:2T:120:ARG:NH2  | 2.27                     | 0.58              |
| 12:1Q:67:ARG:O     | 12:1Q:101:ARG:NH2  | 2.37                     | 0.58              |
| 1:1A:560:C:H5'     | 16:1U:52:ARG:HH21  | 1.67                     | 0.58              |
| 1:1A:674:G:O2'     | 5:1F:74:ARG:HD3    | 2.04                     | 0.58              |
| 8:1I:72:LEU:C      | 8:1I:74:ASN:H      | 2.05                     | 0.58              |
| 1:1A:1352:U:OP2    | 61:1A:4049:HOH:O   | 2.17                     | 0.58              |
| 5:2F:178:PRO:HB3   | 5:2F:198:ALA:HA    | 1.85                     | 0.58              |
| 1:2A:2846:G:N7     | 61:2A:3824:HOH:O   | 2.32                     | 0.58              |
| 6:1G:38:VAL:HG22   | 6:1G:93:THR:HG23   | 1.86                     | 0.58              |
| 4:1E:29:GLY:HA3    | 61:1E:404:HOH:O    | 2.04                     | 0.58              |
| 26:24:62:ARG:HH11  | 26:24:62:ARG:H     | 1.51                     | 0.58              |
| 26:14:24:THR:OG1   | 26:14:25:TYR:N     | 2.37                     | 0.58              |
| 1:2A:1119:C:H2'    | 1:2A:1120:G:C8     | 3.19                     | 0.58              |
| 1:1A:1418:G:OP2    | 61:1A:4048:HOH:O   | 2.17                     | 0.58              |
| 1:1A:414:C:H2'     | 1:1A:415:A:C8      | 2.38                     | 0.58              |
| 17:2V:24:LYS:HG3   | 17:2V:64:HIS:CD2   | 2.34                     | 0.58              |
| 1:2A:411:G:OP1     | 61:2A:3735:HOH:O   | 2.16                     | 0.58              |
| 1:2A:652(B):A:H61  | 1:2A:655:A:H1'     | 1.68                     | 0.58              |
| 1:2A:2674:G:H2'    | 1:2A:2675:A:C8     | 2.39                     | 0.58              |
| 15:1T:24:PRO:HD3   | 15:1T:52:ILE:HD12  | 1.85                     | 0.58              |
| 11:2P:63:PRO:HG2   | 30:28:25:MET:HB2   | 1.85                     | 0.58              |
| 11:1P:140:ALA:O    | 25:23:38:GLU:HG2   | 2.02                     | 0.58              |
| 1:1A:2532:G:O2'    | 1:1A:2657:A:N1     | 2.36                     | 0.58              |
| 25:23:7:LYS:HB2    | 25:23:34:GLU:HG3   | 1.85                     | 0.58              |
| 6:2G:16:ARG:HE     | 6:2G:31:VAL:HG11   | 1.68                     | 0.58              |
| 1:2A:298:G:O2'     | 1:2A:322:A:N1      | 2.31                     | 0.58              |
| 8:2I:92:VAL:HG13   | 8:2I:120:ILE:HB    | 1.84                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:1E:48:GLN:HE21  | 4:1E:78:LEU:HD23  | 1.67                     | 0.58              |
| 8:2I:130:TYR:HB3  | 8:2I:138:ILE:HB   | 1.86                     | 0.58              |
| 17:2V:40:LEU:HB2  | 17:2V:46:VAL:HG22 | 1.85                     | 0.58              |
| 1:2A:1011:G:OP2   | 16:2U:70:ARG:NH2  | 2.37                     | 0.58              |
| 1:2A:223:A:O2'    | 1:2A:420:C:O2     | 2.20                     | 0.58              |
| 26:14:55:ARG:N    | 26:14:56:VAL:HA   | 2.19                     | 0.58              |
| 1:2A:2805:G:H2'   | 1:2A:2807:G:C8    | 2.38                     | 0.58              |
| 1:1A:363(A):A:H2' | 1:1A:363(B):G:C8  | 2.39                     | 0.58              |
| 1:2A:1514:U:H2'   | 1:2A:1515:G:C8    | 2.37                     | 0.58              |
| 7:2H:124:GLU:HB2  | 7:2H:132:ARG:HB3  | 1.84                     | 0.58              |
| 1:1A:1086:A:H3'   | 1:1A:1086:A:N3    | 2.19                     | 0.58              |
| 1:2A:1024:G:HO2'  | 1:2A:1144:G:HO2'  | 1.51                     | 0.58              |
| 1:2A:1025:G:C4    | 1:2A:1135:C:H1'   | 2.38                     | 0.58              |
| 1:1A:1342:A:OP2   | 61:1A:4003:HOH:O  | 2.17                     | 0.58              |
| 1:2A:625:G:N7     | 11:2P:107:LYS:NZ  | 2.45                     | 0.58              |
| 1:1A:1843:C:H5'   | 3:1D:253:GLN:OE1  | 2.04                     | 0.58              |
| 1:1A:2285:C:OP2   | 28:16:6:ARG:NH1   | 2.36                     | 0.58              |
| 1:2A:1805:U:O2    | 3:2D:50:THR:HB    | 2.04                     | 0.58              |
| 21:1Z:149:SER:OG  | 21:1Z:150:LEU:N   | 2.36                     | 0.58              |
| 1:2A:322:A:OP2    | 5:2F:169:ASN:HB2  | 2.04                     | 0.58              |
| 1:1A:1826:G:H4'   | 3:1D:242:ARG:CZ   | 2.34                     | 0.58              |
| 1:2A:2156:G:O5'   | 1:2A:2156:G:H8    | 1.86                     | 0.58              |
| 1:2A:2129:C:N4    | 1:2A:2159:G:H1    | 2.02                     | 0.58              |
| 8:1I:92:VAL:HG13  | 8:1I:120:ILE:HB   | 1.85                     | 0.58              |
| 1:1A:1156:A:P     | 16:1U:55:ARG:HH11 | 2.26                     | 0.58              |
| 1:1A:2327:A:H2'   | 1:1A:2328:A:C8    | 2.38                     | 0.58              |
| 1:1A:2377:A:H2'   | 1:1A:2378:A:C8    | 2.39                     | 0.58              |
| 1:2A:266:G:H5''   | 1:2A:268:C:H41    | 11.02                    | 0.58              |
| 8:2I:57:ARG:O     | 8:2I:61:ARG:HG2   | 2.04                     | 0.57              |
| 1:2A:918:A:N3     | 2:2B:80:U:O2'     | 2.37                     | 0.57              |
| 1:2A:918:A:C5     | 1:2A:919:G:H1'    | 2.39                     | 0.57              |
| 2:1B:88:C:H2'     | 2:1B:89:G:O4'     | 2.04                     | 0.57              |
| 1:1A:1588:C:H2'   | 1:1A:1589:C:H6    | 1.68                     | 0.57              |
| 1:2A:2705:A:OP2   | 61:2A:3738:HOH:O  | 2.17                     | 0.57              |
| 1:2A:1119:C:H2'   | 1:2A:1120:G:H8    | 2.47                     | 0.57              |
| 14:2S:15:ARG:O    | 14:2S:19:LYS:HG2  | 2.04                     | 0.57              |
| 12:2Q:12:GLN:HE21 | 12:2Q:72:LYS:NZ   | 2.01                     | 0.57              |
| 1:2A:111:A:O2'    | 24:22:65:ASN:ND2  | 2.37                     | 0.57              |
| 1:1A:1002:G:C5    | 1:1A:1003:G:H1'   | 4.31                     | 0.57              |
| 12:2Q:16:ARG:HG3  | 12:2Q:18:LYS:H    | 1.68                     | 0.57              |
| 1:1A:1105:U:H2'   | 1:1A:1106:G:C8    | 2.37                     | 0.57              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:2A:457:A:OP1     | 19:2X:68:ARG:NH2   | 2.37                     | 0.57              |
| 1:1A:1292:U:H2'    | 1:1A:1293:C:C6     | 2.39                     | 0.57              |
| 1:2A:27:G:N2       | 1:2A:512:G:H1'     | 2.19                     | 0.57              |
| 10:2O:115:VAL:HG13 | 10:2O:121:VAL:HG21 | 1.87                     | 0.57              |
| 1:2A:323:G:O2'     | 1:2A:1205:U:N3     | 2.36                     | 0.57              |
| 1:2A:1227:G:OP2    | 16:2U:16:LYS:NZ    | 2.37                     | 0.57              |
| 1:1A:1406:U:H2'    | 1:1A:1407:C:C6     | 2.39                     | 0.57              |
| 6:2G:3:LEU:O       | 6:2G:8:LYS:NZ      | 2.30                     | 0.57              |
| 1:1A:1670:C:O2     | 4:1E:129:HIS:NE2   | 2.30                     | 0.57              |
| 1:1A:484:C:H2'     | 1:1A:485:C:H6      | 1.70                     | 0.57              |
| 1:2A:2061:G:H5''   | 1:2A:2503:2MA:C2   | 2.34                     | 0.57              |
| 1:1A:422:A:H2'     | 1:1A:423:A:C8      | 2.38                     | 0.57              |
| 19:2X:31:HIS:CD2   | 19:2X:33:LYS:HB2   | 2.39                     | 0.57              |
| 1:2A:1328:G:O6     | 61:2A:3729:HOH:O   | 2.15                     | 0.57              |
| 1:2A:2646:C:OP2    | 1:2A:2732:G:O2'    | 2.22                     | 0.57              |
| 1:2A:1636:C:H2'    | 1:2A:1637:A:C8     | 2.40                     | 0.57              |
| 1:2A:1365:A:O2'    | 23:21:11:ARG:NH1   | 2.35                     | 0.57              |
| 1:2A:80:G:H1       | 1:2A:106:C:H42     | 1.52                     | 0.57              |
| 1:2A:2136:C:N3     | 1:2A:2155:G:N2     | 2.50                     | 0.57              |
| 1:2A:1816:G:O6     | 3:2D:35:LYS:NZ     | 2.37                     | 0.57              |
| 1:2A:2375:G:N2     | 1:2A:2378:A:OP2    | 2.37                     | 0.57              |
| 1:1A:2748:A:H5'    | 7:1H:4:ILE:HD12    | 1.86                     | 0.57              |
| 1:2A:1839:G:C8     | 1:2A:1927:A:H1'    | 2.40                     | 0.57              |
| 1:1A:2142:C:N3     | 1:1A:2149:G:O6     | 2.37                     | 0.57              |
| 1:1A:1183:G:O2'    | 25:13:29:ARG:NH1   | 2.38                     | 0.57              |
| 1:2A:1030:G:OP2    | 12:2Q:128:LYS:NZ   | 2.38                     | 0.57              |
| 4:1E:111:ARG:HD2   | 4:1E:160:TYR:CD2   | 2.40                     | 0.57              |
| 1:1A:484:C:H2'     | 1:1A:485:C:C6      | 2.40                     | 0.57              |
| 23:21:83:GLU:OE1   | 23:21:83:GLU:N     | 2.37                     | 0.57              |
| 7:1H:56:SER:HB3    | 7:1H:61:HIS:ND1    | 2.20                     | 0.57              |
| 5:1F:155:LEU:HB2   | 5:1F:189:THR:HG21  | 1.85                     | 0.57              |
| 1:2A:2499:C:O2     | 61:2A:3733:HOH:O   | 2.15                     | 0.57              |
| 1:2A:2742:C:OP1    | 31:29:35:ARG:HD2   | 2.04                     | 0.57              |
| 1:2A:8:A:H2'       | 1:2A:9:U:C6        | 2.40                     | 0.57              |
| 1:1A:747:U:O2      | 1:1A:2014:A:H1'    | 2.04                     | 0.57              |
| 9:2N:33:LEU:HA     | 9:2N:38:HIS:HD2    | 1.70                     | 0.57              |
| 1:1A:1713:U:H2'    | 1:1A:1714:G:H8     | 1.70                     | 0.57              |
| 1:1A:2818:G:OP2    | 13:1R:42:LYS:NZ    | 2.28                     | 0.57              |
| 1:1A:971:C:O2'     | 1:1A:983:A:N3      | 2.31                     | 0.57              |
| 4:2E:27:LEU:HD22   | 15:2T:1:MET:HE1    | 1.87                     | 0.57              |
| 1:1A:1063:G:H2'    | 1:1A:1064:C:C6     | 2.40                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1A:1090:U:C2    | 1:1A:1102:C:H1'   | 2.40                     | 0.57              |
| 1:1A:1356:G:O6    | 61:1A:4038:HOH:O  | 2.14                     | 0.57              |
| 8:2I:77:LEU:HD23  | 8:2I:142:VAL:HG13 | 1.86                     | 0.57              |
| 1:2A:2646:C:H2'   | 1:2A:2647:U:O4'   | 2.05                     | 0.57              |
| 4:1E:111:ARG:HD3  | 4:1E:118:LYS:HD3  | 1.86                     | 0.57              |
| 15:1T:127:ALA:C   | 15:1T:129:ARG:H   | 2.07                     | 0.57              |
| 1:1A:1045:A:H5'   | 1:1A:1046:A:H5'   | 1.85                     | 0.57              |
| 1:1A:71:A:N7      | 19:1X:31:HIS:HE1  | 2.03                     | 0.57              |
| 1:2A:2133:G:N2    | 1:2A:2157:G:H1'   | 2.20                     | 0.57              |
| 4:2E:48:GLN:HE21  | 4:2E:78:LEU:HD23  | 1.69                     | 0.57              |
| 1:1A:2142:C:H2'   | 1:1A:2143:C:C6    | 2.40                     | 0.57              |
| 6:1G:43:LEU:HD11  | 6:1G:153:ARG:HD2  | 1.86                     | 0.57              |
| 1:1A:1913:A:H4'   | 1:1A:1914:C:H5''  | 1.87                     | 0.57              |
| 19:1X:43:VAL:HG21 | 19:1X:81:VAL:HG11 | 1.86                     | 0.57              |
| 2:2B:17:C:H2'     | 2:2B:18:G:O4'     | 2.05                     | 0.57              |
| 1:2A:792:G:N3     | 1:2A:2072:G:O2'   | 2.34                     | 0.57              |
| 1:2A:2291:U:H2'   | 1:2A:2292:C:C6    | 2.40                     | 0.57              |
| 1:1A:1800:C:P     | 3:1D:183:ARG:HH12 | 2.28                     | 0.57              |
| 2:2B:22:U:H3      | 2:2B:61:G:H1      | 1.51                     | 0.57              |
| 1:1A:911:A:N6     | 12:1Q:11:LYS:O    | 2.35                     | 0.57              |
| 8:1I:130:TYR:N    | 8:1I:138:ILE:O    | 2.36                     | 0.56              |
| 1:1A:2141:G:O6    | 1:1A:2150:U:O2    | 2.23                     | 0.56              |
| 1:1A:2140:C:N3    | 1:1A:2151:G:O6    | 2.38                     | 0.56              |
| 8:1I:6:LEU:HD11   | 8:1I:37:VAL:HG23  | 1.87                     | 0.56              |
| 1:2A:272(H):C:H2' | 1:2A:272(I):U:C6  | 2.39                     | 0.56              |
| 1:1A:2430:A:N3    | 1:1A:2430:A:H2'   | 2.20                     | 0.56              |
| 15:2T:127:ALA:C   | 15:2T:129:ARG:H   | 2.06                     | 0.56              |
| 1:2A:1027:A:C2    | 1:2A:2488:A:H5'   | 2.40                     | 0.56              |
| 1:1A:1803:A:O2'   | 3:1D:259:THR:HG21 | 2.04                     | 0.56              |
| 1:2A:1639:U:H2'   | 1:2A:1640:C:H5''  | 1.87                     | 0.56              |
| 26:14:44:THR:O    | 26:14:46:GLN:N    | 2.38                     | 0.56              |
| 2:2B:7:G:H21      | 14:2S:38:GLN:NE2  | 2.03                     | 0.56              |
| 1:2A:1783:A:HO2'  | 1:2A:2607:G:HO2'  | 1.54                     | 0.56              |
| 1:2A:1243:G:O2'   | 11:2P:4:SER:O     | 2.21                     | 0.56              |
| 1:2A:336:C:H2'    | 1:2A:337:C:C6     | 2.71                     | 0.56              |
| 1:1A:2130:U:O2'   | 1:1A:2158:A:N1    | 2.32                     | 0.56              |
| 1:2A:2803:C:H2'   | 1:2A:2804:C:C6    | 2.40                     | 0.56              |
| 1:2A:571:A:N6     | 1:2A:2499:C:O3'   | 2.38                     | 0.56              |
| 1:1A:1265:A:OP2   | 61:1A:4051:HOH:O  | 2.18                     | 0.56              |
| 3:1D:37:LEU:HD22  | 3:1D:87:ASN:HD21  | 1.69                     | 0.56              |
| 1:2A:251:A:C5     | 1:2A:252:G:H1'    | 2.41                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1A:247:G:H4'    | 1:1A:386:G:C5     | 2.39                     | 0.56              |
| 5:2F:158:THR:O    | 5:2F:164:ARG:NH1  | 2.37                     | 0.56              |
| 23:11:83:GLU:N    | 23:11:83:GLU:OE1  | 2.38                     | 0.56              |
| 1:2A:668:G:H5'    | 1:2A:669:G:OP2    | 2.06                     | 0.56              |
| 1:1A:621:A:OP2    | 11:1P:108:LYS:NZ  | 2.34                     | 0.56              |
| 7:2H:17:VAL:HG13  | 7:2H:26:VAL:HG22  | 1.87                     | 0.56              |
| 1:1A:1778:U:H2'   | 1:1A:1784:A:N6    | 2.20                     | 0.56              |
| 1:1A:2107:C:H42   | 1:1A:2182:G:H1    | 1.52                     | 0.56              |
| 1:2A:2584:U:H2'   | 1:2A:2585:U:H2'   | 1.88                     | 0.56              |
| 8:1I:116:LEU:HD21 | 8:1I:119:PRO:HA   | 1.88                     | 0.56              |
| 8:2I:123:LEU:HA   | 8:2I:144:VAL:HG23 | 1.87                     | 0.56              |
| 1:2A:2682:U:O2'   | 15:2T:58:ASN:ND2  | 2.38                     | 0.56              |
| 1:1A:2279:G:OP2   | 22:10:11:ARG:NH1  | 2.39                     | 0.56              |
| 1:2A:1002:G:H1    | 1:2A:1038:C:H42   | 43.00                    | 0.56              |
| 1:2A:1412:A:H2'   | 1:2A:1413:G:C8    | 2.40                     | 0.56              |
| 30:18:6:THR:HG23  | 30:18:64:TYR:HD2  | 1.71                     | 0.56              |
| 6:2G:106:LEU:HG   | 6:2G:111:LEU:HD11 | 1.87                     | 0.56              |
| 1:1A:1540:U:H2'   | 1:1A:1541:G:O4'   | 2.06                     | 0.56              |
| 1:1A:2355:C:H1'   | 22:10:39:ARG:HH21 | 1.70                     | 0.56              |
| 1:2A:577:G:O2'    | 1:2A:1254:A:OP1   | 2.20                     | 0.56              |
| 3:2D:12:SER:HB3   | 3:2D:208:LYS:HB3  | 1.86                     | 0.56              |
| 3:1D:71:ASP:HB3   | 3:1D:103:ARG:HH12 | 1.70                     | 0.56              |
| 17:2V:56:SER:H    | 17:2V:100:ARG:HB2 | 1.70                     | 0.56              |
| 1:2A:2105:C:H2'   | 1:2A:2106:G:C8    | 2.40                     | 0.56              |
| 6:2G:131:TYR:HB3  | 6:2G:159:VAL:HG13 | 1.87                     | 0.56              |
| 1:2A:2218:U:N3    | 23:21:55:GLY:O    | 2.34                     | 0.56              |
| 1:1A:288:C:H2'    | 1:1A:289:A:H8     | 1.71                     | 0.56              |
| 6:2G:27:ASN:HB3   | 6:2G:30:GLU:HG3   | 1.86                     | 0.56              |
| 1:2A:884:C:N4     | 1:2A:893:C:N3     | 2.53                     | 0.56              |
| 1:2A:2149:G:C6    | 1:2A:2150:U:C2    | 2.94                     | 0.56              |
| 1:2A:2165:G:H2'   | 1:2A:2166:G:O4'   | 2.05                     | 0.56              |
| 1:1A:2183:C:H2'   | 1:1A:2184:G:C8    | 2.40                     | 0.56              |
| 1:2A:2555:U:OP2   | 61:2A:3739:HOH:O  | 2.18                     | 0.56              |
| 30:28:23:VAL:HG11 | 30:28:47:LYS:HD3  | 1.87                     | 0.56              |
| 1:2A:1337:G:H2'   | 1:2A:1338:G:H8    | 1.71                     | 0.56              |
| 1:1A:848:G:H2'    | 1:1A:849:A:C8     | 2.41                     | 0.56              |
| 1:1A:65:C:H5'     | 19:1X:71:GLY:HA3  | 1.87                     | 0.56              |
| 28:26:34:LEU:HB2  | 28:26:51:GLU:HB2  | 1.88                     | 0.56              |
| 1:2A:2320:A:H2'   | 1:2A:2320:A:N3    | 2.21                     | 0.56              |
| 7:1H:3:ARG:HH21   | 7:1H:65:HIS:HB3   | 1.70                     | 0.56              |
| 1:1A:1364:G:P     | 23:11:3:LYS:HG3   | 2.46                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1A:2791:C:H2'   | 1:1A:2792:G:H8    | 1.70                     | 0.56              |
| 30:18:23:VAL:HG11 | 30:18:47:LYS:HD3  | 1.88                     | 0.56              |
| 15:2T:29:ARG:HB3  | 15:2T:87:ASP:HB2  | 1.88                     | 0.56              |
| 5:1F:156:LEU:HD21 | 5:1F:163:VAL:HG12 | 1.87                     | 0.56              |
| 10:1O:2:ILE:HD12  | 10:1O:6:THR:HG21  | 1.87                     | 0.56              |
| 1:2A:473:G:H2'    | 1:2A:474:G:H8     | 2.68                     | 0.56              |
| 1:1A:2206:G:H3'   | 1:1A:2207:G:C8    | 2.41                     | 0.56              |
| 1:2A:1266:G:N2    | 1:2A:1269:A:OP2   | 13.50                    | 0.56              |
| 12:2Q:2:LEU:HD23  | 12:2Q:69:PHE:CD1  | 2.41                     | 0.56              |
| 1:1A:2102:U:H3    | 1:1A:2187:G:H1    | 1.51                     | 0.56              |
| 2:2B:42:C:C4      | 2:2B:43:C:C4      | 2.94                     | 0.55              |
| 1:1A:1055:G:H21   | 1:1A:1085:A:H2    | 1.52                     | 0.55              |
| 11:2P:38:GLN:O    | 11:2P:39:LYS:HB3  | 2.06                     | 0.55              |
| 1:1A:2870:C:H2'   | 1:1A:2871:C:O4'   | 2.05                     | 0.55              |
| 13:1R:44:LEU:HD22 | 13:1R:48:VAL:HG23 | 1.88                     | 0.55              |
| 1:2A:764:A:N1     | 1:2A:1789:A:O2'   | 2.39                     | 0.55              |
| 1:2A:900:A:H2'    | 1:2A:901:A:H8     | 1.71                     | 0.55              |
| 1:2A:2169:A:H2'   | 1:2A:2170:A:C8    | 2.42                     | 0.55              |
| 26:24:41:PRO:HG3  | 26:24:49:PHE:CZ   | 2.40                     | 0.55              |
| 1:1A:1837:C:O2'   | 1:1A:1927:A:N3    | 2.32                     | 0.55              |
| 1:2A:2109:U:H3    | 1:2A:2180:U:H3    | 1.52                     | 0.55              |
| 12:2Q:111:GLU:O   | 12:2Q:115:MET:HG2 | 2.06                     | 0.55              |
| 28:26:6:ARG:NH2   | 61:26:5001:HOH:O  | 2.38                     | 0.55              |
| 1:1A:641:C:O2'    | 1:1A:2350:C:OP1   | 2.14                     | 0.55              |
| 18:1W:15:ARG:NH1  | 61:1W:3103:HOH:O  | 2.38                     | 0.55              |
| 1:2A:600:G:O6     | 61:2A:3737:HOH:O  | 2.17                     | 0.55              |
| 23:21:56:GLN:HE21 | 23:21:87:PRO:HG3  | 1.71                     | 0.55              |
| 1:1A:381:G:O6     | 61:1A:4046:HOH:O  | 2.16                     | 0.55              |
| 1:2A:2314:C:H2'   | 1:2A:2315:G:C8    | 2.41                     | 0.55              |
| 21:2Z:30:ASN:HA   | 21:2Z:89:PHE:HE1  | 1.70                     | 0.55              |
| 2:1B:75:G:H22     | 21:1Z:73:GLN:NE2  | 2.05                     | 0.55              |
| 6:2G:18:GLU:OE1   | 6:2G:21:ARG:NH1   | 2.40                     | 0.55              |
| 7:2H:20:ALA:HB1   | 7:2H:21:PRO:HD2   | 1.88                     | 0.55              |
| 1:2A:903:C:H2'    | 1:2A:904:C:C6     | 2.42                     | 0.55              |
| 4:2E:52:LEU:HB3   | 4:2E:76:ARG:HD3   | 1.88                     | 0.55              |
| 2:2B:4:C:H42      | 2:2B:117:G:H1     | 1.53                     | 0.55              |
| 5:1F:53:THR:CG2   | 5:1F:55:GLY:H     | 2.19                     | 0.55              |
| 2:2B:55:U:H4'     | 6:2G:28:VAL:HG22  | 1.89                     | 0.55              |
| 1:1A:2336:A:H61   | 22:10:43:THR:CG2  | 2.19                     | 0.55              |
| 1:2A:305:U:H2'    | 1:2A:306:U:C6     | 2.42                     | 0.55              |
| 1:2A:2702:U:H4'   | 1:2A:2703:C:OP1   | 2.06                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 20:1Y:92:ASN:N    | 20:1Y:93:GLY:HA2  | 2.21                     | 0.55              |
| 9:2N:37:LYS:NZ    | 61:2N:201:HOH:O   | 2.22                     | 0.55              |
| 6:1G:73:ALA:HB3   | 6:1G:85:GLY:H     | 1.72                     | 0.55              |
| 13:2R:44:LEU:HD22 | 13:2R:48:VAL:HG23 | 1.87                     | 0.55              |
| 22:10:2:ALA:N     | 61:10:201:HOH:O   | 2.40                     | 0.55              |
| 1:1A:1235:G:O6    | 61:1A:4050:HOH:O  | 2.18                     | 0.55              |
| 1:2A:2313:C:H4'   | 6:2G:91:ARG:HD3   | 1.88                     | 0.55              |
| 23:21:53:VAL:HG22 | 23:21:74:VAL:HG13 | 1.88                     | 0.55              |
| 3:1D:147:LEU:HD13 | 3:1D:155:LEU:HD11 | 1.88                     | 0.55              |
| 28:26:6:ARG:NH1   | 28:26:26:ASN:HB2  | 2.21                     | 0.55              |
| 13:2R:33:ARG:HB2  | 13:2R:115:GLU:HB3 | 1.89                     | 0.55              |
| 17:1V:55:ALA:HB2  | 17:1V:101:GLY:HA2 | 1.89                     | 0.55              |
| 2:1B:1:U:HO2'     | 2:1B:2:C:H6       | 1.54                     | 0.55              |
| 1:2A:443:A:H1'    | 1:2A:1201:C:O4'   | 2.06                     | 0.55              |
| 1:2A:2689:U:P     | 1:2A:2719:G:H22   | 2.30                     | 0.55              |
| 2:2B:7:G:N2       | 14:2S:38:GLN:HE22 | 2.04                     | 0.55              |
| 1:2A:1889:A:H2'   | 1:2A:1890:A:C8    | 2.42                     | 0.55              |
| 1:2A:140:G:H1'    | 1:2A:141:A:H2     | 1.71                     | 0.55              |
| 12:2Q:31:ASP:OD1  | 12:2Q:134:ARG:NH1 | 2.26                     | 0.55              |
| 6:1G:129:GLY:O    | 6:1G:161:THR:OG1  | 2.24                     | 0.55              |
| 1:2A:667:U:O2     | 30:28:2:PRO:HD2   | 2.07                     | 0.55              |
| 1:1A:1025:G:C4    | 1:1A:1135:C:H1'   | 2.42                     | 0.55              |
| 1:2A:1449:A:O2'   | 1:2A:1529:G:N2    | 2.27                     | 0.55              |
| 1:1A:2627:G:O2'   | 1:1A:2781:A:N1    | 2.27                     | 0.55              |
| 21:2Z:149:SER:OG  | 21:2Z:150:LEU:N   | 2.39                     | 0.54              |
| 1:2A:2892:A:H2'   | 1:2A:2893:G:H5'   | 1.89                     | 0.54              |
| 1:2A:2788:C:OP1   | 4:2E:61:ARG:NH2   | 2.40                     | 0.54              |
| 3:1D:12:SER:HB3   | 3:1D:208:LYS:HB3  | 1.89                     | 0.54              |
| 7:1H:127:GLU:OE1  | 7:1H:130:ARG:NE   | 2.36                     | 0.54              |
| 3:2D:159:ALA:HB1  | 3:2D:198:ASN:O    | 2.08                     | 0.54              |
| 7:1H:22:GLY:HA2   | 7:1H:37:VAL:O     | 2.07                     | 0.54              |
| 1:2A:1188:U:H4'   | 17:2V:79:VAL:HG22 | 1.89                     | 0.54              |
| 1:1A:2506:U:OP1   | 4:1E:144:ARG:NH2  | 2.39                     | 0.54              |
| 1:2A:2441:C:OP2   | 1:2A:2586:C:O2'   | 2.20                     | 0.54              |
| 1:1A:1044:G:H5'   | 1:1A:1045:A:OP2   | 2.07                     | 0.54              |
| 1:2A:740:U:H2'    | 1:2A:741:G:C8     | 2.41                     | 0.54              |
| 1:1A:1186:G:OP1   | 61:1A:4053:HOH:O  | 2.18                     | 0.54              |
| 7:2H:58:GLU:OE2   | 7:2H:60:ARG:NH2   | 2.40                     | 0.54              |
| 1:1A:879:G:O5'    | 1:1A:879:G:H8     | 1.91                     | 0.54              |
| 1:2A:776:G:N1     | 1:2A:802:A:OP1    | 22.89                    | 0.54              |
| 1:2A:1292:U:H2'   | 1:2A:1293:C:C6    | 2.42                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1A:266:G:H2'    | 1:1A:266:G:N3     | 3.20                     | 0.54              |
| 1:2A:902:C:H2'    | 1:2A:903:C:H6     | 1.72                     | 0.54              |
| 1:2A:2162:G:H4'   | 1:2A:2172:U:H2'   | 1.89                     | 0.54              |
| 1:2A:2166:G:H3'   | 1:2A:2167:U:H5''  | 1.87                     | 0.54              |
| 1:2A:2262:U:OP2   | 22:20:16:SER:OG   | 2.19                     | 0.54              |
| 21:2Z:99:TYR:HA   | 21:2Z:124:ILE:O   | 2.07                     | 0.54              |
| 7:1H:144:VAL:O    | 7:1H:148:ILE:HG13 | 2.06                     | 0.54              |
| 13:1R:56:LYS:NZ   | 13:1R:90:ARG:O    | 2.41                     | 0.54              |
| 6:2G:15:VAL:HG13  | 6:2G:175:LEU:HD23 | 1.88                     | 0.54              |
| 61:1A:4234:HOH:O  | 9:1N:73:THR:HG21  | 2.06                     | 0.54              |
| 21:2Z:57:ILE:HD12 | 21:2Z:71:VAL:HG23 | 1.89                     | 0.54              |
| 10:2O:24:VAL:HG12 | 10:2O:33:ALA:HB2  | 1.89                     | 0.54              |
| 1:2A:1496:A:N3    | 1:2A:1577:C:O2'   | 2.38                     | 0.54              |
| 1:1A:1047:G:H2'   | 1:1A:1110:G:H22   | 1.71                     | 0.54              |
| 21:1Z:150:LEU:HG  | 21:1Z:151:HIS:H   | 1.72                     | 0.54              |
| 1:2A:219:G:N3     | 1:2A:234:C:O2'    | 2.39                     | 0.54              |
| 1:1A:2139:C:C2    | 1:1A:2152:G:N2    | 2.75                     | 0.54              |
| 9:1N:62:VAL:HG11  | 9:1N:66:LYS:HB2   | 1.89                     | 0.54              |
| 15:1T:109:GLU:O   | 15:1T:113:LYS:HG2 | 2.08                     | 0.54              |
| 1:1A:192:C:OP1    | 61:1A:4054:HOH:O  | 2.18                     | 0.54              |
| 21:2Z:55:HIS:CE1  | 21:2Z:135:GLU:HG3 | 2.43                     | 0.54              |
| 7:2H:3:ARG:NH1    | 7:2H:5:GLY:H      | 2.05                     | 0.54              |
| 2:2B:24:G:H4'     | 2:2B:25:A:N7      | 2.23                     | 0.54              |
| 25:23:10:LYS:HB3  | 25:23:53:LEU:HA   | 1.90                     | 0.54              |
| 21:2Z:73:GLN:O    | 21:2Z:87:ASP:N    | 2.38                     | 0.54              |
| 1:2A:857:C:OP2    | 22:20:77:ARG:NH2  | 2.40                     | 0.54              |
| 1:2A:796:C:H2'    | 1:2A:797:C:C6     | 2.43                     | 0.54              |
| 3:2D:108:PRO:HB3  | 3:2D:143:HIS:CE1  | 2.41                     | 0.54              |
| 4:2E:36:ARG:HG2   | 4:2E:47:VAL:HG12  | 1.87                     | 0.54              |
| 1:2A:1600:C:OP1   | 19:2X:58:HIS:NE2  | 2.28                     | 0.54              |
| 2:1B:1:U:O2'      | 2:1B:2:C:O5'      | 2.25                     | 0.54              |
| 1:2A:2815:C:H5'   | 27:25:29:THR:HG21 | 1.89                     | 0.54              |
| 1:2A:1993:U:OP2   | 61:2A:3742:HOH:O  | 2.18                     | 0.54              |
| 9:1N:67:LEU:HA    | 9:1N:87:LEU:HD22  | 1.89                     | 0.54              |
| 2:2B:42:C:O2'     | 6:2G:67:LYS:O     | 2.16                     | 0.54              |
| 19:1X:31:HIS:CD2  | 19:1X:33:LYS:H    | 2.25                     | 0.54              |
| 1:2A:2331:G:O2'   | 1:2A:2336:A:N6    | 2.40                     | 0.54              |
| 11:1P:63:PRO:HG2  | 30:18:25:MET:HB2  | 1.90                     | 0.54              |
| 2:2B:117:G:N7     | 61:2B:3101:HOH:O  | 2.33                     | 0.54              |
| 6:1G:115:ARG:HB3  | 6:1G:136:ARG:NH2  | 2.22                     | 0.54              |
| 15:2T:51:ARG:HG3  | 15:2T:98:LYS:HD2  | 1.90                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 17:2V:25:LEU:H     | 17:2V:92:THR:HG1   | 1.56                     | 0.54              |
| 1:2A:566:U:H5''    | 11:2P:29:LYS:HE3   | 1.90                     | 0.54              |
| 16:1U:49:HIS:HA    | 16:1U:52:ARG:HB3   | 1.89                     | 0.54              |
| 1:1A:1588:C:H2'    | 1:1A:1589:C:C6     | 2.43                     | 0.54              |
| 1:2A:1336:A:H2'    | 1:2A:1337:G:C8     | 2.43                     | 0.54              |
| 1:1A:253:C:OP2     | 30:18:5:LYS:NZ     | 2.28                     | 0.54              |
| 7:2H:126:PRO:HG2   | 7:2H:130:ARG:HD2   | 1.90                     | 0.54              |
| 14:2S:10:ARG:NH2   | 14:2S:91:PRO:O     | 2.33                     | 0.54              |
| 1:2A:971:C:H2'     | 1:2A:972:G:O4'     | 2.08                     | 0.54              |
| 1:2A:172:C:H2'     | 1:2A:173:G:H8      | 1.72                     | 0.54              |
| 1:1A:2130:U:H2'    | 1:1A:2131:G:H21    | 1.73                     | 0.54              |
| 1:2A:570:G:H2'     | 1:2A:2030:A:C5     | 2.43                     | 0.54              |
| 1:2A:526:A:N3      | 1:2A:2044:C:H1'    | 2.23                     | 0.54              |
| 12:2Q:125:LEU:HD12 | 12:2Q:129:THR:HG21 | 1.89                     | 0.54              |
| 1:2A:1405:U:H2'    | 1:2A:1406:U:C6     | 2.42                     | 0.54              |
| 1:2A:1697:G:OP2    | 1:2A:1698:A:O2'    | 2.16                     | 0.53              |
| 1:2A:1434:A:H2'    | 1:2A:1435:G:C8     | 2.42                     | 0.53              |
| 4:1E:116:VAL:HG13  | 4:1E:122:PHE:HB2   | 1.90                     | 0.53              |
| 1:1A:2313:C:H4'    | 6:1G:91:ARG:HD3    | 1.90                     | 0.53              |
| 2:2B:22:U:H3       | 2:2B:61:G:H22      | 1.56                     | 0.53              |
| 21:2Z:55:HIS:HE1   | 21:2Z:135:GLU:HG3  | 1.72                     | 0.53              |
| 1:1A:900:A:H2'     | 1:1A:901:A:O4'     | 2.08                     | 0.53              |
| 1:1A:271(K):U:H4'  | 1:1A:271(L):U:OP2  | 2.09                     | 0.53              |
| 11:1P:138:LEU:HD23 | 11:1P:145:PRO:HB3  | 1.90                     | 0.53              |
| 7:2H:11:VAL:HG21   | 7:2H:50:VAL:HG23   | 1.90                     | 0.53              |
| 1:2A:839:U:H2'     | 1:2A:840:C:C6      | 2.43                     | 0.53              |
| 1:2A:1593:G:H2'    | 1:2A:1594:G:C8     | 2.43                     | 0.53              |
| 5:2F:21:ALA:CB     | 5:2F:22:ALA:HA     | 2.38                     | 0.53              |
| 1:2A:111:A:O3'     | 24:22:65:ASN:ND2   | 2.42                     | 0.53              |
| 1:1A:1799:G:O2'    | 3:1D:181:GLU:OE2   | 2.25                     | 0.53              |
| 1:2A:1562:A:H2'    | 1:2A:1563:G:C8     | 2.43                     | 0.53              |
| 1:2A:127:A:H5''    | 1:2A:128:C:C6      | 2.43                     | 0.53              |
| 1:1A:1063:G:H1     | 1:1A:1075:C:N4     | 2.05                     | 0.53              |
| 6:2G:11:TYR:CZ     | 6:2G:16:ARG:HD3    | 2.43                     | 0.53              |
| 2:2B:75:G:N2       | 21:2Z:87:ASP:OD1   | 2.40                     | 0.53              |
| 1:1A:2573:C:H3'    | 61:1A:4014:HOH:O   | 2.09                     | 0.53              |
| 14:2S:64:GLU:CD    | 14:2S:64:GLU:H     | 4.07                     | 0.53              |
| 1:1A:2564:A:C2     | 1:1A:2647:U:H4'    | 2.42                     | 0.53              |
| 11:2P:63:PRO:HD3   | 30:28:27:THR:HG22  | 1.90                     | 0.53              |
| 1:1A:2150:U:H2'    | 1:1A:2151:G:H8     | 1.73                     | 0.53              |
| 1:2A:1899:G:N3     | 1:2A:1899:G:H2'    | 2.22                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:2Z:9:TYR:OH    | 21:2Z:63:ASP:OD2  | 2.26                     | 0.53              |
| 6:1G:64:THR:HB    | 6:1G:94:LEU:HD21  | 1.90                     | 0.53              |
| 20:1Y:54:LYS:H    | 20:1Y:56:PRO:HD3  | 1.72                     | 0.53              |
| 2:2B:91:C:OP1     | 12:2Q:16:ARG:HD3  | 2.08                     | 0.53              |
| 8:2I:3:VAL:HG12   | 8:2I:38:LEU:HA    | 1.91                     | 0.53              |
| 8:2I:102:SER:O    | 8:2I:106:GLY:N    | 2.40                     | 0.53              |
| 21:2Z:30:ASN:HA   | 21:2Z:89:PHE:CE1  | 2.44                     | 0.53              |
| 1:1A:2290:G:OP2   | 61:1A:4057:HOH:O  | 2.19                     | 0.53              |
| 1:1A:2839:G:H5'   | 13:1R:46:GLY:HA2  | 1.89                     | 0.53              |
| 6:2G:109:VAL:HG21 | 26:24:14:ILE:HG21 | 1.90                     | 0.53              |
| 16:1U:69:CYS:HB3  | 16:1U:74:LEU:HD12 | 1.89                     | 0.53              |
| 1:1A:886:C:H4'    | 1:1A:886:C:OP1    | 2.08                     | 0.53              |
| 1:2A:2062:A:H2'   | 1:2A:2062:A:N3    | 2.23                     | 0.53              |
| 1:1A:1058:G:OP1   | 1:1A:1058:G:H4'   | 2.09                     | 0.53              |
| 1:1A:2134:A:OP2   | 1:1A:2157:G:N2    | 2.42                     | 0.53              |
| 1:2A:2674:G:H5''  | 10:2O:26:LYS:HG2  | 1.91                     | 0.53              |
| 1:2A:995:C:O2     | 9:2N:3:THR:OG1    | 2.19                     | 0.53              |
| 4:1E:48:GLN:NE2   | 4:1E:78:LEU:HD23  | 2.23                     | 0.53              |
| 1:1A:2150:U:H2'   | 1:1A:2151:G:C8    | 2.43                     | 0.53              |
| 1:1A:1993:U:OP2   | 61:1A:4055:HOH:O  | 2.18                     | 0.53              |
| 1:2A:1656:C:H2'   | 1:2A:1657:C:H6    | 1.74                     | 0.53              |
| 16:2U:65:ILE:HD11 | 16:2U:95:LEU:HB3  | 1.91                     | 0.53              |
| 9:1N:30:ILE:HG22  | 9:1N:34:LEU:HD22  | 1.90                     | 0.53              |
| 1:2A:403:U:H4'    | 1:2A:404:C:H5'    | 1.90                     | 0.53              |
| 1:2A:1147:C:H2'   | 1:2A:1148:A:C8    | 2.42                     | 0.53              |
| 1:2A:2375:G:O2'   | 1:2A:2377:A:N7    | 2.32                     | 0.53              |
| 11:1P:141:ALA:HA  | 25:23:38:GLU:HG2  | 1.91                     | 0.53              |
| 10:1O:23:ARG:HD3  | 10:1O:24:VAL:N    | 2.24                     | 0.53              |
| 1:2A:384:U:H2'    | 1:2A:385:C:H6     | 1.72                     | 0.53              |
| 11:2P:77:ARG:HB2  | 11:2P:78:PRO:HD2  | 1.90                     | 0.53              |
| 1:2A:993:G:N7     | 1:2A:1213:A:N6    | 48.89                    | 0.53              |
| 18:2W:67:ASP:N    | 18:2W:67:ASP:OD1  | 2.41                     | 0.53              |
| 1:2A:629:G:H2'    | 1:2A:630:G:O4'    | 2.37                     | 0.53              |
| 2:2B:83:G:H1      | 2:2B:94:C:N4      | 2.04                     | 0.53              |
| 2:2B:98:G:H3'     | 2:2B:99:G:H8      | 1.74                     | 0.53              |
| 1:2A:41:C:H2'     | 1:2A:42:G:C8      | 2.43                     | 0.53              |
| 1:2A:2114:A:H62   | 1:2A:2115:G:H21   | 1.57                     | 0.53              |
| 1:2A:2285:C:OP2   | 28:26:6:ARG:NH1   | 2.41                     | 0.53              |
| 17:2V:62:LEU:HD11 | 17:2V:95:LEU:HB2  | 1.89                     | 0.53              |
| 1:2A:2835:A:N6    | 1:2A:2879:C:OP2   | 2.39                     | 0.53              |
| 1:1A:2051:A:H5'   | 1:1A:2578:G:O4'   | 2.08                     | 0.53              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:1A:1866:C:H2'    | 1:1A:1876:A:O4'   | 2.09                     | 0.53              |
| 18:2W:34:ASN:OD1   | 18:2W:37:ARG:NH1  | 2.32                     | 0.53              |
| 1:1A:883:G:H22     | 1:1A:893:C:H42    | 1.56                     | 0.53              |
| 1:2A:2143:C:H2'    | 1:2A:2144:U:O4'   | 2.09                     | 0.53              |
| 1:1A:2135:A:N6     | 1:1A:2156:G:O2'   | 2.37                     | 0.53              |
| 5:1F:110:LEU:HD22  | 5:1F:205:ARG:HD2  | 1.90                     | 0.53              |
| 1:1A:2223:G:OP1    | 3:1D:172:TYR:OH   | 2.20                     | 0.53              |
| 1:1A:1593:G:H2'    | 1:1A:1594:G:C8    | 2.44                     | 0.53              |
| 21:2Z:150:LEU:HG   | 21:2Z:151:HIS:H   | 1.74                     | 0.53              |
| 1:2A:172:C:H2'     | 1:2A:173:G:C8     | 2.44                     | 0.53              |
| 13:1R:33:ARG:HH22  | 27:15:57:VAL:HG12 | 1.74                     | 0.53              |
| 1:2A:19:C:H2'      | 1:2A:20:C:H6      | 1.73                     | 0.53              |
| 1:2A:578:A:OP2     | 61:2A:3746:HOH:O  | 2.19                     | 0.53              |
| 1:1A:2432:A:C4     | 23:11:33:LYS:HG3  | 2.44                     | 0.53              |
| 6:2G:64:THR:HG22   | 6:2G:94:LEU:HD11  | 1.90                     | 0.52              |
| 1:2A:2135:A:H5'    | 1:2A:2159:G:O2'   | 2.09                     | 0.52              |
| 1:1A:1798:U:H5'    | 3:1D:259:THR:CG2  | 2.37                     | 0.52              |
| 1:1A:111:A:O2'     | 24:12:65:ASN:ND2  | 2.41                     | 0.52              |
| 1:2A:2148:G:H2'    | 1:2A:2149:G:C8    | 2.44                     | 0.52              |
| 14:1S:11:LYS:HG3   | 14:1S:91:PRO:HD3  | 1.91                     | 0.52              |
| 1:1A:1274:A:N3     | 1:1A:1297:C:H1'   | 2.23                     | 0.52              |
| 1:1A:1278:A:OP1    | 13:1R:36:THR:HG23 | 2.08                     | 0.52              |
| 14:2S:27:SER:HA    | 14:2S:88:ASP:HB3  | 1.90                     | 0.52              |
| 3:2D:83:GLU:OE1    | 3:2D:104:TYR:OH   | 2.18                     | 0.52              |
| 1:2A:191:A:H2'     | 1:2A:192:C:C6     | 2.44                     | 0.52              |
| 8:1I:87:LYS:NZ     | 8:1I:122:GLU:OE2  | 2.36                     | 0.52              |
| 23:11:71:TYR:O     | 23:11:75:GLU:HG2  | 2.10                     | 0.52              |
| 1:2A:322:A:H5'     | 1:2A:340:A:H1'    | 1.91                     | 0.52              |
| 1:2A:1410:G:H2'    | 1:2A:1411:C:C6    | 2.43                     | 0.52              |
| 1:2A:2731:G:H5''   | 4:2E:203:LYS:HE3  | 1.91                     | 0.52              |
| 1:1A:1996:C:H4'    | 1:1A:1997:G:OP1   | 2.09                     | 0.52              |
| 1:1A:2291:U:H2'    | 1:1A:2292:C:C6    | 2.44                     | 0.52              |
| 1:1A:1636:C:H2'    | 1:1A:1637:A:C8    | 2.43                     | 0.52              |
| 1:1A:800:A:OP1     | 1:1A:800:A:H8     | 1.93                     | 0.52              |
| 1:2A:1482:G:H2'    | 1:2A:1484:G:H8    | 1.74                     | 0.52              |
| 16:2U:107:ALA:O    | 16:2U:111:GLU:HG2 | 2.09                     | 0.52              |
| 19:2X:12:VAL:HG22  | 19:2X:29:TRP:CE2  | 2.44                     | 0.52              |
| 1:2A:1010:A:OP2    | 61:2A:3748:HOH:O  | 2.19                     | 0.52              |
| 1:2A:1360:A:OP1    | 1:2A:1360:A:H8    | 5.36                     | 0.52              |
| 1:2A:1509(B):A:H2' | 1:2A:1510:G:H8    | 1.75                     | 0.52              |
| 1:1A:494:G:H4'     | 18:1W:6:ILE:HB    | 1.91                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:2A:271(H):G:HO2' | 1:2A:271(I):G:H8   | 1.55                     | 0.52              |
| 1:1A:475:U:OP1     | 61:1A:4052:HOH:O   | 2.18                     | 0.52              |
| 1:2A:491:G:O6      | 18:2W:49:LYS:HE2   | 2.09                     | 0.52              |
| 1:2A:2136:C:N4     | 1:2A:2155:G:N1     | 2.57                     | 0.52              |
| 1:2A:2134:A:HO2'   | 1:2A:2159:G:H21    | 1.49                     | 0.52              |
| 22:20:38:VAL:HG21  | 22:20:45:PHE:HD2   | 1.75                     | 0.52              |
| 1:2A:2128:C:O4'    | 1:2A:2173:A:O2'    | 2.27                     | 0.52              |
| 13:2R:63:ARG:O     | 13:2R:67:LEU:HB2   | 2.09                     | 0.52              |
| 1:1A:2788:C:OP1    | 4:1E:61:ARG:NH2    | 2.42                     | 0.52              |
| 1:1A:65:C:H2'      | 1:1A:66:C:H6       | 1.74                     | 0.52              |
| 3:2D:34:VAL:HB     | 3:2D:61:LEU:HD23   | 1.91                     | 0.52              |
| 5:2F:152:GLU:OE1   | 5:2F:191:ARG:NE    | 2.43                     | 0.52              |
| 29:17:30:VAL:HG22  | 29:17:33:ARG:HH21  | 1.75                     | 0.52              |
| 6:2G:49:ASP:OD1    | 6:2G:49:ASP:N      | 2.40                     | 0.52              |
| 1:2A:1572:A:H5'    | 61:2A:3992:HOH:O   | 2.09                     | 0.52              |
| 1:1A:1669:A:H5''   | 1:1A:2550:G:OP1    | 2.09                     | 0.52              |
| 1:2A:1028:A:H2'    | 1:2A:1029:A:C8     | 2.44                     | 0.52              |
| 3:2D:242:ARG:HD2   | 3:2D:246:PRO:HG3   | 1.90                     | 0.52              |
| 1:2A:1783:A:H5'    | 1:2A:2608:G:H4'    | 1.92                     | 0.52              |
| 1:2A:2148:G:H2'    | 1:2A:2149:G:H8     | 1.75                     | 0.52              |
| 1:1A:34:C:H5''     | 1:1A:35:G:OP2      | 2.09                     | 0.52              |
| 4:2E:47:VAL:HG11   | 4:2E:86:PRO:HD2    | 1.91                     | 0.52              |
| 1:1A:886:C:H2'     | 1:1A:887:A:H5''    | 1.90                     | 0.52              |
| 1:2A:1833:U:O2'    | 1:2A:1969:A:N1     | 2.34                     | 0.52              |
| 5:2F:183:VAL:O     | 5:2F:187:VAL:HG23  | 2.10                     | 0.52              |
| 1:1A:1566:A:OP1    | 3:1D:211:ARG:NH1   | 2.42                     | 0.52              |
| 1:1A:796:C:H2'     | 1:1A:797:C:C6      | 2.45                     | 0.52              |
| 1:2A:1278:A:H5''   | 13:2R:36:THR:HG22  | 1.91                     | 0.52              |
| 1:1A:2591:C:H2'    | 1:1A:2592:G:C8     | 2.45                     | 0.52              |
| 1:1A:2506:U:O2     | 58:1A:3915:HGR:H23 | 2.10                     | 0.52              |
| 1:2A:1882:C:H2'    | 1:2A:1883:G:O4'    | 2.10                     | 0.52              |
| 1:1A:443:A:H1'     | 1:1A:1201:C:O4'    | 2.10                     | 0.52              |
| 1:2A:2294:C:H2'    | 1:2A:2295:C:O4'    | 2.10                     | 0.52              |
| 14:2S:87:PHE:CZ    | 14:2S:102:ALA:HB2  | 2.44                     | 0.52              |
| 5:2F:145:GLU:OE1   | 5:2F:145:GLU:N     | 2.43                     | 0.52              |
| 1:2A:1666:G:H1'    | 10:2O:3:GLN:HE21   | 1.75                     | 0.52              |
| 6:1G:18:GLU:HG3    | 6:1G:22:ARG:HD3    | 1.92                     | 0.52              |
| 16:2U:49:HIS:HA    | 16:2U:52:ARG:HB3   | 1.91                     | 0.52              |
| 1:2A:1264:G:H2'    | 1:2A:2014:A:N6     | 2.25                     | 0.52              |
| 8:2I:72:LEU:HD21   | 8:2I:107:VAL:HG11  | 1.89                     | 0.52              |
| 1:2A:1278:A:H4'    | 13:2R:34:ILE:HD12  | 1.90                     | 0.52              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:1A:630:G:OP2   | 30:18:15:LYS:NZ   | 2.28                     | 0.52              |
| 7:1H:149:ARG:HD2 | 7:1H:164:TYR:CE2  | 2.44                     | 0.52              |
| 1:2A:2074:U:H2'  | 1:2A:2075:U:C6    | 2.45                     | 0.52              |
| 1:1A:1068:G:OP2  | 1:1A:1068:G:H8    | 4.46                     | 0.52              |
| 1:2A:1204:A:N6   | 1:2A:1240:U:H2'   | 2.24                     | 0.52              |
| 6:2G:28:VAL:O    | 6:2G:31:VAL:HG12  | 2.09                     | 0.52              |
| 1:1A:1341:U:O4'  | 19:1X:57:LEU:HD23 | 2.10                     | 0.52              |
| 7:1H:4:ILE:O     | 7:1H:69:ARG:HD2   | 2.09                     | 0.52              |
| 1:2A:1991:U:H2'  | 1:2A:1992:G:H5''  | 1.92                     | 0.52              |
| 1:2A:2478:A:C2   | 1:2A:2529:G:H2'   | 2.45                     | 0.52              |
| 2:1B:66:A:H61    | 2:1B:108:U:H2'    | 1.75                     | 0.52              |
| 1:1A:2533:A:H2'  | 1:1A:2534:A:O4'   | 2.10                     | 0.52              |
| 1:1A:1423:G:OP1  | 10:1O:49:ARG:NH2  | 97.79                    | 0.52              |
| 1:2A:840:C:OP2   | 1:2A:932:G:N2     | 2.41                     | 0.52              |
| 1:1A:918:A:H5''  | 2:1B:98:G:O2'     | 2.10                     | 0.52              |
| 1:1A:1803:A:H4'  | 3:1D:259:THR:HG23 | 1.90                     | 0.52              |
| 1:2A:637:A:H2'   | 11:2P:117:GLU:OE2 | 2.10                     | 0.52              |
| 2:1B:2:C:H2'     | 2:1B:3:C:C6       | 2.45                     | 0.52              |
| 1:2A:2815:C:H2'  | 1:2A:2816:C:H6    | 1.75                     | 0.52              |
| 1:2A:2360:A:H2'  | 1:2A:2361:A:O4'   | 2.09                     | 0.52              |
| 1:1A:2166:G:N7   | 1:1A:2168:G:N2    | 2.58                     | 0.52              |
| 1:2A:2183:C:H2'  | 1:2A:2184:G:H8    | 1.75                     | 0.52              |
| 1:2A:1022:G:N7   | 9:2N:66:LYS:HE2   | 2.25                     | 0.52              |
| 12:2Q:16:ARG:HG2 | 12:2Q:18:LYS:NZ   | 2.24                     | 0.52              |
| 8:1I:31:LEU:HD21 | 8:1I:38:LEU:HG    | 1.91                     | 0.52              |
| 8:1I:104:GLN:C   | 8:1I:106:GLY:H    | 2.13                     | 0.52              |
| 1:2A:2332:U:H5'  | 1:2A:2336:A:N6    | 2.25                     | 0.52              |
| 26:24:59:PHE:HA  | 26:24:61:ARG:N    | 2.24                     | 0.52              |
| 4:2E:28:ALA:HB3  | 4:2E:93:VAL:HG12  | 1.90                     | 0.52              |
| 1:2A:524:U:H2'   | 1:2A:525:U:C6     | 2.45                     | 0.52              |
| 1:1A:993:G:H2'   | 1:1A:995:C:H41    | 14.59                    | 0.51              |
| 1:2A:900:A:H2'   | 1:2A:901:A:C8     | 2.45                     | 0.51              |
| 1:2A:1410:G:H2'  | 1:2A:1411:C:H6    | 1.75                     | 0.51              |
| 1:1A:2882:A:OP1  | 13:1R:96:ARG:HD3  | 2.10                     | 0.51              |
| 1:1A:64:A:C5     | 19:1X:66:LEU:HD13 | 2.45                     | 0.51              |
| 21:2Z:23:LYS:HB3 | 21:2Z:38:TYR:CD1  | 2.45                     | 0.51              |
| 1:1A:1359:A:H2'  | 1:1A:1360:A:H5'   | 1.92                     | 0.51              |
| 1:1A:1792:G:O2'  | 1:1A:1830:C:OP1   | 2.26                     | 0.51              |
| 1:1A:1683:C:H2'  | 1:1A:1684:C:C6    | 2.44                     | 0.51              |
| 1:2A:700:G:O2'   | 1:2A:1632:A:N3    | 2.34                     | 0.51              |
| 18:2W:4:LYS:HD2  | 18:2W:6:ILE:HD11  | 1.92                     | 0.51              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 6:2G:11:TYR:O     | 6:2G:16:ARG:HG2    | 2.10                     | 0.51              |
| 1:1A:831:G:N2     | 11:1P:53:GLY:O     | 2.44                     | 0.51              |
| 1:2A:910:A:N1     | 1:2A:2277:G:H1'    | 2.25                     | 0.51              |
| 1:1A:582:G:H2'    | 1:1A:583:G:C8      | 2.45                     | 0.51              |
| 61:2A:3742:HOH:O  | 4:2E:127:ASP:OD2   | 2.19                     | 0.51              |
| 1:2A:2573:C:N4    | 58:2A:3652:HGR:O12 | 2.32                     | 0.51              |
| 1:2A:573:G:OP1    | 61:2A:3745:HOH:O   | 2.19                     | 0.51              |
| 1:1A:687:C:H5''   | 29:17:2:LYS:HE2    | 1.92                     | 0.51              |
| 1:2A:1357:U:H2'   | 1:2A:1358:G:O4'    | 2.10                     | 0.51              |
| 1:2A:856:C:H2'    | 1:2A:857:C:C6      | 2.45                     | 0.51              |
| 1:2A:2322:A:H2'   | 1:2A:2323:G:O4'    | 2.10                     | 0.51              |
| 3:2D:166:GLN:HB2  | 3:2D:174:ILE:HG22  | 1.91                     | 0.51              |
| 1:2A:1337:G:H2'   | 1:2A:1338:G:C8     | 2.45                     | 0.51              |
| 1:1A:614(C):A:C4  | 5:1F:180:GLY:HA2   | 2.45                     | 0.51              |
| 1:2A:245:G:O6     | 30:28:8:LYS:NZ     | 2.34                     | 0.51              |
| 1:2A:2094:G:P     | 8:2I:22:LYS:HD2    | 2.50                     | 0.51              |
| 11:2P:95:VAL:HG13 | 11:2P:125:VAL:HA   | 1.92                     | 0.51              |
| 1:2A:938:G:OP2    | 30:28:52:LYS:NZ    | 2.40                     | 0.51              |
| 4:1E:8:LYS:NZ     | 4:1E:188:VAL:O     | 2.44                     | 0.51              |
| 28:16:14:THR:O    | 28:16:17:LYS:NZ    | 2.41                     | 0.51              |
| 1:2A:1022:G:N2    | 1:2A:1023:U:O4     | 2.41                     | 0.51              |
| 2:2B:24:G:H4'     | 2:2B:25:A:C8       | 2.45                     | 0.51              |
| 1:2A:2323:G:HO2'  | 1:2A:2337:G:HO2'   | 1.57                     | 0.51              |
| 1:2A:2376:A:H3'   | 1:2A:2377:A:H8     | 1.75                     | 0.51              |
| 8:2I:110:ASP:N    | 8:2I:130:TYR:OH    | 2.42                     | 0.51              |
| 5:2F:132:VAL:HG11 | 5:2F:163:VAL:HG22  | 1.92                     | 0.51              |
| 1:1A:1936:A:OP1   | 1:1A:1937:A:H5'    | 2.09                     | 0.51              |
| 1:1A:2537:U:H2'   | 1:1A:2538:C:C6     | 2.45                     | 0.51              |
| 24:12:64:LEU:HD21 | 24:12:68:ARG:HE    | 1.74                     | 0.51              |
| 1:1A:2347:C:O2'   | 28:16:21:TYR:OH    | 2.29                     | 0.51              |
| 1:2A:2120:G:H2'   | 1:2A:2121:G:H8     | 1.75                     | 0.51              |
| 1:2A:2126:A:N6    | 1:2A:2162:G:HO2'   | 2.07                     | 0.51              |
| 9:1N:73:THR:OG1   | 9:1N:82:LEU:HD11   | 2.11                     | 0.51              |
| 1:1A:2022:U:O2'   | 1:1A:2617:C:H5'    | 2.11                     | 0.51              |
| 1:1A:668:G:H5'    | 1:1A:669:G:OP2     | 2.10                     | 0.51              |
| 10:1O:4:PRO:O     | 10:1O:5:GLN:HB2    | 2.11                     | 0.51              |
| 2:2B:18:G:H2'     | 2:2B:19:G:C8       | 2.46                     | 0.51              |
| 1:2A:940:G:N3     | 1:2A:1191:G:H4'    | 2.26                     | 0.51              |
| 1:2A:2364:C:H2'   | 1:2A:2365:G:O4'    | 2.10                     | 0.51              |
| 1:2A:652(B):A:N6  | 1:2A:655:A:H1'     | 2.26                     | 0.51              |
| 1:2A:1474:C:H2'   | 1:2A:1475:G:C8     | 2.45                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1A:2732:G:H3'   | 1:1A:2733:A:O4'   | 2.10                     | 0.51              |
| 1:2A:600:G:N2     | 1:2A:605:C:O3'    | 2.44                     | 0.51              |
| 1:2A:1665:A:H4'   | 10:2O:67:LYS:HB2  | 1.92                     | 0.51              |
| 24:22:16:LEU:O    | 24:22:67:LYS:NZ   | 2.43                     | 0.51              |
| 61:1A:4181:HOH:O  | 19:1X:50:LYS:HE2  | 2.10                     | 0.51              |
| 1:2A:2139:C:N4    | 1:2A:2152:G:C6    | 2.75                     | 0.51              |
| 1:2A:2136:C:N4    | 1:2A:2155:G:H1    | 2.08                     | 0.51              |
| 6:1G:82:LEU:HD21  | 6:1G:88:ILE:HG21  | 1.92                     | 0.51              |
| 1:2A:990:A:OP2    | 61:2A:3732:HOH:O  | 2.19                     | 0.51              |
| 1:1A:671:C:H2'    | 1:1A:672:C:C6     | 2.46                     | 0.51              |
| 17:1V:46:VAL:HG23 | 17:1V:52:VAL:HG11 | 1.92                     | 0.51              |
| 5:1F:101:LEU:O    | 5:1F:106:ARG:NH1  | 2.42                     | 0.51              |
| 1:2A:516:C:OP1    | 27:25:13:LYS:NZ   | 2.44                     | 0.51              |
| 10:2O:119:PRO:HB2 | 15:2T:68:TYR:CE2  | 2.45                     | 0.51              |
| 1:1A:2086:U:H2'   | 1:1A:2087:G:C8    | 2.46                     | 0.51              |
| 1:2A:2805:G:H2'   | 1:2A:2807:G:H8    | 1.75                     | 0.51              |
| 1:1A:2572:A:N7    | 4:1E:144:ARG:HD2  | 2.26                     | 0.51              |
| 26:14:63:TYR:N    | 26:14:64:GLY:HA2  | 2.26                     | 0.51              |
| 1:1A:534:U:H2'    | 1:1A:535:C:C6     | 2.45                     | 0.51              |
| 8:1I:4:ILE:HG12   | 8:1I:18:VAL:HG22  | 1.93                     | 0.51              |
| 5:2F:64:ILE:HG21  | 5:2F:78:ILE:HG23  | 1.92                     | 0.51              |
| 2:2B:11:C:H3'     | 2:2B:12:C:H6      | 1.74                     | 0.51              |
| 1:2A:686:G:N2     | 1:2A:788:A:H61    | 2.09                     | 0.51              |
| 1:1A:1059:G:O6    | 1:1A:1088:A:H1'   | 2.11                     | 0.51              |
| 3:1D:2:ALA:N      | 3:1D:200:ASP:OD2  | 2.44                     | 0.51              |
| 6:2G:3:LEU:HD12   | 6:2G:8:LYS:NZ     | 2.26                     | 0.51              |
| 28:16:6:ARG:NH1   | 28:16:26:ASN:HB2  | 2.26                     | 0.51              |
| 21:1Z:137:ILE:HA  | 21:1Z:156:LYS:HE2 | 1.93                     | 0.51              |
| 20:2Y:1:MET:HG2   | 20:2Y:2:ARG:H     | 1.75                     | 0.51              |
| 1:2A:2662:A:O5'   | 1:2A:2662:A:H8    | 1.94                     | 0.51              |
| 1:2A:852:G:H2'    | 1:2A:853:G:H8     | 1.76                     | 0.51              |
| 26:14:52:THR:O    | 26:14:54:GLY:N    | 2.43                     | 0.51              |
| 1:1A:1164:G:H2'   | 1:1A:1165:U:C6    | 2.46                     | 0.51              |
| 18:2W:6:ILE:HG22  | 18:2W:8:ARG:HG3   | 1.93                     | 0.51              |
| 1:1A:1779:U:H2'   | 61:1A:4121:HOH:O  | 2.10                     | 0.51              |
| 1:1A:2128:C:H2'   | 1:1A:2129:C:O4'   | 2.11                     | 0.51              |
| 1:1A:1354:A:H2'   | 1:1A:1355:G:O4'   | 2.11                     | 0.51              |
| 1:2A:2261:C:H1'   | 1:2A:2388:A:N3    | 2.25                     | 0.51              |
| 1:2A:141:A:N1     | 1:2A:142:A:N6     | 2.58                     | 0.51              |
| 1:1A:1429:G:H2'   | 1:1A:1430:C:C6    | 2.45                     | 0.51              |
| 3:2D:17:THR:O     | 3:2D:211:ARG:NH2  | 2.35                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1A:2271:G:OP1   | 22:10:18:ALA:HB1  | 2.11                     | 0.51              |
| 19:2X:4:ALA:HB1   | 19:2X:42:ALA:HA   | 1.93                     | 0.51              |
| 1:2A:2461:C:H2'   | 1:2A:2462:U:C6    | 2.46                     | 0.51              |
| 21:2Z:80:ARG:HD3  | 21:2Z:82:ARG:NH2  | 2.26                     | 0.51              |
| 1:1A:2144:U:H3    | 1:1A:2147:G:H22   | 1.58                     | 0.50              |
| 1:1A:2646:C:H2'   | 1:1A:2647:U:O4'   | 2.11                     | 0.50              |
| 1:2A:1495:A:H2'   | 1:2A:1496:A:C8    | 2.46                     | 0.50              |
| 8:1I:40:THR:O     | 8:1I:44:LEU:HB2   | 2.11                     | 0.50              |
| 15:2T:19:LEU:HD22 | 15:2T:86:ILE:HG13 | 1.93                     | 0.50              |
| 1:2A:446:G:OP1    | 16:2U:3:ARG:NH1   | 2.44                     | 0.50              |
| 20:1Y:34:LYS:NZ   | 61:1Y:5001:HOH:O  | 2.41                     | 0.50              |
| 2:2B:55:U:O3'     | 6:2G:27:ASN:ND2   | 2.44                     | 0.50              |
| 1:2A:1012:U:C5    | 9:2N:28:THR:HG21  | 2.45                     | 0.50              |
| 1:2A:614(B):G:H2' | 5:2F:44:ARG:HD2   | 1.93                     | 0.50              |
| 1:2A:2809:A:H62   | 1:2A:2891:G:H2'   | 1.76                     | 0.50              |
| 25:23:46:ASN:O    | 25:23:50:VAL:HG22 | 2.10                     | 0.50              |
| 1:1A:1074:G:H3'   | 1:1A:1075:C:H5''  | 1.93                     | 0.50              |
| 1:2A:2183:C:H2'   | 1:2A:2184:G:C8    | 2.46                     | 0.50              |
| 1:1A:2161:C:O2'   | 1:1A:2162:G:H8    | 1.94                     | 0.50              |
| 1:2A:1300:U:H4'   | 1:2A:1301:A:C5'   | 2.41                     | 0.50              |
| 5:2F:103:LYS:HA   | 5:2F:106:ARG:HG3  | 1.94                     | 0.50              |
| 14:2S:14:VAL:O    | 14:2S:18:ILE:HG12 | 2.11                     | 0.50              |
| 1:1A:11:G:O2'     | 1:1A:506:G:N2     | 53.36                    | 0.50              |
| 1:1A:1230:C:H2'   | 1:1A:1231:G:C8    | 2.47                     | 0.50              |
| 1:2A:2461:C:H2'   | 1:2A:2462:U:H6    | 1.76                     | 0.50              |
| 7:2H:28:GLY:HA3   | 7:2H:79:VAL:HB    | 1.92                     | 0.50              |
| 1:1A:466:A:N3     | 1:1A:683:C:H1'    | 2.26                     | 0.50              |
| 1:1A:2780:G:N1    | 9:1N:100:GLU:OE2  | 2.36                     | 0.50              |
| 1:1A:493:G:H2'    | 1:1A:494:G:O4'    | 2.11                     | 0.50              |
| 1:1A:291:C:O2     | 1:1A:309:G:N2     | 48.69                    | 0.50              |
| 1:2A:11:G:C2'     | 1:2A:12:U:H5'     | 2.41                     | 0.50              |
| 6:1G:37:VAL:HG23  | 6:1G:99:MET:HG3   | 1.93                     | 0.50              |
| 1:2A:2567:G:H2'   | 1:2A:2568:C:C6    | 2.47                     | 0.50              |
| 10:1O:104:ARG:CZ  | 15:1T:34:VAL:HG21 | 2.41                     | 0.50              |
| 21:2Z:104:PHE:HA  | 21:2Z:139:VAL:HB  | 1.92                     | 0.50              |
| 1:2A:957:A:H5'    | 12:2Q:76:LYS:HG3  | 1.93                     | 0.50              |
| 10:1O:34:THR:OG1  | 10:1O:35:VAL:N    | 2.44                     | 0.50              |
| 19:2X:35:THR:O    | 19:2X:39:ILE:HG13 | 2.11                     | 0.50              |
| 1:1A:34:C:H2'     | 1:1A:35:G:C8      | 5.69                     | 0.50              |
| 14:2S:64:GLU:HB2  | 26:24:59:PHE:CE2  | 82.26                    | 0.50              |
| 25:23:7:LYS:HZ3   | 25:23:34:GLU:HB2  | 1.76                     | 0.50              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:2A:1582:C:H2'   | 1:2A:1583:A:C8     | 2.46                     | 0.50              |
| 1:2A:2537:U:H2'   | 1:2A:2538:C:C6     | 2.47                     | 0.50              |
| 1:2A:1288:U:O2'   | 1:2A:1647:G:N2     | 2.44                     | 0.50              |
| 1:1A:1796:U:H2'   | 1:1A:1797:C:H6     | 1.77                     | 0.50              |
| 6:1G:11:TYR:O     | 6:1G:16:ARG:HG3    | 2.11                     | 0.50              |
| 1:2A:19:C:H2'     | 1:2A:20:C:C6       | 2.46                     | 0.50              |
| 21:2Z:53:ILE:HG22 | 21:2Z:71:VAL:HB    | 1.92                     | 0.50              |
| 1:1A:242:G:C8     | 30:18:5:LYS:HG2    | 2.47                     | 0.50              |
| 1:2A:2542:A:H4'   | 1:2A:2543:G:C8     | 2.46                     | 0.50              |
| 1:2A:1794:U:H2'   | 1:2A:1795:C:C6     | 2.47                     | 0.50              |
| 22:20:27:GLU:HB2  | 22:20:69:PHE:HD2   | 1.76                     | 0.50              |
| 1:2A:2032:G:H1'   | 4:2E:145:LYS:HD3   | 1.94                     | 0.50              |
| 1:1A:2693:A:H2'   | 1:1A:2694:G:C8     | 2.46                     | 0.50              |
| 13:1R:63:ARG:HG2  | 13:1R:80:PHE:CE2   | 2.47                     | 0.50              |
| 20:2Y:14:LEU:HB2  | 20:2Y:75:ILE:HD11  | 1.93                     | 0.50              |
| 1:2A:2621:A:OP1   | 4:2E:119:ARG:NH2   | 2.45                     | 0.50              |
| 1:2A:1418:G:OP2   | 61:2A:3752:HOH:O   | 2.20                     | 0.50              |
| 27:15:16:ARG:HG3  | 27:15:17:ASP:N     | 2.26                     | 0.50              |
| 1:2A:1817:G:OP1   | 3:2D:88:ARG:NH2    | 2.44                     | 0.50              |
| 1:2A:597:U:H2'    | 1:2A:598:G:C8      | 2.47                     | 0.50              |
| 14:2S:58:LEU:HD12 | 14:2S:65:VAL:HG22  | 1.94                     | 0.50              |
| 4:1E:111:ARG:HD2  | 4:1E:160:TYR:CE2   | 2.47                     | 0.50              |
| 1:2A:682:G:H1     | 1:2A:708:C:H42     | 68.81                    | 0.50              |
| 1:2A:723:G:H2'    | 1:2A:724:U:O4'     | 2.12                     | 0.50              |
| 17:2V:98:GLU:CD   | 17:2V:100:ARG:HH12 | 2.15                     | 0.50              |
| 26:24:64:GLY:C    | 26:24:66:SER:H     | 2.15                     | 0.50              |
| 1:2A:269:U:C4     | 1:2A:271(Y):U:C2   | 3.00                     | 0.50              |
| 19:1X:94:GLY:CA   | 19:1X:95:LEU:HB2   | 2.42                     | 0.50              |
| 1:1A:1379:A:H4'   | 1:1A:1380:G:OP2    | 2.12                     | 0.50              |
| 1:2A:484:C:H2'    | 1:2A:485:C:C6      | 2.46                     | 0.50              |
| 1:2A:58:G:O2'     | 1:2A:73:A:N1       | 2.40                     | 0.50              |
| 7:1H:137:ASP:HB3  | 7:1H:140:LYS:HB3   | 1.93                     | 0.50              |
| 7:1H:24:VAL:HG22  | 7:1H:35:VAL:HB     | 1.93                     | 0.50              |
| 1:2A:2136:C:O2'   | 1:2A:2137:C:O5'    | 2.18                     | 0.50              |
| 1:2A:828:U:H4'    | 1:2A:831:G:N1      | 2.26                     | 0.50              |
| 1:1A:588:U:H2'    | 1:1A:589:C:C6      | 2.47                     | 0.50              |
| 8:1I:72:LEU:HD21  | 8:1I:107:VAL:HG11  | 1.94                     | 0.50              |
| 5:2F:125:LEU:HD23 | 5:2F:194:MET:HB2   | 1.93                     | 0.50              |
| 3:1D:133:LEU:HD12 | 3:1D:189:CYS:HB2   | 1.93                     | 0.50              |
| 7:2H:70:THR:HA    | 7:2H:73:ALA:HB3    | 1.94                     | 0.50              |
| 1:1A:270:A:OP2    | 1:1A:271(X):G:N1   | 2.34                     | 0.50              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:2A:30:G:H2'    | 1:2A:31:C:C6      | 2.46                     | 0.50              |
| 4:1E:73:GLU:N    | 4:1E:73:GLU:OE1   | 2.44                     | 0.50              |
| 1:2A:2886:G:H2'  | 1:2A:2887:U:H6    | 1.76                     | 0.50              |
| 1:2A:2037:G:H2'  | 1:2A:2038:G:C8    | 2.47                     | 0.50              |
| 1:2A:1777:U:H2'  | 1:2A:1778:U:C6    | 2.46                     | 0.50              |
| 2:2B:95:C:H2'    | 2:2B:96:U:C6      | 2.47                     | 0.50              |
| 1:1A:784:A:O4'   | 3:1D:227:ASN:ND2  | 2.44                     | 0.50              |
| 15:2T:39:ARG:NH1 | 15:2T:41:ARG:HB3  | 2.26                     | 0.50              |
| 1:2A:1786:A:OP2  | 61:2A:3750:HOH:O  | 2.19                     | 0.50              |
| 2:2B:11:C:H3'    | 2:2B:12:C:C6      | 2.47                     | 0.50              |
| 6:2G:72:ARG:NH1  | 6:2G:87:PRO:HG3   | 2.27                     | 0.50              |
| 1:1A:954:G:H5''  | 12:1Q:13:GLN:HB3  | 1.94                     | 0.50              |
| 1:2A:956:G:H2'   | 1:2A:957:A:H2'    | 1.93                     | 0.49              |
| 2:2B:48:A:OP2    | 14:2S:30:ARG:NH2  | 2.45                     | 0.49              |
| 1:1A:121:G:H4'   | 1:1A:149:A:H5'    | 1.93                     | 0.49              |
| 2:1B:8:U:O3'     | 14:1S:25:ARG:NH2  | 2.45                     | 0.49              |
| 1:2A:2404:C:O3'  | 11:2P:77:ARG:NH2  | 2.46                     | 0.49              |
| 4:1E:179:GLU:HG3 | 15:1T:9:LEU:HD21  | 1.94                     | 0.49              |
| 1:1A:910:A:N1    | 1:1A:2277:G:H1'   | 2.26                     | 0.49              |
| 12:2Q:85:LYS:HB2 | 22:20:7:LEU:HD22  | 1.94                     | 0.49              |
| 7:1H:3:ARG:HE    | 7:1H:54:ARG:HH12  | 1.60                     | 0.49              |
| 1:1A:127:A:H5''  | 1:1A:128:C:C6     | 2.47                     | 0.49              |
| 1:1A:55:G:O2'    | 1:1A:127:A:N1     | 2.32                     | 0.49              |
| 11:1P:89:ALA:O   | 11:1P:121:LYS:NZ  | 2.26                     | 0.49              |
| 25:23:7:LYS:NZ   | 25:23:32:GLN:O    | 2.45                     | 0.49              |
| 1:1A:1364:G:OP2  | 23:11:3:LYS:HG3   | 2.12                     | 0.49              |
| 26:14:46:GLN:O   | 26:14:48:ARG:N    | 2.45                     | 0.49              |
| 1:2A:228:A:HO2'  | 1:2A:229:A:H4'    | 1.77                     | 0.49              |
| 1:2A:1656:C:H2'  | 1:2A:1657:C:C6    | 2.47                     | 0.49              |
| 1:2A:1442:G:N3   | 1:2A:1442:G:H2'   | 2.83                     | 0.49              |
| 1:1A:700:G:H2'   | 1:1A:701:G:O4'    | 2.13                     | 0.49              |
| 1:1A:1584:C:O2'  | 1:1A:1586:A:H5'   | 2.12                     | 0.49              |
| 1:2A:1364:G:P    | 23:21:3:LYS:HG3   | 2.51                     | 0.49              |
| 5:2F:28:ILE:HG23 | 5:2F:112:MET:HE3  | 1.94                     | 0.49              |
| 8:1I:127:VAL:HA  | 8:1I:140:LEU:O    | 2.12                     | 0.49              |
| 11:1P:121:LYS:O  | 11:1P:123:LEU:N   | 2.45                     | 0.49              |
| 1:2A:529:A:H62   | 1:2A:2041:U:H3    | 1.60                     | 0.49              |
| 1:2A:1268:A:C2   | 1:2A:2013:A:C4    | 3.00                     | 0.49              |
| 14:1S:10:ARG:O   | 14:1S:14:VAL:HG13 | 2.11                     | 0.49              |
| 30:18:33:ASN:HA  | 30:18:36:LYS:HD2  | 1.95                     | 0.49              |
| 8:1I:80:PRO:HA   | 8:1I:145:VAL:HG23 | 1.95                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:2F:155:LEU:HB2  | 5:2F:189:THR:HG21 | 1.93                     | 0.49              |
| 25:13:10:LYS:HB3  | 25:13:53:LEU:HA   | 1.94                     | 0.49              |
| 1:1A:1094:U:H2'   | 1:1A:1095:A:C8    | 2.47                     | 0.49              |
| 1:2A:1002:G:C4    | 1:2A:1003:G:H8    | 3.56                     | 0.49              |
| 1:2A:740:U:H2'    | 1:2A:741:G:H8     | 1.77                     | 0.49              |
| 1:2A:2630:G:H2'   | 1:2A:2631:G:H8    | 1.77                     | 0.49              |
| 1:2A:2286:A:H4'   | 1:2A:2287:A:O4'   | 2.12                     | 0.49              |
| 1:2A:184:C:H2'    | 1:2A:185:U:H6     | 1.77                     | 0.49              |
| 1:2A:721:C:H2'    | 1:2A:722:A:C8     | 2.47                     | 0.49              |
| 1:1A:2639:A:O2'   | 9:1N:97:ARG:NH2   | 2.46                     | 0.49              |
| 6:2G:101:ILE:HG22 | 6:2G:105:LYS:HE2  | 1.94                     | 0.49              |
| 1:2A:2483:C:H2'   | 1:2A:2484:G:O4'   | 2.11                     | 0.49              |
| 28:26:9:LEU:HA    | 28:26:54:ILE:HB   | 1.94                     | 0.49              |
| 12:2Q:52:VAL:HA   | 12:2Q:55:VAL:HG22 | 1.92                     | 0.49              |
| 8:1I:81:VAL:O     | 8:1I:146:ALA:HA   | 2.12                     | 0.49              |
| 3:2D:96:HIS:CD2   | 3:2D:102:LYS:HG2  | 2.47                     | 0.49              |
| 1:2A:2626:C:H2'   | 1:2A:2627:G:O4'   | 2.12                     | 0.49              |
| 1:2A:414:C:H2'    | 1:2A:415:A:C8     | 2.48                     | 0.49              |
| 22:10:10:THR:HA   | 61:10:206:HOH:O   | 2.12                     | 0.49              |
| 1:2A:900:A:HO2'   | 1:2A:901:A:P      | 2.34                     | 0.49              |
| 1:1A:1054:A:C6    | 1:1A:1055:G:C6    | 3.01                     | 0.49              |
| 1:1A:576:U:H2'    | 1:1A:577:G:C8     | 2.46                     | 0.49              |
| 1:2A:2317:C:H2'   | 1:2A:2318:G:C8    | 2.48                     | 0.49              |
| 1:2A:2351:G:HO2'  | 1:2A:2352:A:H8    | 1.58                     | 0.49              |
| 1:1A:2630:G:H2'   | 1:1A:2631:G:C8    | 2.47                     | 0.49              |
| 9:2N:38:HIS:ND1   | 9:2N:39:ARG:HG3   | 2.27                     | 0.49              |
| 1:1A:911:A:H2'    | 12:1Q:9:TYR:OH    | 2.11                     | 0.49              |
| 17:1V:52:VAL:HG23 | 17:1V:55:ALA:HB3  | 1.95                     | 0.49              |
| 1:2A:478:A:N1     | 1:2A:500:G:H4'    | 2.27                     | 0.49              |
| 1:2A:218:A:C2     | 1:2A:235:U:H4'    | 2.48                     | 0.49              |
| 3:2D:242:ARG:HH11 | 3:2D:242:ARG:CG   | 2.17                     | 0.49              |
| 7:1H:3:ARG:NH1    | 7:1H:5:GLY:H      | 2.09                     | 0.49              |
| 1:2A:674:G:H2'    | 1:2A:675:A:C8     | 4.99                     | 0.49              |
| 11:2P:39:LYS:HD2  | 11:2P:45:LEU:HD11 | 1.93                     | 0.49              |
| 1:2A:911:A:N6     | 12:2Q:11:LYS:O    | 2.45                     | 0.49              |
| 1:1A:2331:G:O2'   | 1:1A:2336:A:N1    | 2.40                     | 0.49              |
| 1:1A:1713:U:H2'   | 1:1A:1714:G:C8    | 2.48                     | 0.49              |
| 19:1X:61:GLY:HA3  | 19:1X:73:ARG:O    | 2.12                     | 0.49              |
| 1:1A:125:G:N3     | 29:17:48:LYS:HG2  | 2.27                     | 0.49              |
| 1:2A:2746:U:H4'   | 7:2H:139:GLN:HA   | 1.95                     | 0.49              |
| 1:1A:2418:A:H2'   | 1:1A:2419:U:C6    | 2.47                     | 0.49              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:2A:76:C:N3       | 1:2A:93:G:N2      | 28.83                    | 0.49              |
| 2:2B:33:G:N3       | 2:2B:50:G:N2      | 2.61                     | 0.49              |
| 1:2A:784:A:C6      | 3:2D:229:VAL:HG11 | 2.48                     | 0.49              |
| 1:2A:2144:U:O2'    | 1:2A:2147:G:O6    | 2.31                     | 0.49              |
| 21:2Z:153:SER:CB   | 21:2Z:167:PRO:HB3 | 2.42                     | 0.49              |
| 8:1I:72:LEU:O      | 8:1I:74:ASN:N     | 2.46                     | 0.49              |
| 1:1A:2727:G:O2'    | 10:1O:70:LYS:NZ   | 2.41                     | 0.49              |
| 19:2X:31:HIS:CD2   | 19:2X:33:LYS:H    | 2.30                     | 0.49              |
| 17:2V:62:LEU:CD1   | 17:2V:95:LEU:HB2  | 2.42                     | 0.49              |
| 26:14:63:TYR:CD1   | 26:14:63:TYR:N    | 2.80                     | 0.49              |
| 1:1A:2693:A:H2'    | 1:1A:2694:G:H8    | 1.77                     | 0.49              |
| 1:2A:2758:A:C4     | 7:2H:67:LEU:HD21  | 2.48                     | 0.49              |
| 9:1N:75:TYR:CE2    | 9:1N:77:GLY:HA2   | 2.47                     | 0.49              |
| 1:1A:1468:C:OP1    | 61:1A:4060:HOH:O  | 2.20                     | 0.49              |
| 1:2A:2660:A:N7     | 7:2H:175:LYS:NZ   | 2.46                     | 0.49              |
| 1:1A:2611:U:H6     | 1:1A:2611:U:H5'   | 1.77                     | 0.49              |
| 1:2A:1579:A:H2'    | 1:2A:1580:A:C8    | 2.47                     | 0.49              |
| 1:1A:1059:G:H2'    | 1:1A:1060:U:C5    | 2.47                     | 0.49              |
| 1:1A:1062:G:C5     | 1:1A:1088:A:H2'   | 2.48                     | 0.49              |
| 12:2Q:24:GLY:HA2   | 12:2Q:67:ARG:NH2  | 2.28                     | 0.49              |
| 1:2A:1816:G:H3'    | 3:2D:62:TYR:CE1   | 2.47                     | 0.49              |
| 1:1A:1039:G:H1     | 1:1A:1116:C:N4    | 2.10                     | 0.49              |
| 1:1A:2789:C:O2     | 1:1A:2894:G:N2    | 2.43                     | 0.49              |
| 5:1F:53:THR:HG22   | 5:1F:55:GLY:H     | 1.78                     | 0.49              |
| 1:1A:1416:G:O2'    | 1:1A:1417:C:OP2   | 2.20                     | 0.49              |
| 24:22:13:ALA:HA    | 24:22:16:LEU:HD12 | 1.95                     | 0.49              |
| 1:2A:2648:C:H2'    | 1:2A:2649:U:C6    | 2.47                     | 0.49              |
| 1:2A:1800:C:OP2    | 3:2D:183:ARG:NH2  | 2.43                     | 0.49              |
| 1:1A:86:C:H4'      | 1:1A:104:U:H1'    | 1.95                     | 0.49              |
| 1:1A:2801(A):A:H1' | 1:1A:2895:U:H1'   | 1.93                     | 0.49              |
| 1:2A:782:A:H5'     | 1:2A:783:A:N7     | 2.28                     | 0.49              |
| 28:26:12:GLU:OE1   | 28:26:19:ARG:NH1  | 2.46                     | 0.49              |
| 1:2A:1007:C:O2     | 1:2A:1022:G:N1    | 17.91                    | 0.49              |
| 1:2A:1328:G:H2'    | 1:2A:1330:C:C5    | 2.48                     | 0.49              |
| 1:2A:784:A:H5''    | 61:2A:3702:HOH:O  | 2.13                     | 0.49              |
| 1:2A:1155:A:H5''   | 16:2U:55:ARG:NH1  | 2.24                     | 0.49              |
| 1:2A:2140:C:H2'    | 1:2A:2141:G:H5'   | 1.94                     | 0.49              |
| 1:2A:345:A:N3      | 1:2A:346:A:N6     | 2.61                     | 0.49              |
| 2:1B:24:G:N7       | 2:1B:56:G:H2'     | 2.28                     | 0.49              |
| 1:1A:1371:G:H2'    | 1:1A:1372:U:H5    | 1.77                     | 0.49              |
| 7:2H:144:VAL:O     | 7:2H:148:ILE:HG12 | 2.13                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:1E:47:VAL:HG23  | 4:1E:84:PHE:O     | 2.12                     | 0.49              |
| 6:2G:11:TYR:O     | 6:2G:15:VAL:HB    | 2.13                     | 0.49              |
| 1:1A:2128:C:H42   | 1:1A:2161:C:H42   | 1.58                     | 0.49              |
| 2:2B:83:G:H5''    | 25:23:52:HIS:CE1  | 2.47                     | 0.49              |
| 1:2A:1796:U:H2'   | 1:2A:1797:C:H6    | 1.76                     | 0.49              |
| 1:1A:674:G:H2'    | 1:1A:675:A:C8     | 5.05                     | 0.49              |
| 9:2N:21:LYS:O     | 9:2N:61:ARG:N     | 2.38                     | 0.49              |
| 1:2A:71:A:N7      | 19:2X:31:HIS:HE1  | 2.11                     | 0.49              |
| 19:2X:31:HIS:HD2  | 19:2X:33:LYS:HB2  | 1.78                     | 0.49              |
| 1:2A:479:A:N3     | 1:2A:481:G:H5''   | 2.27                     | 0.49              |
| 1:2A:2543:G:H2'   | 1:2A:2544:G:C8    | 2.47                     | 0.49              |
| 9:2N:67:LEU:HA    | 9:2N:87:LEU:HD22  | 1.95                     | 0.49              |
| 28:26:35:GLU:HG2  | 28:26:50:ARG:HD3  | 1.94                     | 0.49              |
| 6:2G:57:ALA:HA    | 6:2G:90:LEU:HD13  | 1.95                     | 0.49              |
| 1:1A:579:G:H2'    | 1:1A:580:C:C6     | 2.48                     | 0.49              |
| 9:2N:22:THR:HB    | 9:2N:25:ARG:HB2   | 1.95                     | 0.49              |
| 2:2B:33:G:C6      | 2:2B:34:U:C4      | 3.01                     | 0.48              |
| 1:2A:94(A):G:H2'  | 1:2A:95:G:O4'     | 2.13                     | 0.48              |
| 9:1N:62:VAL:CG1   | 9:1N:66:LYS:HB2   | 2.43                     | 0.48              |
| 1:2A:2345:G:H4'   | 1:2A:2346:A:H5''  | 1.95                     | 0.48              |
| 1:1A:1262:A:OP2   | 18:1W:97:LYS:NZ   | 2.44                     | 0.48              |
| 1:2A:2478:A:OP2   | 31:29:2:LYS:NZ    | 2.43                     | 0.48              |
| 1:2A:2528:U:H5''  | 31:29:31:LYS:HE2  | 1.95                     | 0.48              |
| 1:1A:530:G:N1     | 1:1A:2023:G:OP1   | 2.34                     | 0.48              |
| 1:2A:1429:G:H2'   | 1:2A:1430:C:C6    | 2.48                     | 0.48              |
| 16:2U:76:TYR:CZ   | 16:2U:80:ILE:HG13 | 2.47                     | 0.48              |
| 27:25:49:CYS:SG   | 27:25:51:TYR:HB2  | 2.53                     | 0.48              |
| 29:27:34:ARG:HE   | 29:27:42:LEU:HA   | 1.78                     | 0.48              |
| 10:2O:63:VAL:HG11 | 10:2O:85:VAL:HG23 | 1.94                     | 0.48              |
| 28:16:44:ARG:HG2  | 28:16:44:ARG:HH11 | 1.78                     | 0.48              |
| 15:1T:60:THR:HG22 | 15:1T:77:PRO:HA   | 1.94                     | 0.48              |
| 1:1A:1082:U:C4    | 1:1A:1086:A:N1    | 2.79                     | 0.48              |
| 2:2B:55:U:O2'     | 6:2G:27:ASN:ND2   | 2.45                     | 0.48              |
| 18:2W:46:PHE:O    | 18:2W:50:VAL:HG23 | 2.13                     | 0.48              |
| 1:2A:754:C:H2'    | 1:2A:755:C:C6     | 2.47                     | 0.48              |
| 1:2A:1514:U:H2'   | 1:2A:1515:G:H8    | 1.77                     | 0.48              |
| 1:1A:2375:G:O2'   | 1:1A:2377:A:N7    | 2.38                     | 0.48              |
| 1:2A:647:G:H8     | 1:2A:647:G:O5'    | 1.96                     | 0.48              |
| 1:2A:1406:U:H2'   | 1:2A:1407:C:C6    | 2.48                     | 0.48              |
| 1:2A:927:G:H2'    | 1:2A:928:G:O4'    | 2.12                     | 0.48              |
| 1:1A:1091:G:C6    | 1:1A:1101:U:C2    | 3.01                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:2A:1006:C:H2'   | 1:2A:1007:C:C6    | 3.24                     | 0.48              |
| 1:2A:9:U:OP1      | 9:2N:115:ARG:NH2  | 2.45                     | 0.48              |
| 1:2A:2137:C:H2'   | 1:2A:2138:C:C6    | 2.48                     | 0.48              |
| 1:2A:1502:C:H2'   | 1:2A:1503:U:H6    | 1.78                     | 0.48              |
| 2:2B:105:A:OP1    | 21:2Z:72:ARG:NH1  | 2.47                     | 0.48              |
| 1:2A:2345:G:N3    | 1:2A:2381:C:H2'   | 2.28                     | 0.48              |
| 1:2A:2314:C:H2'   | 1:2A:2315:G:H8    | 1.78                     | 0.48              |
| 20:1Y:7:VAL:HG21  | 20:1Y:72:VAL:HG12 | 1.93                     | 0.48              |
| 7:2H:73:ALA:O     | 7:2H:76:VAL:HG22  | 2.13                     | 0.48              |
| 1:2A:2649:U:H2'   | 1:2A:2650:U:C6    | 2.49                     | 0.48              |
| 12:2Q:112:GLU:HG3 | 12:2Q:113:GLN:N   | 2.29                     | 0.48              |
| 1:1A:250:G:OP2    | 30:18:13:ARG:NH2  | 2.46                     | 0.48              |
| 1:1A:2243:U:H2'   | 1:1A:2244:U:C6    | 2.48                     | 0.48              |
| 20:2Y:38:ILE:HD11 | 20:2Y:66:PRO:HG3  | 1.94                     | 0.48              |
| 12:2Q:12:GLN:HE21 | 12:2Q:72:LYS:HZ2  | 1.60                     | 0.48              |
| 1:2A:2756:U:H1'   | 1:2A:2757:A:H5''  | 1.95                     | 0.48              |
| 1:2A:2655:G:O2'   | 1:2A:2664:G:O6    | 2.21                     | 0.48              |
| 1:1A:2773:C:H2'   | 1:1A:2774:C:H6    | 1.78                     | 0.48              |
| 1:1A:1363:C:OP1   | 23:11:61:ARG:NH2  | 2.46                     | 0.48              |
| 4:2E:9:VAL:HB     | 15:2T:3:ARG:HG2   | 1.96                     | 0.48              |
| 26:14:33:VAL:HG12 | 26:14:35:VAL:H    | 1.78                     | 0.48              |
| 1:1A:1178:C:H2'   | 1:1A:1179:C:H6    | 1.77                     | 0.48              |
| 2:2B:30:C:H2'     | 2:2B:31:C:H5'     | 1.95                     | 0.48              |
| 1:1A:1028:A:N6    | 1:1A:1125:G:H2'   | 2.28                     | 0.48              |
| 2:2B:75:G:H1      | 21:2Z:73:GLN:NE2  | 2.11                     | 0.48              |
| 1:1A:1512:U:H2'   | 1:1A:1513:C:C6    | 2.48                     | 0.48              |
| 1:2A:2156:G:H2'   | 1:2A:2157:G:C2    | 2.48                     | 0.48              |
| 6:1G:126:ASP:HB3  | 6:1G:128:ARG:H    | 1.78                     | 0.48              |
| 26:14:59:PHE:C    | 26:14:61:ARG:H    | 2.16                     | 0.48              |
| 21:2Z:105:VAL:N   | 21:2Z:139:VAL:O   | 2.45                     | 0.48              |
| 1:2A:1794:U:H2'   | 1:2A:1795:C:H6    | 1.78                     | 0.48              |
| 1:2A:1971:A:OP1   | 61:2A:3756:HOH:O  | 2.20                     | 0.48              |
| 1:2A:2820:A:C5    | 13:2R:4:LEU:HD11  | 2.49                     | 0.48              |
| 6:1G:131:TYR:HB3  | 6:1G:159:VAL:HG13 | 1.95                     | 0.48              |
| 1:1A:2504:U:OP2   | 61:1A:4059:HOH:O  | 2.20                     | 0.48              |
| 7:2H:149:ARG:HH12 | 7:2H:163:TYR:HA   | 1.78                     | 0.48              |
| 19:2X:20:GLY:O    | 19:2X:25:LYS:N    | 2.37                     | 0.48              |
| 2:1B:91:C:H5'     | 12:1Q:18:LYS:HA   | 1.95                     | 0.48              |
| 1:1A:2273:A:H2'   | 1:1A:2274:A:C8    | 2.48                     | 0.48              |
| 2:2B:13:A:O2'     | 2:2B:14:U:H3'     | 2.13                     | 0.48              |
| 1:2A:1371:G:H2'   | 1:2A:1372:U:H5    | 1.77                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1A:1518:U:H2'   | 1:1A:1519:G:O4'   | 2.13                     | 0.48              |
| 1:2A:2639:A:OP2   | 61:2A:3753:HOH:O  | 2.20                     | 0.48              |
| 18:1W:7:ALA:HB2   | 18:1W:50:VAL:HG22 | 1.95                     | 0.48              |
| 16:2U:65:ILE:CD1  | 16:2U:95:LEU:HB3  | 2.44                     | 0.48              |
| 1:2A:1388:G:H2'   | 1:2A:1389:G:H8    | 1.79                     | 0.48              |
| 1:2A:2191:G:H2'   | 1:2A:2192:G:O4'   | 2.13                     | 0.48              |
| 1:1A:1580:A:H8    | 1:1A:1580:A:OP2   | 1.97                     | 0.48              |
| 14:1S:27:SER:HA   | 14:1S:88:ASP:HB3  | 1.95                     | 0.48              |
| 1:2A:1721:G:H2'   | 1:2A:1740:G:O6    | 2.14                     | 0.48              |
| 1:2A:1027:A:C6    | 1:2A:1126:A:C4    | 3.02                     | 0.48              |
| 26:14:53:GLU:HB2  | 26:14:55:ARG:O    | 2.14                     | 0.48              |
| 1:2A:911:A:H2'    | 12:2Q:9:TYR:OH    | 2.14                     | 0.48              |
| 1:1A:1641:A:H2'   | 1:1A:1642:G:O4'   | 2.14                     | 0.48              |
| 15:1T:24:PRO:HA   | 15:1T:49:VAL:HG23 | 1.96                     | 0.48              |
| 1:2A:361:G:N2     | 1:2A:362:U:H3     | 2.11                     | 0.48              |
| 1:2A:709:U:H2'    | 1:2A:710:G:C8     | 2.49                     | 0.48              |
| 19:1X:94:GLY:HA3  | 19:1X:95:LEU:HB2  | 1.94                     | 0.48              |
| 1:2A:415:A:H2'    | 1:2A:416:C:O4'    | 2.13                     | 0.48              |
| 1:1A:2408:U:H2'   | 1:1A:2409:G:C8    | 2.48                     | 0.48              |
| 1:1A:1846:G:H5''  | 1:1A:1847:A:OP2   | 2.13                     | 0.48              |
| 28:26:44:ARG:HH11 | 28:26:44:ARG:HG2  | 1.78                     | 0.48              |
| 7:2H:88:LEU:HD11  | 7:2H:165:ALA:HA   | 1.96                     | 0.48              |
| 1:1A:1048:A:N1    | 1:1A:1112:G:O2'   | 2.42                     | 0.48              |
| 14:2S:53:SER:O    | 14:2S:57:LYS:N    | 2.46                     | 0.48              |
| 1:2A:833:U:H2'    | 1:2A:834:C:C6     | 3.28                     | 0.48              |
| 1:2A:923:C:H2'    | 1:2A:924:C:H6     | 1.79                     | 0.48              |
| 12:1Q:42:ILE:HG12 | 12:1Q:103:MET:HE1 | 1.96                     | 0.48              |
| 1:2A:526:A:OP1    | 61:2A:3755:HOH:O  | 2.20                     | 0.48              |
| 11:1P:42:SER:O    | 61:1P:301:HOH:O   | 2.20                     | 0.48              |
| 1:1A:2846:G:H2'   | 1:1A:2847:U:O4'   | 2.14                     | 0.48              |
| 1:1A:2512:C:H2'   | 1:1A:2513:G:O4'   | 2.14                     | 0.48              |
| 3:2D:275:LYS:HE3  | 3:2D:276:LYS:HA   | 1.96                     | 0.48              |
| 10:2O:104:ARG:NH2 | 15:2T:36:GLU:OE2  | 2.42                     | 0.48              |
| 2:2B:113:G:N2     | 14:2S:45:GLY:O    | 2.21                     | 0.48              |
| 1:1A:1072:C:H3'   | 1:1A:1094:U:O4    | 2.13                     | 0.48              |
| 1:2A:1024:G:C6    | 1:2A:1025:G:C6    | 3.01                     | 0.48              |
| 1:2A:948:G:H21    | 1:2A:985:C:P      | 2.36                     | 0.48              |
| 1:1A:2687:U:H2'   | 1:1A:2688:U:O4'   | 2.12                     | 0.48              |
| 1:2A:2167:U:H2'   | 1:2A:2168:G:N3    | 2.29                     | 0.48              |
| 1:1A:107:C:H2'    | 1:1A:108:U:H6     | 1.76                     | 0.48              |
| 1:2A:521:G:H2'    | 1:2A:522:G:H8     | 1.79                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:1D:37:LEU:HD22  | 3:1D:87:ASN:ND2   | 2.29                     | 0.48              |
| 1:2A:1562:A:H2'   | 1:2A:1563:G:H8    | 1.79                     | 0.48              |
| 1:1A:535:C:O3'    | 16:1U:53:ARG:NH1  | 2.45                     | 0.48              |
| 16:2U:28:ARG:NH1  | 16:2U:38:THR:OG1  | 2.47                     | 0.48              |
| 9:1N:114:ARG:HD2  | 61:1N:3102:HOH:O  | 2.14                     | 0.48              |
| 19:1X:60:ARG:HH22 | 29:17:47:ARG:HH12 | 1.61                     | 0.48              |
| 11:1P:98:GLU:O    | 11:1P:102:ARG:HG3 | 2.14                     | 0.48              |
| 1:1A:2340:G:H2'   | 1:1A:2341:G:H8    | 1.79                     | 0.48              |
| 2:2B:115:G:H2'    | 2:2B:116:G:O4'    | 2.14                     | 0.48              |
| 2:2B:90:A:C5      | 2:2B:91:C:H1'     | 2.49                     | 0.48              |
| 1:2A:848:G:N3     | 1:2A:933:A:H1'    | 2.29                     | 0.48              |
| 1:2A:330:A:H2     | 1:2A:1210:A:HO2'  | 1.60                     | 0.48              |
| 1:2A:94:C:H2'     | 1:2A:94(A):G:O4'  | 2.13                     | 0.48              |
| 1:2A:614(A):U:H4' | 1:2A:614(B):G:H5' | 1.96                     | 0.48              |
| 1:1A:1442:G:H2'   | 1:1A:1442:G:N3    | 2.81                     | 0.48              |
| 28:16:12:GLU:OE1  | 28:16:52:VAL:HG21 | 2.13                     | 0.48              |
| 20:2Y:13:VAL:HG12 | 20:2Y:74:PRO:HA   | 1.96                     | 0.48              |
| 1:2A:2224:G:H4'   | 1:2A:2226:C:C2    | 2.49                     | 0.48              |
| 1:2A:2049:G:N7    | 61:2A:3846:HOH:O  | 2.35                     | 0.48              |
| 11:2P:97:PRO:HD3  | 11:2P:126:VAL:O   | 2.13                     | 0.48              |
| 1:1A:1068:G:O2'   | 1:1A:1070:A:N7    | 2.47                     | 0.47              |
| 2:2B:32:C:H42     | 2:2B:50:G:H1      | 1.61                     | 0.47              |
| 6:2G:16:ARG:HB2   | 6:2G:17:PRO:HD3   | 1.95                     | 0.47              |
| 1:2A:890:A:H2'    | 1:2A:892:G:C8     | 2.46                     | 0.47              |
| 20:1Y:9:LYS:HA    | 20:1Y:10:GLY:HA2  | 1.59                     | 0.47              |
| 1:2A:2645:G:N2    | 1:2A:2767:C:OP2   | 2.46                     | 0.47              |
| 1:1A:947:G:H2'    | 1:1A:948:G:C8     | 2.49                     | 0.47              |
| 1:2A:2815:C:H2'   | 1:2A:2816:C:C6    | 2.49                     | 0.47              |
| 14:1S:14:VAL:O    | 14:1S:18:ILE:HG12 | 2.13                     | 0.47              |
| 1:2A:1352:U:OP2   | 61:2A:3754:HOH:O  | 2.20                     | 0.47              |
| 1:2A:2347:C:O2'   | 28:26:21:TYR:OH   | 2.25                     | 0.47              |
| 1:2A:118:A:N3     | 1:2A:178:G:H1'    | 2.29                     | 0.47              |
| 1:1A:1047:G:H2'   | 1:1A:1110:G:N2    | 2.29                     | 0.47              |
| 1:2A:1199:U:H2'   | 1:2A:1200:C:C6    | 2.49                     | 0.47              |
| 20:2Y:9:LYS:HA    | 20:2Y:10:GLY:HA2  | 1.59                     | 0.47              |
| 1:1A:918:A:N3     | 2:1B:80:U:O2'     | 2.42                     | 0.47              |
| 1:2A:2134:A:N3    | 1:2A:2134:A:H2'   | 2.29                     | 0.47              |
| 1:2A:674:G:O2'    | 5:2F:74:ARG:HD3   | 2.15                     | 0.47              |
| 1:2A:2321:G:N3    | 1:2A:2321:G:H2'   | 2.28                     | 0.47              |
| 1:2A:1518:U:H2'   | 1:2A:1519:G:O4'   | 2.14                     | 0.47              |
| 1:1A:1421:G:N2    | 1:1A:1495:A:N1    | 2.58                     | 0.47              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 3:2D:145:VAL:HG13 | 3:2D:191:ALA:HB2   | 1.96                     | 0.47              |
| 20:1Y:6:HIS:HE1   | 20:1Y:72:VAL:O     | 1.97                     | 0.47              |
| 20:1Y:13:VAL:HG12 | 20:1Y:74:PRO:HA    | 1.96                     | 0.47              |
| 10:2O:4:PRO:O     | 10:2O:5:GLN:HB2    | 2.14                     | 0.47              |
| 1:2A:1608:A:H1'   | 1:2A:1610:A:OP2    | 2.13                     | 0.47              |
| 1:2A:614(C):A:C4  | 5:2F:180:GLY:HA2   | 2.49                     | 0.47              |
| 1:1A:272(A):U:O2' | 1:1A:272(B):G:O5'  | 2.25                     | 0.47              |
| 9:2N:123:TYR:CZ   | 9:2N:129:PRO:HD2   | 2.49                     | 0.47              |
| 3:2D:260:ARG:NH2  | 3:2D:266:SER:OG    | 2.46                     | 0.47              |
| 12:2Q:39:PRO:HD3  | 12:2Q:99:PRO:HG3   | 1.96                     | 0.47              |
| 1:2A:2065:C:H2'   | 1:2A:2066:C:H6     | 1.79                     | 0.47              |
| 1:1A:218:A:C2     | 1:1A:235:U:H4'     | 2.49                     | 0.47              |
| 1:2A:2136:C:H1'   | 1:2A:2137:C:H5'    | 1.96                     | 0.47              |
| 1:1A:784:A:C6     | 3:1D:229:VAL:HG11  | 2.49                     | 0.47              |
| 1:1A:226:G:H21    | 1:1A:228:A:H62     | 1.60                     | 0.47              |
| 31:29:3:VAL:HG22  | 31:29:35:ARG:HD3   | 1.95                     | 0.47              |
| 1:2A:576:U:H2'    | 1:2A:577:G:C8      | 2.50                     | 0.47              |
| 21:1Z:105:VAL:O   | 21:1Z:141:VAL:HG22 | 2.15                     | 0.47              |
| 1:2A:531:C:H4'    | 1:2A:532:A:H5''    | 1.96                     | 0.47              |
| 4:1E:7:VAL:CG1    | 4:1E:27:LEU:HB3    | 2.44                     | 0.47              |
| 1:2A:2238:G:N3    | 1:2A:2238:G:H2'    | 2.29                     | 0.47              |
| 3:1D:233:HIS:CE1  | 3:1D:242:ARG:HG2   | 2.49                     | 0.47              |
| 1:1A:741:G:H2'    | 1:1A:742:G:O4'     | 2.48                     | 0.47              |
| 1:2A:952:G:H5''   | 1:2A:953:A:OP2     | 2.15                     | 0.47              |
| 1:1A:2139:C:N3    | 1:1A:2152:G:C2     | 2.82                     | 0.47              |
| 8:2I:5:LEU:HD11   | 8:2I:19:VAL:HG22   | 1.96                     | 0.47              |
| 1:1A:360:G:H3'    | 1:1A:361:G:H8      | 1.80                     | 0.47              |
| 7:1H:3:ARG:HH22   | 7:1H:66:GLY:N      | 2.12                     | 0.47              |
| 1:2A:1490:A:O2'   | 3:2D:99:ASP:OD1    | 2.31                     | 0.47              |
| 26:24:62:ARG:HA   | 26:24:62:ARG:HD3   | 1.61                     | 0.47              |
| 7:1H:56:SER:OG    | 7:1H:57:ASP:N      | 2.46                     | 0.47              |
| 1:2A:1268:A:H2'   | 1:2A:1269:A:O4'    | 2.13                     | 0.47              |
| 1:2A:2062:A:N6    | 58:2A:3652:HGR:O6  | 2.43                     | 0.47              |
| 1:1A:1371:G:N7    | 61:1A:4156:HOH:O   | 2.35                     | 0.47              |
| 13:2R:57:ARG:HH21 | 13:2R:62:ALA:HB2   | 1.80                     | 0.47              |
| 6:2G:33:ARG:O     | 6:2G:161:THR:HG23  | 2.14                     | 0.47              |
| 1:1A:2108:C:H2'   | 1:1A:2109:U:H6     | 1.79                     | 0.47              |
| 13:2R:18:LEU:HD21 | 13:2R:22:ARG:CZ    | 2.44                     | 0.47              |
| 3:1D:19:ALA:HB3   | 3:1D:21:PHE:CE1    | 2.50                     | 0.47              |
| 1:1A:1899:G:N3    | 1:1A:1899:G:H2'    | 2.29                     | 0.47              |
| 4:1E:119:ARG:HH11 | 4:1E:119:ARG:HG3   | 1.79                     | 0.47              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:1A:2804:C:H2'   | 1:1A:2805:G:C8     | 2.49                     | 0.47              |
| 1:1A:2364:C:H2'   | 1:1A:2365:G:O4'    | 2.15                     | 0.47              |
| 17:2V:37:VAL:O    | 17:2V:52:VAL:HG22  | 2.13                     | 0.47              |
| 5:2F:32:LEU:O     | 5:2F:36:VAL:HG23   | 2.14                     | 0.47              |
| 1:1A:1688:U:O2    | 1:1A:1700:A:H5'    | 2.13                     | 0.47              |
| 1:1A:657:U:H2'    | 1:1A:658:C:C6      | 2.49                     | 0.47              |
| 1:2A:1169:G:H8    | 1:2A:1169:G:O5'    | 1.98                     | 0.47              |
| 12:2Q:16:ARG:HD3  | 12:2Q:17:LEU:H     | 1.79                     | 0.47              |
| 1:1A:1300:U:H4'   | 1:1A:1301:A:H5''   | 1.95                     | 0.47              |
| 1:2A:228:A:O2'    | 1:2A:229:A:H4'     | 2.14                     | 0.47              |
| 1:1A:272:G:N7     | 1:1A:421:U:H2'     | 2.30                     | 0.47              |
| 1:1A:2690:C:OP1   | 13:1R:17:ARG:NH1   | 2.30                     | 0.47              |
| 21:2Z:69:THR:HG22 | 21:2Z:90:VAL:HA    | 1.96                     | 0.47              |
| 16:1U:108:GLU:O   | 16:1U:112:ARG:HG2  | 2.13                     | 0.47              |
| 1:1A:1338:G:N7    | 19:1X:62:LYS:NZ    | 2.49                     | 0.47              |
| 1:2A:656:G:H2'    | 1:2A:657:U:O4'     | 2.15                     | 0.47              |
| 1:2A:2161:C:H2'   | 1:2A:2162:G:C8     | 2.49                     | 0.47              |
| 6:2G:125:PHE:HD1  | 6:2G:131:TYR:HD1   | 1.62                     | 0.47              |
| 6:2G:5:VAL:HG13   | 6:2G:8:LYS:HZ1     | 1.79                     | 0.47              |
| 1:2A:2705:A:H2'   | 1:2A:2706:G:O4'    | 2.14                     | 0.47              |
| 1:1A:614:U:H5'    | 1:1A:614(C):A:N6   | 2.29                     | 0.47              |
| 4:1E:52:LEU:HD12  | 4:1E:77:ILE:HD11   | 1.97                     | 0.47              |
| 1:2A:2273:A:H2'   | 1:2A:2274:A:C8     | 2.50                     | 0.47              |
| 1:2A:2771:C:H5''  | 4:2E:202:LYS:HD3   | 1.95                     | 0.47              |
| 1:1A:721:C:H2'    | 1:1A:722:A:C8      | 2.49                     | 0.47              |
| 12:2Q:36:ALA:HB2  | 12:2Q:103:MET:SD   | 2.54                     | 0.47              |
| 1:1A:1466:G:H2'   | 1:1A:1547:C:N4     | 2.30                     | 0.47              |
| 1:1A:2121:G:H1    | 1:1A:2177:C:H42    | 1.62                     | 0.47              |
| 1:1A:2252:G:N7    | 22:10:4:LYS:NZ     | 2.63                     | 0.47              |
| 11:1P:15:ARG:HD3  | 61:1P:313:HOH:O    | 2.14                     | 0.47              |
| 1:1A:1028:A:H61   | 1:1A:1125:G:H2'    | 1.80                     | 0.47              |
| 1:2A:893:C:H2'    | 1:2A:894:C:C6      | 2.49                     | 0.47              |
| 2:2B:75:G:N3      | 21:2Z:85:HIS:CE1   | 2.83                     | 0.47              |
| 1:2A:2206:G:H5''  | 1:2A:2207:G:N1     | 2.29                     | 0.47              |
| 11:2P:84:ASN:O    | 11:2P:88:LEU:HG    | 2.14                     | 0.47              |
| 1:2A:536:A:H2'    | 1:2A:537:C:C6      | 2.50                     | 0.47              |
| 3:2D:167:GLY:O    | 3:2D:174:ILE:N     | 2.44                     | 0.47              |
| 1:2A:272:G:H4'    | 1:2A:272(A):U:H5'' | 1.96                     | 0.47              |
| 1:1A:2206:G:H4'   | 1:1A:2206:G:OP2    | 2.12                     | 0.47              |
| 1:2A:2356:C:H2'   | 1:2A:2357:U:O4'    | 2.15                     | 0.47              |
| 2:1B:78:A:H2'     | 2:1B:79:C:O4'      | 2.15                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:2E:9:VAL:HG22    | 4:2E:25:VAL:HB     | 1.96                     | 0.47              |
| 1:2A:1607:C:H5''   | 1:2A:1608:A:H5'    | 1.97                     | 0.47              |
| 17:2V:52:VAL:CG2   | 17:2V:55:ALA:HB3   | 2.44                     | 0.47              |
| 2:2B:45:A:O4'      | 6:2G:95:ARG:NH1    | 2.47                     | 0.47              |
| 1:1A:1709:U:H2'    | 1:1A:1710:C:C6     | 2.50                     | 0.47              |
| 1:2A:2312:U:H5'    | 6:2G:88:ILE:HD11   | 1.96                     | 0.47              |
| 20:1Y:87:LYS:HB3   | 20:1Y:95:LYS:HD2   | 1.96                     | 0.47              |
| 1:2A:824:A:H1'     | 1:2A:2358:G:N7     | 2.29                     | 0.47              |
| 11:2P:121:LYS:HG2  | 11:2P:122:PRO:HD2  | 1.95                     | 0.47              |
| 1:2A:2512:C:H2'    | 1:2A:2513:G:O4'    | 2.13                     | 0.47              |
| 21:2Z:126:VAL:HG13 | 21:2Z:161:VAL:HG23 | 1.97                     | 0.47              |
| 6:1G:62:LEU:HA     | 26:14:27:THR:HG21  | 1.97                     | 0.47              |
| 1:2A:2747:G:O6     | 1:2A:2755:C:H5''   | 2.15                     | 0.47              |
| 1:1A:2712:U:H1'    | 1:1A:2712(A):A:C8  | 2.50                     | 0.47              |
| 1:1A:919:G:N2      | 1:1A:2269:A:OP2    | 2.48                     | 0.47              |
| 1:2A:946:G:N2      | 1:2A:972:G:H1'     | 2.29                     | 0.47              |
| 3:2D:242:ARG:NH1   | 3:2D:242:ARG:HG3   | 2.19                     | 0.47              |
| 1:2A:2129:C:N3     | 1:2A:2159:G:N2     | 2.63                     | 0.47              |
| 1:1A:686:G:N2      | 1:1A:788:A:H61     | 2.13                     | 0.47              |
| 1:2A:1226:A:OP1    | 17:2V:84:LYS:HE2   | 2.14                     | 0.47              |
| 8:2I:102:SER:OG    | 8:2I:103:ARG:N     | 2.48                     | 0.47              |
| 1:1A:1876:A:H2'    | 1:1A:1877:A:C8     | 2.49                     | 0.47              |
| 1:2A:817:C:H2'     | 1:2A:818:G:O4'     | 2.15                     | 0.47              |
| 11:2P:95:VAL:HA    | 11:2P:99:LEU:HD21  | 1.97                     | 0.47              |
| 1:1A:1431:U:H2'    | 1:1A:1432:C:C6     | 2.50                     | 0.47              |
| 3:2D:132:PRO:HG2   | 3:2D:135:PHE:CD2   | 2.50                     | 0.47              |
| 8:1I:47:LEU:HD23   | 8:1I:47:LEU:HA     | 1.77                     | 0.47              |
| 2:1B:31:C:H4'      | 6:1G:29:TRP:CH2    | 2.49                     | 0.47              |
| 1:1A:143:G:H2'     | 1:1A:143(A):C:C6   | 2.49                     | 0.47              |
| 16:1U:76:TYR:CZ    | 16:1U:80:ILE:HG13  | 2.50                     | 0.47              |
| 1:1A:2127:G:H2'    | 1:1A:2128:C:C6     | 2.50                     | 0.47              |
| 1:1A:883:G:H22     | 1:1A:893:C:N4      | 2.12                     | 0.47              |
| 1:1A:1797:C:H4'    | 3:1D:257:LEU:O     | 2.15                     | 0.47              |
| 1:2A:2291:U:OP1    | 1:2A:2380:C:O2'    | 2.33                     | 0.47              |
| 6:2G:107:LEU:HA    | 6:2G:111:LEU:HD13  | 1.97                     | 0.47              |
| 1:2A:1653:G:O3'    | 13:2R:2:ARG:HB2    | 2.15                     | 0.47              |
| 1:2A:309:G:N3      | 1:2A:329:G:O2'     | 2.45                     | 0.47              |
| 1:2A:1339:G:O3'    | 19:2X:16:LYS:NZ    | 2.45                     | 0.47              |
| 13:2R:33:ARG:HB2   | 13:2R:115:GLU:CB   | 2.44                     | 0.47              |
| 61:1A:5109:HOH:O   | 4:1E:145:LYS:HE2   | 2.15                     | 0.47              |
| 1:1A:1223:G:N2     | 1:1A:1226:A:OP2    | 2.37                     | 0.47              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:2A:29:U:H2'     | 1:2A:30:G:C8       | 2.50                     | 0.47              |
| 6:2G:76:SER:N     | 6:2G:84:LYS:HB2    | 2.30                     | 0.47              |
| 26:24:40:HIS:HB3  | 26:24:43:TYR:HB2   | 1.97                     | 0.47              |
| 1:1A:2747:G:O6    | 1:1A:2755:C:H5''   | 2.15                     | 0.47              |
| 1:1A:1268:A:C2    | 1:1A:2013:A:C4     | 3.03                     | 0.47              |
| 29:17:12:ARG:NH2  | 29:17:44:PRO:HB3   | 2.29                     | 0.47              |
| 1:1A:833:U:H2'    | 1:1A:834:C:H6      | 2.45                     | 0.47              |
| 6:2G:110:ALA:O    | 6:2G:140:ILE:HG23  | 2.15                     | 0.47              |
| 1:2A:730:C:H3'    | 61:2A:3790:HOH:O   | 2.14                     | 0.47              |
| 11:1P:88:LEU:HD22 | 11:1P:95:VAL:HG21  | 1.96                     | 0.47              |
| 24:12:52:ASP:O    | 24:12:56:GLN:HG3   | 2.14                     | 0.47              |
| 1:2A:212:G:H2'    | 1:2A:213:A:O4'     | 2.14                     | 0.47              |
| 2:1B:95:C:H2'     | 2:1B:96:U:C6       | 2.50                     | 0.47              |
| 12:2Q:37:LEU:HD21 | 12:2Q:130:LYS:HE2  | 1.97                     | 0.47              |
| 7:1H:17:VAL:HG13  | 7:1H:26:VAL:HG22   | 1.96                     | 0.47              |
| 1:2A:940:G:H2'    | 1:2A:941:A:O4'     | 2.15                     | 0.47              |
| 1:2A:2378:A:O5'   | 1:2A:2378:A:H8     | 1.98                     | 0.47              |
| 1:1A:2149:G:H2'   | 1:1A:2150:U:O4'    | 2.14                     | 0.47              |
| 1:2A:699:A:H2'    | 1:2A:700:G:O4'     | 2.14                     | 0.47              |
| 1:2A:1777:U:H2'   | 1:2A:1778:U:H6     | 1.78                     | 0.47              |
| 1:2A:1894:C:H2'   | 1:2A:1895:C:H6     | 1.79                     | 0.47              |
| 3:2D:218:ARG:HB3  | 3:2D:219:PRO:HD2   | 1.96                     | 0.47              |
| 3:1D:150:LYS:HA   | 3:1D:150:LYS:HD3   | 1.81                     | 0.47              |
| 1:2A:1019:U:O2'   | 1:2A:1021:A:H2     | 1.98                     | 0.46              |
| 1:1A:1002:G:H3'   | 1:1A:1003:G:C4'    | 4.77                     | 0.46              |
| 1:1A:1188:U:H4'   | 17:1V:79:VAL:HG22  | 1.97                     | 0.46              |
| 1:2A:2615:U:C2    | 27:25:7:PRO:HA     | 2.50                     | 0.46              |
| 1:1A:1815:A:OP1   | 1:1A:1815:A:H8     | 1.98                     | 0.46              |
| 8:2I:124:GLY:H    | 8:2I:144:VAL:HG23  | 1.80                     | 0.46              |
| 1:1A:2572:A:C8    | 4:1E:144:ARG:HD2   | 2.50                     | 0.46              |
| 1:1A:687:C:H2'    | 1:1A:688:U:O4'     | 2.14                     | 0.46              |
| 1:2A:2821:A:H2'   | 1:2A:2822:G:C8     | 2.50                     | 0.46              |
| 1:2A:2530:A:H62   | 7:2H:172:LYS:NZ    | 2.13                     | 0.46              |
| 1:2A:2786:U:O2'   | 4:2E:62:PRO:O      | 2.27                     | 0.46              |
| 1:1A:2667:C:H2'   | 1:1A:2668:G:O4'    | 2.14                     | 0.46              |
| 10:2O:92:GLU:HG2  | 10:2O:113:LYS:HD2  | 1.97                     | 0.46              |
| 10:2O:90:GLN:O    | 10:2O:92:GLU:HG3   | 2.16                     | 0.46              |
| 1:2A:1394:U:OP1   | 61:2A:3757:HOH:O   | 2.20                     | 0.46              |
| 1:2A:493:G:H2'    | 1:2A:494:G:O4'     | 2.16                     | 0.46              |
| 14:2S:110:LEU:HA  | 14:2S:110:LEU:HD12 | 1.82                     | 0.46              |
| 1:2A:1203:G:O6    | 61:2A:3747:HOH:O   | 2.19                     | 0.46              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:2A:958:U:OP1     | 12:2Q:74:TYR:OH   | 2.19                     | 0.46              |
| 21:1Z:163:LEU:HD23 | 21:1Z:167:PRO:HG3 | 1.96                     | 0.46              |
| 1:2A:300:A:N3      | 1:2A:319:C:H1'    | 2.31                     | 0.46              |
| 1:2A:121:G:H4'     | 1:2A:149:A:H5'    | 1.97                     | 0.46              |
| 1:2A:18:C:H4'      | 16:2U:23:GLY:O    | 2.15                     | 0.46              |
| 1:2A:2351:G:O5'    | 1:2A:2351:G:H8    | 1.98                     | 0.46              |
| 13:1R:33:ARG:NH2   | 27:15:57:VAL:HG12 | 2.29                     | 0.46              |
| 26:24:59:PHE:N     | 26:24:60:GLN:HB2  | 2.30                     | 0.46              |
| 6:2G:111:LEU:HD23  | 6:2G:117:PHE:CZ   | 2.49                     | 0.46              |
| 12:1Q:35:VAL:HG13  | 12:1Q:130:LYS:HB3 | 1.97                     | 0.46              |
| 1:1A:2791:C:H2'    | 1:1A:2792:G:C8    | 2.48                     | 0.46              |
| 2:1B:74:U:H2'      | 2:1B:75:G:O4'     | 2.15                     | 0.46              |
| 2:1B:1:U:O2'       | 2:1B:2:C:H6       | 1.98                     | 0.46              |
| 15:2T:11:GLU:O     | 15:2T:15:VAL:HG23 | 2.15                     | 0.46              |
| 1:2A:500:G:N1      | 1:2A:503:A:OP2    | 2.46                     | 0.46              |
| 17:1V:5:VAL:HG21   | 17:1V:35:LEU:HD23 | 1.97                     | 0.46              |
| 1:2A:839:U:H4'     | 1:2A:840:C:OP2    | 4.68                     | 0.46              |
| 3:2D:118:VAL:HG22  | 3:2D:119:ALA:H    | 1.80                     | 0.46              |
| 1:2A:887:A:H4'     | 1:2A:888:C:C5     | 2.50                     | 0.46              |
| 1:2A:858:U:O2      | 1:2A:2268:A:H2'   | 2.15                     | 0.46              |
| 7:1H:20:ALA:HB1    | 7:1H:21:PRO:HD2   | 1.97                     | 0.46              |
| 1:2A:2206:G:H3'    | 1:2A:2207:G:C5    | 2.51                     | 0.46              |
| 1:2A:1475:G:C2     | 1:2A:1517:G:C2    | 3.04                     | 0.46              |
| 1:2A:528:A:C2      | 1:2A:2043:C:H4'   | 2.51                     | 0.46              |
| 1:1A:2319:G:H22    | 14:1S:3:ARG:CD    | 2.28                     | 0.46              |
| 7:1H:13:LYS:HA     | 7:1H:14:GLY:HA2   | 1.67                     | 0.46              |
| 3:2D:155:LEU:HA    | 3:2D:155:LEU:HD23 | 4.47                     | 0.46              |
| 1:2A:873:G:O3'     | 12:2Q:63:LYS:NZ   | 2.43                     | 0.46              |
| 1:2A:2820:A:O2'    | 1:2A:2821:A:OP1   | 2.32                     | 0.46              |
| 1:1A:833:U:H2'     | 1:1A:834:C:C6     | 2.95                     | 0.46              |
| 17:2V:31:ALA:O     | 17:2V:61:VAL:HG12 | 2.15                     | 0.46              |
| 6:2G:46:ALA:HB2    | 6:2G:53:LEU:HG    | 1.97                     | 0.46              |
| 1:2A:1539:G:H2'    | 1:2A:1540:U:O4'   | 2.16                     | 0.46              |
| 1:2A:1810:A:H2'    | 1:2A:1811:G:O4'   | 2.15                     | 0.46              |
| 1:1A:1178:C:O5'    | 1:1A:1178:C:H6    | 1.98                     | 0.46              |
| 1:2A:1015:G:H2'    | 1:2A:1016:G:C8    | 2.46                     | 0.46              |
| 7:1H:3:ARG:HE      | 7:1H:54:ARG:NH1   | 2.13                     | 0.46              |
| 3:2D:69:ARG:NH2    | 3:2D:128:GLY:O    | 2.48                     | 0.46              |
| 1:1A:2105:C:H2'    | 1:1A:2106:G:H8    | 1.77                     | 0.46              |
| 1:1A:363:G:H2'     | 1:1A:363(A):A:C8  | 2.48                     | 0.46              |
| 11:2P:17:LYS:HE3   | 11:2P:27:HIS:CE1  | 2.50                     | 0.46              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:2A:407:G:H2'    | 1:2A:408:G:C8      | 2.51                     | 0.46              |
| 2:2B:119:G:H2'    | 2:2B:120:A:C8      | 2.51                     | 0.46              |
| 10:2O:102:VAL:HB  | 10:2O:106:LEU:HD12 | 1.98                     | 0.46              |
| 18:1W:67:ASP:N    | 18:1W:67:ASP:OD1   | 2.48                     | 0.46              |
| 14:2S:106:ARG:HE  | 14:2S:112:PHE:C    | 2.18                     | 0.46              |
| 16:1U:58:ARG:HA   | 16:1U:61:TRP:CE3   | 2.51                     | 0.46              |
| 1:2A:1824:G:N3    | 3:2D:254:THR:OG1   | 2.46                     | 0.46              |
| 1:1A:1794:U:H2'   | 1:1A:1795:C:H6     | 1.80                     | 0.46              |
| 12:1Q:31:ASP:OD1  | 12:1Q:134:ARG:NH1  | 2.43                     | 0.46              |
| 1:2A:953:A:OP2    | 12:2Q:16:ARG:NH2   | 2.48                     | 0.46              |
| 1:2A:631:A:H1'    | 11:2P:66:GLY:HA2   | 1.97                     | 0.46              |
| 1:2A:857:C:H4'    | 22:20:23:VAL:HG21  | 1.97                     | 0.46              |
| 1:1A:686:G:H8     | 29:17:6:GLN:O      | 1.98                     | 0.46              |
| 1:2A:2393:A:H2'   | 1:2A:2394:C:O4'    | 2.16                     | 0.46              |
| 1:2A:994:C:O2'    | 1:2A:996:A:OP1     | 2.19                     | 0.46              |
| 1:2A:18:C:O2'     | 1:2A:554:U:OP1     | 2.32                     | 0.46              |
| 5:1F:64:ILE:HG21  | 5:1F:78:ILE:HG23   | 1.97                     | 0.46              |
| 1:1A:414:C:H2'    | 1:1A:415:A:H8      | 1.79                     | 0.46              |
| 1:1A:2119:A:C2    | 1:1A:2170:A:H2'    | 2.51                     | 0.46              |
| 1:2A:1404:C:H2'   | 1:2A:1405:U:H6     | 1.81                     | 0.46              |
| 1:2A:384:U:H2'    | 1:2A:385:C:C6      | 2.49                     | 0.46              |
| 1:2A:2891:G:O5'   | 1:2A:2891:G:H8     | 1.98                     | 0.46              |
| 1:1A:1441:G:H2'   | 1:1A:1442:G:H8     | 1.80                     | 0.46              |
| 1:2A:2745:C:H2'   | 1:2A:2746:U:O4'    | 2.16                     | 0.46              |
| 7:2H:90:LYS:HD3   | 7:2H:159:GLU:HG3   | 1.98                     | 0.46              |
| 10:2O:15:GLY:O    | 10:2O:47:ILE:HG12  | 2.15                     | 0.46              |
| 1:1A:639:U:H2'    | 1:1A:640:C:C6      | 2.51                     | 0.46              |
| 12:1Q:34:LEU:HB2  | 12:1Q:118:LEU:HD22 | 1.98                     | 0.46              |
| 1:1A:1043:C:O2    | 1:1A:1112:G:N2     | 2.32                     | 0.46              |
| 9:2N:62:VAL:HG11  | 9:2N:66:LYS:HB2    | 1.97                     | 0.46              |
| 1:2A:1286:A:H2'   | 1:2A:1287:A:H4'    | 6.44                     | 0.46              |
| 17:2V:24:LYS:HA   | 17:2V:92:THR:OG1   | 2.16                     | 0.46              |
| 1:2A:1031:G:O2'   | 31:29:7:VAL:O      | 2.23                     | 0.46              |
| 1:2A:831:G:N2     | 11:2P:53:GLY:O     | 2.49                     | 0.46              |
| 4:2E:32:PRO:HB2   | 4:2E:72:VAL:HG21   | 1.96                     | 0.46              |
| 18:2W:25:ARG:NH2  | 18:2W:74:ALA:O     | 2.48                     | 0.46              |
| 1:2A:236:C:H2'    | 1:2A:237:C:H6      | 1.79                     | 0.46              |
| 14:2S:26:LEU:HD22 | 14:2S:87:PHE:CD1   | 2.50                     | 0.46              |
| 1:2A:1777:U:O2'   | 1:2A:1778:U:H5'    | 2.16                     | 0.46              |
| 9:1N:48:MET:O     | 9:1N:48:MET:HG2    | 2.15                     | 0.46              |
| 1:1A:1258:C:H2'   | 1:1A:1259:G:O4'    | 2.16                     | 0.46              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:1A:2641:G:H5'   | 9:1N:83:LYS:HE2    | 1.97                     | 0.46              |
| 1:1A:2118:U:OP1   | 1:1A:2148:G:O2'    | 2.20                     | 0.46              |
| 1:2A:389:G:N1     | 11:2P:70:GLN:HG3   | 2.31                     | 0.46              |
| 24:22:32:LEU:HD21 | 24:22:54:LYS:HG2   | 1.98                     | 0.46              |
| 16:2U:104:GLN:NE2 | 16:2U:105:VAL:HG23 | 2.30                     | 0.46              |
| 1:2A:79:G:H2'     | 1:2A:80:G:H8       | 1.81                     | 0.46              |
| 26:14:57:GLU:HB3  | 26:14:58:ARG:HG2   | 1.97                     | 0.46              |
| 1:2A:2892:A:C2'   | 1:2A:2893:G:H5'    | 2.46                     | 0.46              |
| 1:2A:330:A:H2     | 1:2A:1210:A:H2'    | 1.81                     | 0.46              |
| 1:2A:1252:G:N1    | 16:2U:37:GLU:OE2   | 2.47                     | 0.46              |
| 1:1A:2051:A:H4'   | 4:1E:141:ILE:HG12  | 1.98                     | 0.46              |
| 1:2A:1482:G:H2'   | 1:2A:1484:G:C8     | 2.51                     | 0.46              |
| 1:2A:1778:U:H2'   | 1:2A:1784:A:N6     | 2.31                     | 0.46              |
| 6:2G:161:THR:HG22 | 6:2G:163:ALA:H     | 1.81                     | 0.46              |
| 1:1A:1794:U:H2'   | 1:1A:1795:C:C6     | 2.50                     | 0.46              |
| 11:2P:50:ARG:HD3  | 30:28:7:HIS:CD2    | 2.51                     | 0.46              |
| 4:2E:135:HIS:NE2  | 61:2E:401:HOH:O    | 2.36                     | 0.46              |
| 1:2A:1197:G:H2'   | 1:2A:1198:U:C6     | 2.51                     | 0.46              |
| 1:1A:2822:G:N7    | 61:1A:4163:HOH:O   | 2.36                     | 0.46              |
| 1:2A:2313:C:H5''  | 6:2G:91:ARG:HD3    | 1.97                     | 0.46              |
| 1:2A:322:A:OP1    | 5:2F:168:ARG:HD2   | 2.15                     | 0.46              |
| 1:2A:195:A:OP1    | 11:2P:46:LYS:NZ    | 2.46                     | 0.46              |
| 17:2V:15:GLU:O    | 17:2V:18:LEU:HB2   | 2.16                     | 0.46              |
| 1:1A:893:C:H2'    | 1:1A:894:C:C6      | 2.51                     | 0.46              |
| 1:2A:2298:A:N3    | 1:2A:2321:G:N2     | 2.64                     | 0.46              |
| 1:2A:597:U:H2'    | 1:2A:598:G:H8      | 1.81                     | 0.46              |
| 8:2I:122:GLU:O    | 8:2I:126:TYR:OH    | 2.26                     | 0.46              |
| 1:2A:2168:G:H8    | 1:2A:2170:A:N7     | 2.13                     | 0.46              |
| 1:1A:2629:A:HO2'  | 1:1A:2630:G:P      | 2.38                     | 0.46              |
| 1:1A:1364:G:N7    | 23:11:3:LYS:HD2    | 2.30                     | 0.46              |
| 1:2A:200:U:O4     | 1:2A:250:G:N2      | 2.48                     | 0.46              |
| 1:2A:250:G:C6     | 1:2A:251:A:C6      | 3.04                     | 0.46              |
| 1:2A:646:A:H2'    | 1:2A:647:G:O4'     | 2.14                     | 0.46              |
| 1:1A:629:G:H2'    | 1:1A:630:G:O4'     | 2.49                     | 0.46              |
| 1:1A:1710:C:O2'   | 1:1A:2858:C:N3     | 2.45                     | 0.46              |
| 9:2N:103:VAL:O    | 9:2N:107:LEU:HG    | 2.16                     | 0.46              |
| 12:1Q:87:LYS:HA   | 12:1Q:87:LYS:HD2   | 4.07                     | 0.46              |
| 24:12:70:GLN:HG3  | 24:12:70:GLN:O     | 2.16                     | 0.46              |
| 13:1R:18:LEU:HD21 | 13:1R:22:ARG:NH1   | 2.30                     | 0.46              |
| 5:1F:56:GLU:OE1   | 5:1F:93:LYS:NZ     | 2.47                     | 0.46              |
| 1:1A:1815:A:P     | 3:1D:54:ARG:HH22   | 2.39                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:2A:924:C:H2'    | 1:2A:925:C:C6     | 2.51                     | 0.46              |
| 1:1A:1041:C:N4    | 1:1A:1114:G:H1    | 2.07                     | 0.46              |
| 15:2T:49:VAL:HG12 | 15:2T:63:VAL:HG22 | 1.96                     | 0.46              |
| 1:2A:323:G:C8     | 5:2F:171:PRO:HG3  | 2.51                     | 0.46              |
| 1:1A:528:A:O2'    | 1:1A:529:A:H5'    | 2.16                     | 0.46              |
| 13:2R:33:ARG:NH2  | 27:25:57:VAL:O    | 2.44                     | 0.46              |
| 1:2A:2683:C:OP1   | 15:2T:53:ARG:NH2  | 2.45                     | 0.46              |
| 1:2A:852:G:H2'    | 1:2A:853:G:C8     | 2.51                     | 0.46              |
| 1:2A:398:G:OP1    | 1:2A:2090:G:O2'   | 2.27                     | 0.46              |
| 13:1R:18:LEU:HD21 | 13:1R:22:ARG:CZ   | 2.46                     | 0.46              |
| 1:1A:2287:A:O2'   | 1:1A:2289:G:N7    | 2.37                     | 0.46              |
| 1:1A:996:A:H4'    | 16:1U:91:ASP:OD2  | 2.16                     | 0.46              |
| 10:1O:64:ARG:HD2  | 10:1O:79:PHE:CD1  | 2.51                     | 0.46              |
| 14:1S:39:ILE:HB   | 14:1S:49:VAL:HG13 | 1.98                     | 0.46              |
| 1:2A:1469:A:H2'   | 1:2A:1470:G:O4'   | 2.16                     | 0.46              |
| 1:1A:2238:G:H2'   | 1:1A:2238:G:N3    | 2.30                     | 0.46              |
| 21:2Z:121:HIS:HB3 | 21:2Z:123:ASP:O   | 2.16                     | 0.46              |
| 1:2A:2239:G:OP2   | 61:2A:3758:HOH:O  | 2.21                     | 0.46              |
| 1:2A:1857:G:C6    | 1:2A:1858:G:N1    | 2.84                     | 0.46              |
| 26:14:49:PHE:HB3  | 26:14:50:VAL:H    | 1.41                     | 0.46              |
| 1:1A:1057:A:H3'   | 1:1A:1058:G:H5''  | 1.98                     | 0.46              |
| 1:2A:195:A:H5''   | 1:2A:196:A:O5'    | 2.15                     | 0.46              |
| 7:2H:38:SER:HB3   | 7:2H:41:MET:HG2   | 1.97                     | 0.46              |
| 1:1A:2722:G:H5''  | 1:1A:2820:A:N7    | 2.31                     | 0.46              |
| 25:23:52:HIS:CD2  | 25:23:53:LEU:HG   | 2.51                     | 0.46              |
| 3:1D:3:VAL:HG22   | 3:1D:17:THR:HB    | 1.98                     | 0.46              |
| 26:14:62:ARG:HD3  | 26:14:62:ARG:HA   | 1.78                     | 0.46              |
| 1:2A:1121:C:H2'   | 1:2A:1122:G:O4'   | 2.16                     | 0.46              |
| 1:2A:2180:U:H2'   | 1:2A:2181:G:O4'   | 2.16                     | 0.46              |
| 11:2P:96:THR:O    | 11:2P:99:LEU:HG   | 2.15                     | 0.46              |
| 7:2H:154:PRO:HB3  | 7:2H:163:TYR:CE1  | 2.50                     | 0.46              |
| 21:1Z:8:TYR:HB2   | 21:1Z:38:TYR:CE2  | 2.51                     | 0.46              |
| 10:1O:78:ARG:HD2  | 61:1O:303:HOH:O   | 2.16                     | 0.46              |
| 4:1E:28:ALA:HB3   | 4:1E:93:VAL:HG12  | 1.97                     | 0.46              |
| 1:2A:241:A:H8     | 1:2A:241:A:OP1    | 1.98                     | 0.46              |
| 1:2A:2349:G:OP1   | 61:2A:3759:HOH:O  | 2.21                     | 0.46              |
| 1:1A:1517:G:N3    | 1:1A:1919:A:O2'   | 104.72                   | 0.46              |
| 20:2Y:43:ASN:HB3  | 20:2Y:65:ALA:HB3  | 1.97                     | 0.45              |
| 1:1A:1026:U:H4'   | 1:1A:1027:A:OP1   | 2.15                     | 0.45              |
| 1:1A:2127:G:H21   | 1:1A:2173:A:H1'   | 1.80                     | 0.45              |
| 1:2A:1354:A:H4'   | 3:2D:38:LYS:HE2   | 1.97                     | 0.45              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:2A:1301:A:H2     | 1:2A:1626:G:N3    | 2.14                     | 0.45              |
| 1:1A:34:C:H2'      | 1:1A:35:G:H8      | 4.95                     | 0.45              |
| 25:13:7:LYS:HB2    | 25:13:34:GLU:HG3  | 1.98                     | 0.45              |
| 5:1F:178:PRO:HB2   | 5:1F:201:VAL:CG2  | 2.46                     | 0.45              |
| 1:2A:581:C:H2'     | 1:2A:582:G:C8     | 2.51                     | 0.45              |
| 1:2A:150:C:H2'     | 1:2A:151:C:C6     | 2.52                     | 0.45              |
| 1:2A:1582:C:H2'    | 1:2A:1583:A:H8    | 1.80                     | 0.45              |
| 1:1A:1153:C:H2'    | 1:1A:1154:G:O4'   | 2.16                     | 0.45              |
| 1:2A:1379:A:O5'    | 1:2A:1379:A:H8    | 1.99                     | 0.45              |
| 28:16:40:CYS:HA    | 28:16:41:PRO:HD3  | 1.80                     | 0.45              |
| 7:2H:97:ARG:O      | 7:2H:103:LEU:HD12 | 2.16                     | 0.45              |
| 21:2Z:154:ASP:OD1  | 21:2Z:154:ASP:N   | 2.49                     | 0.45              |
| 1:1A:196:A:N3      | 1:1A:196:A:H2'    | 2.31                     | 0.45              |
| 1:1A:2163:C:N4     | 1:1A:2164:C:O2    | 2.49                     | 0.45              |
| 1:1A:1066:U:H2'    | 1:1A:1068:G:OP2   | 2.16                     | 0.45              |
| 1:2A:2184:G:H2'    | 1:2A:2185:C:C6    | 2.52                     | 0.45              |
| 1:2A:1007:C:N3     | 1:2A:1022:G:C6    | 16.97                    | 0.45              |
| 2:2B:27:C:H5''     | 14:2S:54:LEU:HD21 | 1.98                     | 0.45              |
| 26:14:56:VAL:HB    | 26:14:57:GLU:H    | 1.53                     | 0.45              |
| 3:1D:242:ARG:HG3   | 3:1D:242:ARG:NH1  | 2.16                     | 0.45              |
| 1:2A:143:G:H2'     | 1:2A:143(A):C:C6  | 2.51                     | 0.45              |
| 1:2A:856:C:HO2'    | 1:2A:857:C:P      | 2.39                     | 0.45              |
| 1:2A:1803:A:H4'    | 3:2D:259:THR:HG23 | 1.97                     | 0.45              |
| 9:1N:66:LYS:HB3    | 9:1N:70:LYS:HB2   | 1.96                     | 0.45              |
| 1:1A:1267:U:OP2    | 1:1A:2012:G:N1    | 2.30                     | 0.45              |
| 5:1F:64:ILE:HD11   | 5:1F:75:HIS:HB2   | 1.98                     | 0.45              |
| 1:1A:107:C:H2'     | 1:1A:108:U:C6     | 2.50                     | 0.45              |
| 1:2A:407:G:H2'     | 1:2A:408:G:H8     | 1.81                     | 0.45              |
| 1:2A:2065:C:H2'    | 1:2A:2066:C:C6    | 2.51                     | 0.45              |
| 1:1A:721:C:H2'     | 1:1A:722:A:H8     | 1.81                     | 0.45              |
| 15:1T:51:ARG:HG3   | 15:1T:98:LYS:HD2  | 1.98                     | 0.45              |
| 1:1A:1745(A):C:H5' | 1:1A:1746:G:OP2   | 2.16                     | 0.45              |
| 12:1Q:81:VAL:HB    | 22:10:7:LEU:HD21  | 1.99                     | 0.45              |
| 1:1A:1099:G:H2'    | 1:1A:1100:C:C6    | 2.51                     | 0.45              |
| 1:2A:1171:G:H22    | 1:2A:1178:C:N4    | 2.14                     | 0.45              |
| 1:2A:999:U:O2'     | 1:2A:1000:A:H5'   | 2.16                     | 0.45              |
| 2:2B:17:C:N4       | 2:2B:109:C:N3     | 2.64                     | 0.45              |
| 2:2B:6:C:H42       | 2:2B:115:G:H1     | 1.63                     | 0.45              |
| 18:1W:68:ARG:HH11  | 18:1W:111:HIS:HA  | 1.81                     | 0.45              |
| 8:2I:93:THR:HG22   | 8:2I:119:PRO:HB3  | 1.97                     | 0.45              |
| 7:2H:85:LYS:HD3    | 7:2H:164:TYR:CE1  | 2.52                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 6:2G:111:LEU:HD23  | 6:2G:117:PHE:CE1   | 2.51                     | 0.45              |
| 1:1A:2142:C:O2     | 1:1A:2149:G:N1     | 2.38                     | 0.45              |
| 1:2A:1366:A:H2'    | 1:2A:1367:A:O4'    | 2.17                     | 0.45              |
| 10:2O:2:ILE:HB     | 10:2O:33:ALA:HB3   | 1.98                     | 0.45              |
| 1:2A:370:G:OP2     | 1:2A:370:G:H8      | 2.00                     | 0.45              |
| 1:2A:928:G:H8      | 1:2A:928:G:O5'     | 1.99                     | 0.45              |
| 1:2A:1379:A:H4'    | 1:2A:1380:G:OP2    | 2.12                     | 0.45              |
| 12:2Q:19:GLY:O     | 12:2Q:99:PRO:HD2   | 2.16                     | 0.45              |
| 1:2A:2251:OMG:C8   | 1:2A:2450:A:H4'    | 2.51                     | 0.45              |
| 1:1A:1386:C:H2'    | 1:1A:1387:C:C6     | 2.52                     | 0.45              |
| 21:1Z:126:VAL:HG13 | 21:1Z:161:VAL:HG23 | 1.98                     | 0.45              |
| 1:1A:1394:U:H2'    | 1:1A:1395:A:O4'    | 2.17                     | 0.45              |
| 3:2D:150:LYS:HD2   | 3:2D:150:LYS:N     | 2.30                     | 0.45              |
| 1:1A:303:U:H2'     | 1:1A:304:G:C8      | 2.51                     | 0.45              |
| 1:2A:1941:C:C5     | 1:2A:1942:5MC:HM52 | 2.51                     | 0.45              |
| 1:1A:2529:G:H5''   | 1:1A:2530:A:H5''   | 1.97                     | 0.45              |
| 6:1G:179:PRO:HG3   | 26:14:43:TYR:OH    | 2.16                     | 0.45              |
| 6:2G:142:PRO:HG2   | 6:2G:143:GLU:OE2   | 2.17                     | 0.45              |
| 1:2A:1002:G:H1     | 1:2A:1038:C:N4     | 42.67                    | 0.45              |
| 2:1B:92:C:OP1      | 21:1Z:79:ARG:NH1   | 2.49                     | 0.45              |
| 5:2F:40:GLN:HE22   | 5:2F:184:TYR:H     | 1.63                     | 0.45              |
| 27:25:16:ARG:HG3   | 27:25:17:ASP:N     | 2.31                     | 0.45              |
| 1:1A:2334:G:H5'    | 14:1S:9:ARG:HG2    | 1.99                     | 0.45              |
| 8:2I:80:PRO:HA     | 8:2I:145:VAL:HG23  | 1.98                     | 0.45              |
| 1:1A:620:G:H5'     | 1:1A:620:G:N3      | 2.32                     | 0.45              |
| 1:2A:1266:G:O5'    | 18:2W:15:ARG:NH2   | 2.49                     | 0.45              |
| 1:2A:2683:C:OP1    | 15:2T:55:ASN:ND2   | 2.49                     | 0.45              |
| 1:2A:776:G:H4'     | 1:2A:777:A:O5'     | 2.16                     | 0.45              |
| 8:1I:12:LEU:HD23   | 8:1I:12:LEU:HA     | 1.79                     | 0.45              |
| 4:2E:144:ARG:HB3   | 4:2E:145:LYS:H     | 1.52                     | 0.45              |
| 10:1O:79:PHE:CD1   | 15:1T:72:VAL:HG22  | 2.51                     | 0.45              |
| 6:2G:142:PRO:HB2   | 26:24:31:ILE:HG21  | 1.98                     | 0.45              |
| 2:1B:106:G:H5'     | 21:1Z:31:ARG:HG2   | 1.98                     | 0.45              |
| 18:1W:71:VAL:HA    | 18:1W:107:LEU:HD12 | 1.98                     | 0.45              |
| 21:2Z:35:ARG:HA    | 21:2Z:35:ARG:HD2   | 1.79                     | 0.45              |
| 1:1A:694:U:OP1     | 3:1D:59:LYS:NZ     | 2.41                     | 0.45              |
| 17:1V:74:LYS:HB2   | 17:1V:83:ARG:HB2   | 1.99                     | 0.45              |
| 2:2B:14:U:OP2      | 2:2B:70:C:O2'      | 2.22                     | 0.45              |
| 2:2B:55:U:H2'      | 2:2B:56:G:O4'      | 2.16                     | 0.45              |
| 1:2A:84:A:H5''     | 20:2Y:8:LYS:HE3    | 1.98                     | 0.45              |
| 1:1A:1083:U:H2'    | 1:1A:1085:A:OP2    | 2.16                     | 0.45              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:1A:1802:A:H2'   | 1:1A:1803:A:C8     | 2.51                     | 0.45              |
| 1:2A:2144:U:H1'   | 1:2A:2148:G:N2     | 2.31                     | 0.45              |
| 13:1R:33:ARG:HH21 | 13:1R:113:LEU:HD22 | 1.82                     | 0.45              |
| 1:2A:2315:G:H2'   | 1:2A:2316:C:C6     | 2.52                     | 0.45              |
| 1:2A:686:G:H21    | 1:2A:788:A:H61     | 1.64                     | 0.45              |
| 21:1Z:156:LYS:HE3 | 21:1Z:158:PRO:HD3  | 1.98                     | 0.45              |
| 1:2A:484:C:H2'    | 1:2A:485:C:H6      | 1.82                     | 0.45              |
| 1:1A:434:U:H2'    | 1:1A:435:C:O4'     | 7.83                     | 0.45              |
| 1:2A:2818:G:OP2   | 13:2R:42:LYS:NZ    | 2.48                     | 0.45              |
| 61:2A:4140:HOH:O  | 5:2F:68:LYS:HE2    | 2.17                     | 0.45              |
| 1:2A:438:G:H2'    | 1:2A:440:G:C8      | 2.51                     | 0.45              |
| 31:19:32:HIS:O    | 31:19:34:GLN:HG3   | 2.16                     | 0.45              |
| 11:2P:6:LEU:HD23  | 11:2P:6:LEU:HA     | 1.75                     | 0.45              |
| 7:1H:71:LEU:HA    | 7:1H:71:LEU:HD12   | 1.81                     | 0.45              |
| 21:2Z:92:SER:O    | 21:2Z:130:PRO:HG3  | 2.16                     | 0.45              |
| 1:1A:956:G:H2'    | 1:1A:957:A:H2'     | 1.99                     | 0.45              |
| 9:1N:4:TYR:CD2    | 16:1U:100:VAL:HG11 | 2.51                     | 0.45              |
| 1:2A:1009:A:H5''  | 16:2U:63:VAL:CG2   | 2.46                     | 0.45              |
| 7:2H:3:ARG:HH11   | 7:2H:4:ILE:H       | 1.64                     | 0.45              |
| 1:2A:974:G:C4     | 1:2A:989:G:C2      | 3.05                     | 0.45              |
| 17:2V:27:ALA:O    | 17:2V:64:HIS:HE1   | 2.00                     | 0.45              |
| 3:2D:69:ARG:NE    | 3:2D:130:ALA:HB2   | 2.29                     | 0.45              |
| 1:2A:1637:A:H4'   | 1:2A:2711:A:O2'    | 2.17                     | 0.45              |
| 3:2D:168:ARG:HA   | 3:2D:173:VAL:HA    | 1.99                     | 0.45              |
| 1:2A:2506:U:O2    | 58:2A:3652:HGR:H23 | 2.16                     | 0.45              |
| 1:1A:1218:C:H42   | 1:1A:1231:G:H1     | 1.63                     | 0.45              |
| 1:2A:1790:C:H5''  | 1:2A:1791:A:OP1    | 2.17                     | 0.45              |
| 5:1F:200:GLU:O    | 5:1F:204:ASN:ND2   | 2.47                     | 0.45              |
| 11:1P:116:GLY:O   | 11:1P:137:LYS:NZ   | 2.28                     | 0.45              |
| 29:27:12:ARG:HG2  | 29:27:46:VAL:HB    | 1.98                     | 0.45              |
| 1:2A:2123:G:H2'   | 1:2A:2124:G:C8     | 2.52                     | 0.45              |
| 1:1A:2525:G:C2    | 1:1A:2539:C:C2     | 3.05                     | 0.45              |
| 15:1T:117:ASP:O   | 15:1T:121:ILE:HG13 | 2.16                     | 0.45              |
| 1:2A:863:A:H2'    | 1:2A:864:G:C8      | 2.52                     | 0.45              |
| 1:2A:1651:G:H2'   | 1:2A:1652:A:O4'    | 2.16                     | 0.45              |
| 1:2A:2807:G:C2    | 1:2A:2808:U:H1'    | 2.51                     | 0.45              |
| 1:1A:2156:G:H2'   | 1:1A:2157:G:C4     | 2.52                     | 0.45              |
| 1:2A:2112:G:H2'   | 1:2A:2113:U:O4'    | 2.16                     | 0.45              |
| 1:2A:1272:A:H3'   | 1:2A:1273:U:H5''   | 1.99                     | 0.45              |
| 1:2A:2080:G:OP1   | 23:21:35:THR:OG1   | 2.27                     | 0.45              |
| 1:2A:1235:G:C6    | 1:2A:1236:G:N1     | 2.85                     | 0.45              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:1A:2590:A:O3'   | 3:1D:239:ARG:NH2   | 2.50                     | 0.45              |
| 1:2A:746:A:H2'    | 1:2A:2612:C:H5''   | 1.99                     | 0.45              |
| 1:1A:412:A:H8     | 1:1A:412:A:O5'     | 2.00                     | 0.45              |
| 1:2A:52:A:OP2     | 1:2A:117:G:N1      | 2.39                     | 0.45              |
| 1:2A:2749:A:H3'   | 1:2A:2750:A:H2'    | 1.98                     | 0.45              |
| 1:1A:1271:G:OP2   | 61:1A:4012:HOH:O   | 2.21                     | 0.45              |
| 1:2A:855:G:H2'    | 1:2A:856:C:C6      | 2.51                     | 0.45              |
| 1:2A:34:C:H2'     | 1:2A:35:G:H8       | 4.82                     | 0.45              |
| 1:1A:839:U:H2'    | 1:1A:840:C:C6      | 2.52                     | 0.45              |
| 1:2A:661:C:H2'    | 1:2A:662:G:C8      | 2.51                     | 0.45              |
| 1:2A:1814:G:H2'   | 1:2A:1815:A:C8     | 2.52                     | 0.45              |
| 1:1A:2143:C:C2    | 1:1A:2149:G:C2     | 3.05                     | 0.45              |
| 1:1A:1286:A:H2'   | 1:1A:1287:A:H4'    | 6.64                     | 0.45              |
| 20:2Y:97:ARG:HG3  | 20:2Y:97:ARG:H     | 1.63                     | 0.45              |
| 7:2H:20:ALA:HB3   | 7:2H:23:ARG:HG3    | 1.98                     | 0.45              |
| 1:2A:1592:C:H2'   | 1:2A:1593:G:C8     | 2.45                     | 0.45              |
| 14:2S:11:LYS:HG3  | 14:2S:91:PRO:HD3   | 1.99                     | 0.45              |
| 16:2U:92:ARG:HA   | 16:2U:95:LEU:HB2   | 1.98                     | 0.45              |
| 13:1R:36:THR:HG22 | 13:1R:37:THR:H     | 1.81                     | 0.45              |
| 11:2P:121:LYS:HD2 | 11:2P:123:LEU:HD11 | 1.98                     | 0.45              |
| 1:1A:2712:U:OP1   | 1:1A:2714:G:H4'    | 2.16                     | 0.45              |
| 3:1D:83:GLU:OE1   | 3:1D:104:TYR:OH    | 2.25                     | 0.45              |
| 1:1A:1448:G:H1'   | 1:1A:1528:A:N1     | 2.31                     | 0.45              |
| 1:1A:2660:A:H2'   | 1:1A:2661:G:O4'    | 2.16                     | 0.45              |
| 1:2A:2019:A:N7    | 27:25:9:LYS:HE2    | 2.32                     | 0.45              |
| 1:2A:1455:G:C8    | 13:2R:60:LEU:HD11  | 2.52                     | 0.45              |
| 1:2A:2865:U:C4    | 1:2A:2866:U:C4     | 3.05                     | 0.45              |
| 19:2X:11:PRO:HB3  | 19:2X:92:LEU:HD11  | 1.99                     | 0.45              |
| 1:2A:1782:C:O2'   | 1:2A:2609:U:H5''   | 2.17                     | 0.45              |
| 1:2A:1011:G:H1    | 1:2A:1018:C:H42    | 17.96                    | 0.45              |
| 6:2G:16:ARG:NE    | 6:2G:31:VAL:HG11   | 2.32                     | 0.45              |
| 1:1A:1053:C:N3    | 1:1A:1106:G:N2     | 2.57                     | 0.45              |
| 1:1A:1085:A:HO2'  | 1:1A:1104:C:HO2'   | 1.63                     | 0.45              |
| 1:2A:606:U:H4'    | 1:2A:658:C:H4'     | 1.99                     | 0.45              |
| 1:1A:839:U:H4'    | 1:1A:840:C:OP2     | 4.58                     | 0.45              |
| 1:2A:1131:G:H4'   | 9:2N:82:LEU:HB2    | 1.99                     | 0.45              |
| 1:1A:2445:G:OP1   | 5:1F:74:ARG:NH2    | 2.41                     | 0.45              |
| 5:1F:184:TYR:CE2  | 5:1F:188:ARG:HD2   | 2.52                     | 0.45              |
| 26:24:48:ARG:HA   | 26:24:48:ARG:HD3   | 1.77                     | 0.45              |
| 3:2D:108:PRO:HG2  | 3:2D:111:LEU:HB2   | 1.98                     | 0.45              |
| 1:2A:2846:G:H2'   | 1:2A:2847:U:O4'    | 2.17                     | 0.45              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:1A:1759:A:H1'   | 1:1A:2711:A:C2     | 2.51                     | 0.45              |
| 1:1A:465:G:C6     | 1:1A:466:A:N6      | 2.85                     | 0.45              |
| 1:1A:515:A:H2     | 1:1A:1260:G:N3     | 2.14                     | 0.45              |
| 1:2A:2080:G:H2'   | 1:2A:2081:C:H6     | 1.81                     | 0.45              |
| 20:1Y:1:MET:SD    | 20:1Y:2:ARG:N      | 2.85                     | 0.45              |
| 1:1A:2386:C:H2'   | 1:1A:2387:U:C6     | 2.52                     | 0.45              |
| 3:1D:159:ALA:HB1  | 3:1D:198:ASN:O     | 2.16                     | 0.45              |
| 1:2A:1922:G:H2'   | 1:2A:1923:U:O4'    | 2.17                     | 0.45              |
| 1:1A:238:C:H2'    | 1:1A:239:U:O4'     | 2.17                     | 0.45              |
| 1:1A:658:C:H2'    | 1:1A:659:C:C6      | 2.52                     | 0.44              |
| 1:2A:946:G:H22    | 1:2A:972:G:H1'     | 1.82                     | 0.44              |
| 2:2B:50:G:OP2     | 14:2S:62:LYS:HB2   | 2.17                     | 0.44              |
| 1:2A:320:A:N6     | 5:2F:140:LEU:HD21  | 2.32                     | 0.44              |
| 1:2A:2370:G:C6    | 1:2A:2371:G:C6     | 3.05                     | 0.44              |
| 10:2O:68:GLU:OE1  | 10:2O:78:ARG:NH1   | 2.45                     | 0.44              |
| 1:2A:797:C:H2'    | 1:2A:798:G:O4'     | 2.17                     | 0.44              |
| 1:2A:2164:C:H5''  | 1:2A:2165:G:OP2    | 2.16                     | 0.44              |
| 1:2A:315:G:H2'    | 1:2A:316:C:C6      | 2.52                     | 0.44              |
| 20:1Y:35:TYR:CE2  | 20:1Y:69:ALA:HB3   | 2.52                     | 0.44              |
| 15:2T:23:ARG:NH1  | 15:2T:120:ARG:HD3  | 2.32                     | 0.44              |
| 4:2E:52:LEU:O     | 4:2E:76:ARG:N      | 2.39                     | 0.44              |
| 1:1A:2561:A:H2'   | 1:1A:2562:U:O4'    | 2.17                     | 0.44              |
| 1:2A:2886:G:H2'   | 1:2A:2887:U:C6     | 2.52                     | 0.44              |
| 1:2A:2484:G:C2    | 1:2A:2485:G:C8     | 3.04                     | 0.44              |
| 1:2A:116:C:H2'    | 1:2A:117:G:O4'     | 2.18                     | 0.44              |
| 4:1E:3:GLY:HA3    | 4:1E:81:ILE:HD12   | 1.98                     | 0.44              |
| 3:1D:232:PRO:HB3  | 3:1D:244:ARG:CZ    | 2.47                     | 0.44              |
| 21:1Z:9:TYR:OH    | 21:1Z:61:LEU:HD23  | 2.17                     | 0.44              |
| 1:1A:1032:A:H2    | 1:1A:1122:G:H22    | 1.63                     | 0.44              |
| 16:1U:104:GLN:NE2 | 16:1U:105:VAL:HG23 | 2.32                     | 0.44              |
| 1:1A:1971:A:OP1   | 61:1A:4064:HOH:O   | 2.21                     | 0.44              |
| 25:13:59:VAL:O    | 25:13:60:GLU:HG2   | 2.17                     | 0.44              |
| 15:2T:117:ASP:O   | 15:2T:121:ILE:HG13 | 2.17                     | 0.44              |
| 5:2F:31:HIS:HB2   | 11:2P:9:ASN:OD1    | 2.17                     | 0.44              |
| 8:1I:102:SER:OG   | 8:1I:103:ARG:N     | 2.49                     | 0.44              |
| 1:2A:298:G:H5''   | 1:2A:299:A:OP1     | 2.18                     | 0.44              |
| 1:2A:375:C:H2'    | 1:2A:376:C:C6      | 2.53                     | 0.44              |
| 11:2P:62:LEU:O    | 30:28:13:ARG:NH1   | 2.49                     | 0.44              |
| 2:1B:19:G:H2'     | 2:1B:20:C:O4'      | 2.17                     | 0.44              |
| 15:2T:26:ASP:O    | 15:2T:49:VAL:HG22  | 2.17                     | 0.44              |
| 11:1P:141:ALA:HA  | 25:23:38:GLU:CG    | 2.47                     | 0.44              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:1A:2120:G:O2'   | 1:1A:2121:G:H5'    | 2.18                     | 0.44              |
| 5:2F:110:LEU:HD22 | 5:2F:205:ARG:HD2   | 1.98                     | 0.44              |
| 1:1A:862:G:H2'    | 1:1A:863:A:O4'     | 2.17                     | 0.44              |
| 1:2A:1853:A:N1    | 1:2A:2087:G:H1'    | 2.33                     | 0.44              |
| 1:1A:330:A:HO2'   | 1:1A:331:A:H8      | 1.63                     | 0.44              |
| 1:1A:1072:C:H2'   | 1:1A:1093:G:O6     | 2.17                     | 0.44              |
| 20:1Y:54:LYS:HA   | 20:1Y:56:PRO:HD3   | 1.99                     | 0.44              |
| 1:1A:1035:U:OP1   | 7:1H:59:ARG:NH1    | 2.51                     | 0.44              |
| 1:2A:1042:G:C4    | 1:2A:1043:C:H5     | 2.34                     | 0.44              |
| 1:2A:1200:C:H1'   | 16:2U:2:PRO:HG3    | 1.98                     | 0.44              |
| 1:2A:2365:G:O6    | 30:28:39:LYS:HE3   | 2.17                     | 0.44              |
| 21:1Z:72:ARG:NH2  | 21:1Z:97:GLU:O     | 2.50                     | 0.44              |
| 1:2A:1131:G:C8    | 1:2A:2025:C:H4'    | 2.51                     | 0.44              |
| 1:2A:1131:G:O6    | 1:2A:2040:C:H1'    | 2.17                     | 0.44              |
| 11:2P:59:LEU:HD23 | 30:28:13:ARG:HD2   | 2.00                     | 0.44              |
| 1:2A:793:A:OP2    | 1:2A:2071:A:O2'    | 2.33                     | 0.44              |
| 1:1A:1337:G:H2'   | 1:1A:1338:G:O4'    | 2.16                     | 0.44              |
| 21:2Z:159:PRO:HA  | 21:2Z:161:VAL:HG12 | 1.99                     | 0.44              |
| 31:19:25:VAL:HB   | 31:19:34:GLN:HB2   | 2.00                     | 0.44              |
| 1:1A:1717:G:H2'   | 1:1A:1718:G:H8     | 1.82                     | 0.44              |
| 1:2A:1611:C:OP1   | 61:2A:3760:HOH:O   | 2.21                     | 0.44              |
| 1:1A:2489:G:O6    | 1:1A:2490:G:N1     | 2.51                     | 0.44              |
| 1:1A:1825:A:OP1   | 3:1D:249:PRO:HD3   | 2.18                     | 0.44              |
| 1:2A:1448:G:H4'   | 1:2A:1542:A:OP1    | 2.18                     | 0.44              |
| 1:2A:1450:G:H1    | 1:2A:1462:C:H42    | 1.64                     | 0.44              |
| 14:2S:8:GLU:HG2   | 14:2S:8:GLU:H      | 1.48                     | 0.44              |
| 1:1A:1697:G:OP2   | 1:1A:1698:A:O2'    | 2.23                     | 0.44              |
| 1:2A:1662:C:O2'   | 1:2A:2687:U:OP1    | 2.33                     | 0.44              |
| 1:2A:1319:G:C6    | 1:2A:1320:C:N4     | 2.85                     | 0.44              |
| 1:2A:1011:G:H5''  | 16:2U:77:SER:OG    | 2.17                     | 0.44              |
| 1:2A:468:G:H5''   | 5:2F:60:SER:HB2    | 2.00                     | 0.44              |
| 21:1Z:130:PRO:HA  | 21:1Z:133:ILE:HG13 | 1.99                     | 0.44              |
| 1:1A:250:G:C6     | 1:1A:251:A:C6      | 3.06                     | 0.44              |
| 13:2R:18:LEU:HD21 | 13:2R:22:ARG:NH1   | 2.32                     | 0.44              |
| 1:1A:2461:C:H2'   | 1:1A:2462:U:C6     | 2.52                     | 0.44              |
| 2:1B:7:G:H5'      | 14:1S:29:PHE:CE2   | 2.52                     | 0.44              |
| 22:10:29:GLN:O    | 22:10:67:VAL:HG23  | 2.17                     | 0.44              |
| 1:2A:271(P):C:H2' | 1:2A:271(Q):G:H8   | 1.82                     | 0.44              |
| 1:1A:389:G:N1     | 11:1P:70:GLN:HG3   | 2.32                     | 0.44              |
| 1:1A:1011:G:OP2   | 16:1U:66:ASN:ND2   | 2.45                     | 0.44              |
| 1:1A:667:U:O2     | 30:18:2:PRO:HD2    | 2.16                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:1F:183:VAL:O    | 5:1F:187:VAL:HG23 | 2.17                     | 0.44              |
| 1:2A:387:U:P      | 23:21:20:ARG:HH12 | 2.40                     | 0.44              |
| 1:2A:2249:U:N3    | 1:2A:2253:G:OP2   | 2.48                     | 0.44              |
| 1:2A:1231:G:H2'   | 1:2A:1232:G:C8    | 2.53                     | 0.44              |
| 1:2A:1037:G:H2'   | 1:2A:1038:C:O4'   | 2.17                     | 0.44              |
| 1:1A:1930:G:O2'   | 1:1A:1968:G:O6    | 2.30                     | 0.44              |
| 1:1A:476:G:H4'    | 1:1A:502:A:N1     | 2.32                     | 0.44              |
| 1:1A:2028:U:H2'   | 1:1A:2029:G:O4'   | 2.17                     | 0.44              |
| 15:2T:39:ARG:HH12 | 15:2T:41:ARG:HB3  | 1.82                     | 0.44              |
| 1:1A:2233:U:H2'   | 1:1A:2234:G:C8    | 2.53                     | 0.44              |
| 1:2A:392:C:H5''   | 1:2A:409:C:H5''   | 2.00                     | 0.44              |
| 1:1A:1653:G:O3'   | 13:1R:2:ARG:HB2   | 2.17                     | 0.44              |
| 1:2A:1225:G:C6    | 1:2A:1226:A:C6    | 3.06                     | 0.44              |
| 1:1A:994:C:OP1    | 16:1U:53:ARG:NH2  | 2.51                     | 0.44              |
| 1:2A:2543:G:C2    | 1:2A:2765:A:H2'   | 2.53                     | 0.44              |
| 1:2A:2870:C:H5''  | 13:2R:65:LEU:HD21 | 1.99                     | 0.44              |
| 21:2Z:105:VAL:O   | 21:2Z:140:ASP:HA  | 2.16                     | 0.44              |
| 1:2A:1430:C:H2'   | 1:2A:1431:U:C6    | 2.53                     | 0.44              |
| 1:2A:2010:G:H5''  | 18:2W:42:ARG:HB2  | 1.99                     | 0.44              |
| 1:2A:728:G:H5''   | 3:2D:13:ARG:NH2   | 2.33                     | 0.44              |
| 1:1A:2308:G:O2'   | 1:1A:2310:A:N7    | 2.43                     | 0.44              |
| 1:2A:2275:C:H6    | 1:2A:2275:C:H5'   | 1.82                     | 0.44              |
| 1:1A:1065:U:H5''  | 1:1A:1066:U:OP2   | 2.18                     | 0.44              |
| 1:2A:2046:G:O5'   | 27:25:19:ARG:HA   | 2.17                     | 0.44              |
| 2:2B:66:A:H61     | 2:2B:109:C:H5''   | 1.83                     | 0.44              |
| 1:2A:340:A:H2'    | 1:2A:341:G:O4'    | 2.18                     | 0.44              |
| 8:1I:109:ILE:HG23 | 8:1I:130:TYR:CZ   | 2.52                     | 0.44              |
| 1:2A:336:C:P      | 20:2Y:84:ARG:HG2  | 2.58                     | 0.44              |
| 1:2A:2125:G:N1    | 1:2A:2172:U:OP1   | 2.39                     | 0.44              |
| 1:1A:301:G:H1'    | 1:1A:302:C:C6     | 2.52                     | 0.44              |
| 26:24:46:GLN:C    | 26:24:48:ARG:H    | 2.21                     | 0.44              |
| 20:2Y:56:PRO:C    | 20:2Y:58:GLY:H    | 2.21                     | 0.44              |
| 5:1F:28:ILE:O     | 5:1F:30:PRO:HD3   | 2.18                     | 0.44              |
| 4:2E:72:VAL:HA    | 4:2E:73:GLU:CB    | 2.48                     | 0.44              |
| 1:1A:1693:U:O2    | 3:1D:14:ARG:NH1   | 2.50                     | 0.44              |
| 1:1A:8:A:H2'      | 1:1A:9:U:H6       | 1.83                     | 0.44              |
| 15:2T:127:ALA:C   | 15:2T:129:ARG:N   | 2.70                     | 0.44              |
| 1:2A:1221(A):C:C2 | 1:2A:1229:G:C2    | 3.06                     | 0.44              |
| 26:24:47:GLN:C    | 26:24:49:PHE:H    | 2.20                     | 0.44              |
| 15:1T:108:ARG:HG3 | 15:1T:109:GLU:N   | 2.31                     | 0.44              |
| 1:1A:2881:C:H2'   | 1:1A:2882:A:O4'   | 2.17                     | 0.44              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:1A:1430:C:H2'   | 1:1A:1431:U:C6     | 2.52                     | 0.44              |
| 1:2A:2420:C:H5'   | 28:26:54:ILE:HD11  | 2.00                     | 0.44              |
| 1:1A:303:U:H2'    | 1:1A:304:G:H8      | 1.83                     | 0.44              |
| 10:2O:36:GLY:HA3  | 10:2O:109:LYS:HG3  | 2.00                     | 0.44              |
| 1:1A:2497:A:H5''  | 61:1A:4274:HOH:O   | 2.16                     | 0.44              |
| 4:1E:31:CYS:HA    | 4:1E:32:PRO:HD2    | 1.83                     | 0.44              |
| 1:1A:396:G:H1'    | 23:11:42:GLN:HB3   | 2.00                     | 0.44              |
| 20:1Y:56:PRO:C    | 20:1Y:58:GLY:H     | 2.21                     | 0.44              |
| 16:2U:66:ASN:HD21 | 16:2U:70:ARG:HH21  | 1.64                     | 0.44              |
| 2:2B:13:A:H4'     | 2:2B:15:A:C5       | 2.52                     | 0.44              |
| 3:1D:242:ARG:HD2  | 3:1D:246:PRO:HG3   | 1.98                     | 0.44              |
| 1:1A:1105:U:C2    | 1:1A:1106:G:N7     | 2.86                     | 0.44              |
| 2:2B:73:A:C4      | 2:2B:105:A:C2      | 3.05                     | 0.44              |
| 19:2X:5:TYR:CZ    | 24:22:30:ARG:HD2   | 2.53                     | 0.44              |
| 3:2D:2:ALA:O      | 3:2D:3:VAL:HB      | 2.16                     | 0.44              |
| 1:1A:446:G:OP1    | 16:1U:3:ARG:NH1    | 2.48                     | 0.44              |
| 11:2P:62:LEU:HD11 | 30:28:50:LEU:HD11  | 2.00                     | 0.44              |
| 1:1A:223:A:O4'    | 1:1A:422:A:H5'     | 2.18                     | 0.44              |
| 1:1A:271(P):C:O3' | 8:1I:42:SER:OG     | 2.33                     | 0.44              |
| 16:2U:98:LEU:HD22 | 16:2U:105:VAL:HG11 | 1.99                     | 0.44              |
| 1:1A:1557:C:H5''  | 1:1A:1558:A:OP2    | 2.18                     | 0.44              |
| 10:2O:73:ASP:OD2  | 15:2T:32:TYR:OH    | 2.24                     | 0.44              |
| 12:2Q:22:LYS:O    | 21:2Z:78:LYS:HE3   | 2.17                     | 0.44              |
| 1:2A:1311:G:H2'   | 29:27:47:ARG:HH22  | 1.82                     | 0.44              |
| 24:12:23:LYS:O    | 24:12:27:GLU:HG3   | 2.18                     | 0.44              |
| 1:2A:774:A:N3     | 1:2A:774:A:H2'     | 2.32                     | 0.44              |
| 1:2A:2245:U:O2'   | 1:2A:2436:G:OP2    | 2.29                     | 0.44              |
| 1:1A:2359:C:H2'   | 1:1A:2360:A:O4'    | 2.17                     | 0.44              |
| 1:1A:1024:G:C6    | 1:1A:1025:G:C6     | 3.06                     | 0.44              |
| 1:1A:1149:G:H2'   | 1:1A:1150:C:C6     | 2.53                     | 0.44              |
| 1:1A:557:U:H2'    | 1:1A:558:G:C8      | 2.53                     | 0.44              |
| 1:1A:642:G:N2     | 1:1A:645:C:OP2     | 2.48                     | 0.44              |
| 1:1A:848:G:O6     | 1:1A:928:G:H2'     | 2.18                     | 0.44              |
| 1:2A:918:A:O2'    | 2:2B:97:G:N2       | 2.46                     | 0.44              |
| 7:2H:8:PRO:O      | 7:2H:10:PRO:HD3    | 2.17                     | 0.44              |
| 21:2Z:50:GLN:OE1  | 21:2Z:50:GLN:N     | 2.51                     | 0.44              |
| 1:2A:1201:C:H2'   | 1:2A:1202:C:C6     | 2.53                     | 0.44              |
| 12:2Q:19:GLY:O    | 12:2Q:98:LYS:HE3   | 2.17                     | 0.44              |
| 1:2A:2274:A:C5    | 1:2A:2276:G:C8     | 3.05                     | 0.44              |
| 6:2G:36:LYS:HD3   | 6:2G:95:ARG:NH1    | 2.33                     | 0.44              |
| 1:2A:492:A:H2'    | 1:2A:493:G:O4'     | 2.17                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 27:25:8:LYS:O     | 27:25:9:LYS:HD2   | 2.18                     | 0.44              |
| 1:2A:1231:G:H2'   | 1:2A:1232:G:H8    | 1.83                     | 0.44              |
| 1:2A:1037:G:H1    | 1:2A:1118:C:H42   | 1.65                     | 0.44              |
| 14:2S:68:GLN:HA   | 14:2S:71:ARG:HD3  | 2.00                     | 0.44              |
| 12:2Q:16:ARG:HG2  | 12:2Q:18:LYS:HZ3  | 1.82                     | 0.44              |
| 1:1A:828:U:H4'    | 1:1A:831:G:N1     | 2.32                     | 0.44              |
| 1:2A:2141:G:H2'   | 1:2A:2142:C:O4'   | 2.18                     | 0.44              |
| 10:2O:78:ARG:HH22 | 15:2T:75:ILE:HD11 | 1.82                     | 0.44              |
| 5:1F:184:TYR:O    | 5:1F:188:ARG:HG3  | 2.17                     | 0.44              |
| 6:1G:109:VAL:C    | 6:1G:112:PRO:HD2  | 2.38                     | 0.44              |
| 1:2A:571:A:H5'    | 1:2A:2030:A:N7    | 2.33                     | 0.44              |
| 7:1H:13:LYS:HB3   | 7:1H:13:LYS:HE2   | 1.82                     | 0.44              |
| 1:1A:288:C:H2'    | 1:1A:289:A:C8     | 2.51                     | 0.44              |
| 8:1I:5:LEU:HD11   | 8:1I:19:VAL:HG22  | 1.99                     | 0.44              |
| 1:1A:1360:A:OP1   | 1:1A:1360:A:H8    | 4.96                     | 0.44              |
| 4:1E:51:PHE:O     | 4:1E:77:ILE:HD12  | 2.17                     | 0.44              |
| 1:2A:1232:G:H2'   | 1:2A:1233:C:C6    | 2.53                     | 0.44              |
| 9:2N:108:PRO:O    | 9:2N:113:GLY:HA3  | 2.18                     | 0.44              |
| 1:2A:2785:C:O2'   | 4:2E:66:HIS:ND1   | 2.50                     | 0.44              |
| 30:18:26:LYS:HG2  | 30:18:46:ARG:O    | 2.18                     | 0.44              |
| 19:2X:55:ASN:O    | 19:2X:79:ALA:HA   | 2.18                     | 0.44              |
| 1:1A:548:A:H1'    | 1:1A:549:G:OP1    | 2.17                     | 0.44              |
| 1:1A:1766:U:H2'   | 1:1A:1767:C:H6    | 1.83                     | 0.44              |
| 21:1Z:54:HIS:ND1  | 21:1Z:101:PRO:HG3 | 2.33                     | 0.44              |
| 1:1A:2695:C:H2'   | 1:1A:2696:U:C6    | 2.53                     | 0.44              |
| 1:1A:210:C:H2'    | 1:1A:211:A:C8     | 2.52                     | 0.44              |
| 3:1D:127:VAL:HA   | 3:1D:193:VAL:HG22 | 1.99                     | 0.44              |
| 1:1A:1790:C:H2'   | 1:1A:1791:A:C5    | 2.53                     | 0.44              |
| 1:2A:2526:G:O3'   | 31:29:33:LYS:NZ   | 2.49                     | 0.44              |
| 13:1R:65:LEU:HA   | 13:1R:65:LEU:HD12 | 1.64                     | 0.43              |
| 1:2A:510:C:H2'    | 1:2A:511:U:O4'    | 2.18                     | 0.43              |
| 1:2A:100:G:H3'    | 1:2A:102:G:C5'    | 2.47                     | 0.43              |
| 1:2A:2752:C:H2'   | 1:2A:2753:A:O4'   | 2.18                     | 0.43              |
| 11:1P:59:LEU:HD21 | 30:18:10:ALA:HA   | 2.00                     | 0.43              |
| 1:1A:2691:C:O3'   | 1:1A:2871:C:H4'   | 2.18                     | 0.43              |
| 2:2B:110:G:C6     | 2:2B:111:G:N7     | 2.85                     | 0.43              |
| 15:2T:91:ARG:HD2  | 15:2T:120:ARG:NH1 | 2.33                     | 0.43              |
| 1:2A:2030:A:H4'   | 1:2A:2031:A:C8    | 2.53                     | 0.43              |
| 1:1A:2107:C:N4    | 1:1A:2182:G:H1    | 2.16                     | 0.43              |
| 1:2A:2685:G:OP1   | 15:2T:51:ARG:NH1  | 2.42                     | 0.43              |
| 5:2F:129:PHE:CD2  | 5:2F:163:VAL:HG21 | 2.53                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:2A:2747:G:OP1    | 7:2H:74:ASN:ND2    | 2.51                     | 0.43              |
| 29:27:12:ARG:NH2   | 29:27:44:PRO:HB3   | 2.32                     | 0.43              |
| 1:2A:864:G:N2      | 1:2A:913:U:C2      | 2.86                     | 0.43              |
| 1:1A:478:A:OP1     | 61:1A:4066:HOH:O   | 2.21                     | 0.43              |
| 1:1A:2074:U:H2'    | 1:1A:2075:U:C6     | 2.53                     | 0.43              |
| 21:1Z:14:LYS:HA    | 21:1Z:15:PRO:HD3   | 1.86                     | 0.43              |
| 1:1A:2729:G:O2'    | 4:1E:186:GLY:HA3   | 2.18                     | 0.43              |
| 1:1A:1173:G:OP2    | 1:1A:1173:G:H2'    | 2.19                     | 0.43              |
| 7:2H:54:ARG:HB3    | 7:2H:65:HIS:CG     | 2.53                     | 0.43              |
| 1:2A:894:C:N4      | 1:2A:895:U:O4      | 2.52                     | 0.43              |
| 1:1A:2722:G:H2'    | 1:1A:2723:C:C6     | 2.54                     | 0.43              |
| 2:2B:78:A:H2'      | 2:2B:79:C:O4'      | 2.18                     | 0.43              |
| 1:1A:1331:A:H2'    | 1:1A:1333:C:C5     | 2.53                     | 0.43              |
| 10:2O:17:ARG:HA    | 10:2O:17:ARG:HD3   | 1.79                     | 0.43              |
| 12:1Q:35:VAL:HG12  | 12:1Q:130:LYS:O    | 2.18                     | 0.43              |
| 1:1A:2279:G:O6     | 22:10:14:ARG:HG3   | 2.18                     | 0.43              |
| 1:2A:2689:U:OP2    | 1:2A:2719:G:N2     | 2.49                     | 0.43              |
| 1:2A:1153:C:OP1    | 16:2U:92:ARG:NH2   | 2.51                     | 0.43              |
| 1:2A:2049:G:C2'    | 1:2A:2050:C:H5'    | 2.48                     | 0.43              |
| 19:2X:61:GLY:HA3   | 19:2X:73:ARG:O     | 2.18                     | 0.43              |
| 1:1A:1766:U:H2'    | 1:1A:1767:C:C6     | 2.52                     | 0.43              |
| 27:15:8:LYS:O      | 27:15:9:LYS:HD2    | 2.17                     | 0.43              |
| 9:1N:60:ILE:HD13   | 9:1N:99:LEU:HD12   | 1.99                     | 0.43              |
| 1:1A:1608:A:H1'    | 1:1A:1610:A:OP2    | 2.18                     | 0.43              |
| 20:1Y:20:TYR:HB3   | 20:1Y:23:ARG:HG3   | 2.00                     | 0.43              |
| 1:2A:1002:G:C2     | 1:2A:1003:G:H1'    | 3.02                     | 0.43              |
| 1:2A:1002:G:N3     | 1:2A:1003:G:H1'    | 3.06                     | 0.43              |
| 2:2B:28:C:H2'      | 2:2B:29:A:O4'      | 2.17                     | 0.43              |
| 1:2A:2369:A:H2'    | 1:2A:2370:G:C8     | 2.54                     | 0.43              |
| 5:2F:197:ASP:O     | 5:2F:200:GLU:HB2   | 2.18                     | 0.43              |
| 1:2A:68:G:H2'      | 1:2A:69:C:O4'      | 2.18                     | 0.43              |
| 1:1A:878:A:H3'     | 1:1A:879:G:C8      | 2.53                     | 0.43              |
| 19:1X:50:LYS:HB3   | 19:1X:84:ALA:HB2   | 2.00                     | 0.43              |
| 8:1I:4:ILE:HD11    | 8:1I:44:LEU:HD12   | 2.00                     | 0.43              |
| 10:1O:104:ARG:NH2  | 15:1T:36:GLU:OE2   | 2.39                     | 0.43              |
| 21:2Z:102:LEU:HD23 | 21:2Z:139:VAL:HG21 | 2.01                     | 0.43              |
| 1:2A:1541:G:OP2    | 1:2A:1542:A:O2'    | 2.27                     | 0.43              |
| 1:1A:256:A:H2'     | 1:1A:257:A:C8      | 2.52                     | 0.43              |
| 1:2A:620:G:H8      | 1:2A:622:G:O6      | 2.02                     | 0.43              |
| 1:1A:1906:G:H5''   | 1:1A:1929:G:O2'    | 2.18                     | 0.43              |
| 1:2A:1441:G:H8     | 1:2A:1441:G:O5'    | 2.66                     | 0.43              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:2A:1946:U:H2'   | 1:2A:1947:C:C6     | 2.53                     | 0.43              |
| 1:2A:2243:U:H2'   | 1:2A:2244:U:C6     | 2.53                     | 0.43              |
| 1:1A:2267:A:H5''  | 1:1A:2268:A:H5'    | 1.99                     | 0.43              |
| 1:1A:1056:G:H5''  | 1:1A:1057:A:O4'    | 2.18                     | 0.43              |
| 1:2A:2120:G:H2'   | 1:2A:2121:G:C8     | 2.52                     | 0.43              |
| 1:2A:1359:A:C2    | 1:2A:1360:A:C8     | 3.06                     | 0.43              |
| 19:2X:65:ARG:HB3  | 19:2X:70:LEU:HD23  | 1.99                     | 0.43              |
| 9:1N:28:THR:HG22  | 9:1N:29:LYS:N      | 2.33                     | 0.43              |
| 1:2A:1434:A:N6    | 1:2A:1558:A:H62    | 2.08                     | 0.43              |
| 22:20:45:PHE:HE1  | 22:20:77:ARG:NE    | 2.15                     | 0.43              |
| 1:1A:2790:A:H5'   | 1:1A:2893:G:H21    | 1.83                     | 0.43              |
| 1:1A:1022:G:N7    | 9:1N:66:LYS:HE2    | 2.33                     | 0.43              |
| 1:2A:910:A:C5     | 12:2Q:13:GLN:HG3   | 2.54                     | 0.43              |
| 1:1A:1889:A:N1    | 1:1A:2234:G:H1'    | 2.33                     | 0.43              |
| 1:2A:2694:G:C6    | 1:2A:2695:C:C4     | 3.06                     | 0.43              |
| 6:2G:106:LEU:HG   | 6:2G:111:LEU:CD1   | 2.48                     | 0.43              |
| 1:2A:588:U:H2'    | 1:2A:589:C:C6      | 2.53                     | 0.43              |
| 1:2A:431:U:H6     | 1:2A:431:U:O5'     | 2.01                     | 0.43              |
| 1:1A:1542:A:H8    | 1:1A:1542:A:OP1    | 2.02                     | 0.43              |
| 1:1A:2489:G:C6    | 1:1A:2490:G:N1     | 2.87                     | 0.43              |
| 13:2R:26:LYS:HE2  | 13:2R:70:LEU:O     | 2.18                     | 0.43              |
| 16:2U:93:LYS:NZ   | 17:2V:11:GLN:O     | 2.37                     | 0.43              |
| 1:1A:2685:G:H5'   | 10:1O:68:GLU:OE2   | 2.18                     | 0.43              |
| 24:22:35:LEU:HD12 | 24:22:53:LEU:HD12  | 2.01                     | 0.43              |
| 13:2R:97:VAL:HG22 | 13:2R:114:VAL:HG22 | 2.01                     | 0.43              |
| 1:1A:604:G:C6     | 1:1A:605:C:C4      | 3.06                     | 0.43              |
| 18:1W:11:ARG:HA   | 18:1W:100:THR:HG22 | 2.01                     | 0.43              |
| 1:1A:334:C:HO2'   | 1:1A:1434:A:HO2'   | 124.05                   | 0.43              |
| 1:1A:2098:U:H3    | 1:1A:2191:G:H1     | 1.65                     | 0.43              |
| 1:1A:1177:A:O2'   | 1:1A:1178:C:O4'    | 2.35                     | 0.43              |
| 1:2A:483:A:O2'    | 20:2Y:49:VAL:O     | 2.21                     | 0.43              |
| 20:1Y:92:ASN:HB3  | 20:1Y:94:LYS:N     | 2.18                     | 0.43              |
| 1:2A:1314:C:OP1   | 1:2A:1332:G:H5''   | 2.18                     | 0.43              |
| 1:2A:812:C:H2'    | 1:2A:813:U:C6      | 2.50                     | 0.43              |
| 1:2A:1817:G:C6    | 1:2A:1818:U:C4     | 3.06                     | 0.43              |
| 1:2A:2324:C:H1'   | 1:2A:2337:G:H5'    | 2.00                     | 0.43              |
| 7:2H:101:ARG:HB3  | 7:2H:117:PRO:HG2   | 2.00                     | 0.43              |
| 11:2P:107:LYS:O   | 11:2P:110:TYR:HB2  | 2.19                     | 0.43              |
| 7:1H:126:PRO:HB2  | 7:1H:127:GLU:H     | 1.61                     | 0.43              |
| 1:2A:236:C:H2'    | 1:2A:237:C:C6      | 2.53                     | 0.43              |
| 1:2A:2542:A:H4'   | 1:2A:2543:G:H8     | 1.82                     | 0.43              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:2A:2397:G:N2    | 1:2A:2420:C:H1'    | 2.34                     | 0.43              |
| 1:1A:2108:C:H2'   | 1:1A:2109:U:C6     | 2.53                     | 0.43              |
| 14:2S:85:VAL:HG11 | 14:2S:110:LEU:HG   | 2.00                     | 0.43              |
| 7:2H:96:ALA:HB1   | 7:2H:103:LEU:HD11  | 1.99                     | 0.43              |
| 1:2A:2252:G:H2'   | 1:2A:2253:G:O4'    | 2.19                     | 0.43              |
| 1:2A:312:G:H4'    | 1:2A:331:A:N3      | 2.34                     | 0.43              |
| 1:1A:2584:U:O4    | 61:1A:4062:HOH:O   | 2.21                     | 0.43              |
| 1:1A:1197:G:H2'   | 1:1A:1198:U:C6     | 2.53                     | 0.43              |
| 26:24:53:GLU:H    | 26:24:53:GLU:CD    | 2.22                     | 0.43              |
| 2:2B:31:C:C2'     | 2:2B:32:C:H5'      | 2.49                     | 0.43              |
| 1:2A:299:A:N1     | 1:2A:322:A:O2'     | 2.38                     | 0.43              |
| 1:2A:320:A:H2'    | 5:2F:136:THR:OG1   | 2.17                     | 0.43              |
| 5:2F:150:GLY:HA2  | 5:2F:172:TRP:CE3   | 2.54                     | 0.43              |
| 1:1A:1357:U:H2'   | 1:1A:1358:G:O4'    | 2.19                     | 0.43              |
| 1:2A:811:U:H2'    | 11:2P:21:ARG:HA    | 2.01                     | 0.43              |
| 3:2D:101:GLU:CD   | 3:2D:103:ARG:HH12  | 2.20                     | 0.43              |
| 1:1A:2131:G:H5''  | 1:1A:2132:U:H3'    | 2.00                     | 0.43              |
| 5:2F:40:GLN:NE2   | 5:2F:182:ASN:OD1   | 2.51                     | 0.43              |
| 1:2A:2114:A:N6    | 1:2A:2115:G:H21    | 2.17                     | 0.43              |
| 9:2N:33:LEU:HA    | 9:2N:38:HIS:CD2    | 2.51                     | 0.43              |
| 15:2T:59:THR:HG23 | 15:2T:78:LEU:HB3   | 2.00                     | 0.43              |
| 1:1A:2314:C:H5''  | 6:1G:38:VAL:HG21   | 1.99                     | 0.43              |
| 1:1A:922:U:H2'    | 1:1A:923:C:C6      | 2.54                     | 0.43              |
| 13:1R:26:LYS:HE2  | 13:1R:70:LEU:O     | 2.18                     | 0.43              |
| 1:2A:718:A:H3'    | 1:2A:719:C:H6      | 1.84                     | 0.43              |
| 1:2A:1420:U:O2'   | 1:2A:1421:G:OP1    | 2.32                     | 0.43              |
| 1:1A:1638:C:H2'   | 1:1A:1639:U:O4'    | 2.18                     | 0.43              |
| 1:2A:441:U:H2'    | 1:2A:442:G:C8      | 2.54                     | 0.43              |
| 14:1S:110:LEU:HA  | 14:1S:110:LEU:HD12 | 1.84                     | 0.43              |
| 16:2U:8:VAL:O     | 16:2U:12:ARG:HG3   | 2.19                     | 0.43              |
| 1:2A:2078:C:H2'   | 1:2A:2079:U:O4'    | 2.19                     | 0.43              |
| 1:1A:1065:U:H1'   | 1:1A:1074:G:N1     | 2.34                     | 0.43              |
| 1:2A:1021:A:H3'   | 1:2A:1021:A:C8     | 2.53                     | 0.43              |
| 2:2B:24:G:N7      | 2:2B:56:G:H2'      | 2.33                     | 0.43              |
| 1:2A:902:C:H2'    | 1:2A:903:C:C6      | 2.51                     | 0.43              |
| 3:1D:211:ARG:HG3  | 3:1D:214:TRP:CE3   | 2.53                     | 0.43              |
| 1:1A:785:G:N2     | 1:1A:797:C:O2      | 28.18                    | 0.43              |
| 1:2A:868:U:N3     | 1:2A:869:G:N7      | 2.67                     | 0.43              |
| 1:1A:228:A:OP1    | 11:1P:76:LYS:HE3   | 2.19                     | 0.43              |
| 1:2A:910:A:C6     | 1:2A:911:A:C6      | 3.07                     | 0.43              |
| 1:1A:2864:G:OP1   | 15:1T:119:LYS:HD2  | 2.19                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1A:671:C:H2'    | 1:1A:672:C:H6     | 1.82                     | 0.43              |
| 9:1N:30:ILE:HG23  | 9:1N:52:VAL:HG11  | 2.00                     | 0.43              |
| 1:2A:1882:C:H5''  | 23:21:26:ARG:NH1  | 2.34                     | 0.43              |
| 1:2A:1584:C:O2'   | 1:2A:1586:A:H5'   | 2.19                     | 0.43              |
| 1:2A:1711:C:H2'   | 1:2A:1712:C:C6    | 2.54                     | 0.43              |
| 1:2A:2050:C:N4    | 1:2A:2051:A:N1    | 2.67                     | 0.43              |
| 1:1A:1946:U:H2'   | 1:1A:1947:C:C6    | 2.54                     | 0.43              |
| 1:1A:2576:G:OP1   | 1:1A:2576:G:N2    | 2.51                     | 0.43              |
| 1:2A:271(D):G:H2' | 1:2A:271(E):U:C6  | 2.54                     | 0.43              |
| 16:1U:34:LYS:HD3  | 16:1U:34:LYS:HA   | 1.68                     | 0.43              |
| 10:1O:10:VAL:HG11 | 10:1O:16:ALA:HB1  | 2.01                     | 0.43              |
| 16:2U:27:LEU:HB3  | 16:2U:31:SER:HB3  | 1.99                     | 0.43              |
| 3:1D:43:ARG:HA    | 3:1D:48:ARG:O     | 2.18                     | 0.43              |
| 3:2D:37:LEU:HD22  | 3:2D:87:ASN:HD21  | 1.84                     | 0.43              |
| 2:2B:64:C:H2'     | 2:2B:65:C:C6      | 2.54                     | 0.43              |
| 1:1A:2441:C:OP1   | 61:1A:4063:HOH:O  | 2.21                     | 0.43              |
| 1:1A:2175:C:H2'   | 1:1A:2176:A:O4'   | 2.19                     | 0.43              |
| 20:1Y:20:TYR:CE2  | 20:1Y:43:ASN:HA   | 2.54                     | 0.43              |
| 1:2A:1359:A:C2    | 1:2A:1372:U:O4    | 2.72                     | 0.43              |
| 1:2A:657:U:H2'    | 1:2A:658:C:C6     | 2.54                     | 0.43              |
| 1:1A:281:G:H1'    | 1:1A:360:G:N2     | 2.32                     | 0.43              |
| 1:1A:2849:U:H4'   | 1:1A:2868:A:C2    | 2.53                     | 0.43              |
| 1:2A:2552:2MU:O5' | 1:2A:2552:2MU:H6  | 2.19                     | 0.43              |
| 1:1A:531:C:H4'    | 1:1A:532:A:H5''   | 2.01                     | 0.43              |
| 1:2A:724:U:H2'    | 1:2A:725:G:O4'    | 2.19                     | 0.43              |
| 1:1A:2887:U:H2'   | 1:1A:2888:C:H6    | 1.83                     | 0.43              |
| 1:2A:571:A:C5'    | 1:2A:2030:A:H62   | 2.32                     | 0.43              |
| 1:2A:2685:G:P     | 15:2T:51:ARG:HH12 | 2.42                     | 0.43              |
| 1:2A:108:U:H2'    | 1:2A:109:G:C8     | 2.53                     | 0.43              |
| 1:1A:271(X):G:C2  | 1:1A:271(Y):U:O4  | 2.71                     | 0.43              |
| 1:2A:2051:A:H5'   | 1:2A:2578:G:O4'   | 2.18                     | 0.43              |
| 19:2X:26:TYR:HB3  | 19:2X:92:LEU:HD22 | 2.01                     | 0.43              |
| 1:1A:1851:U:H2'   | 1:1A:1852:C:O4'   | 2.18                     | 0.43              |
| 1:1A:271(A):A:N1  | 1:1A:272(D):G:O2' | 2.44                     | 0.43              |
| 1:1A:2116:G:H2'   | 1:1A:2117:A:C5    | 2.53                     | 0.43              |
| 1:1A:2031:A:C6    | 1:1A:2498:C:H1'   | 2.54                     | 0.43              |
| 1:2A:2579:C:H4'   | 4:2E:134:ILE:HG12 | 2.01                     | 0.43              |
| 8:1I:62:LYS:O     | 8:1I:66:GLU:HG2   | 2.18                     | 0.43              |
| 2:1B:45:A:O4'     | 6:1G:95:ARG:NH1   | 2.52                     | 0.43              |
| 1:2A:1932:A:H2'   | 1:2A:1933:G:O4'   | 2.19                     | 0.43              |
| 6:2G:173:LEU:HB3  | 6:2G:178:PHE:CG   | 2.53                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:2A:65:C:O2'      | 1:2A:456:C:N3      | 2.50                     | 0.43              |
| 1:1A:606:U:H4'     | 1:1A:658:C:H4'     | 2.01                     | 0.43              |
| 14:2S:36:TYR:CD1   | 14:2S:52:SER:HB3   | 2.53                     | 0.43              |
| 6:2G:119:GLY:HA3   | 6:2G:181:ARG:HB3   | 2.00                     | 0.43              |
| 2:2B:38:C:O4'      | 14:2S:95:HIS:NE2   | 2.52                     | 0.43              |
| 1:2A:724:U:C4      | 1:2A:725:G:C6      | 3.07                     | 0.43              |
| 14:2S:15:ARG:HB3   | 14:2S:19:LYS:HE3   | 2.00                     | 0.43              |
| 13:1R:38:VAL:HG12  | 13:1R:42:LYS:HE3   | 2.01                     | 0.43              |
| 1:2A:271(H):G:O2'  | 1:2A:271(I):G:H8   | 2.00                     | 0.43              |
| 1:2A:531:C:H5'     | 61:2A:4395:HOH:O   | 2.17                     | 0.43              |
| 21:2Z:128:VAL:HG13 | 21:2Z:133:ILE:HG12 | 2.00                     | 0.43              |
| 1:2A:1450(A):C:N4  | 1:2A:1451:C:H41    | 2.16                     | 0.43              |
| 1:2A:2633:G:H5''   | 1:2A:2812:G:H5'    | 2.01                     | 0.43              |
| 4:1E:9:VAL:HB      | 15:1T:3:ARG:HG2    | 2.00                     | 0.43              |
| 1:2A:2110:G:H3'    | 1:2A:2111:C:H5'    | 2.01                     | 0.43              |
| 1:2A:1847:A:H3'    | 1:2A:1848:A:H5'    | 2.00                     | 0.43              |
| 1:1A:684:G:OP1     | 29:17:16:HIS:ND1   | 2.46                     | 0.43              |
| 1:1A:1059:G:N1     | 1:1A:1079:C:N4     | 2.42                     | 0.43              |
| 1:1A:784:A:N6      | 3:1D:229:VAL:HG11  | 2.34                     | 0.43              |
| 7:1H:3:ARG:NH2     | 7:1H:65:HIS:HB3    | 2.32                     | 0.43              |
| 9:2N:97:ARG:HA     | 9:2N:100:GLU:HB3   | 2.01                     | 0.43              |
| 1:2A:357:A:H2'     | 1:2A:358:U:C6      | 2.54                     | 0.43              |
| 7:2H:118:PRO:HG2   | 7:2H:121:ILE:HG13  | 2.01                     | 0.43              |
| 27:15:55:ARG:NH1   | 27:15:57:VAL:HG22  | 2.34                     | 0.43              |
| 17:1V:76:LYS:HB2   | 17:1V:81:TYR:HB3   | 2.01                     | 0.43              |
| 3:1D:11:PRO:O      | 3:1D:14:ARG:HB3    | 2.19                     | 0.43              |
| 1:1A:2751:G:H4'    | 7:1H:4:ILE:HD11    | 2.00                     | 0.43              |
| 15:1T:108:ARG:HA   | 15:1T:111:ARG:NH1  | 2.34                     | 0.43              |
| 21:2Z:52:SER:OG    | 21:2Z:53:ILE:N     | 2.48                     | 0.43              |
| 1:1A:191:A:H2'     | 1:1A:192:C:C6      | 2.53                     | 0.43              |
| 1:1A:329:G:OP1     | 1:1A:329:G:H8      | 2.02                     | 0.43              |
| 1:1A:2340:G:H2'    | 1:1A:2341:G:C8     | 2.53                     | 0.43              |
| 1:1A:2352:A:N6     | 1:1A:2365:G:O2'    | 2.52                     | 0.43              |
| 1:2A:1455:G:H8     | 13:2R:60:LEU:HD11  | 1.84                     | 0.43              |
| 11:1P:47:ASP:OD2   | 11:1P:49:ARG:NH2   | 2.48                     | 0.43              |
| 4:1E:143:ASN:HD22  | 4:1E:147:PRO:CD    | 2.32                     | 0.43              |
| 4:2E:2:LYS:NZ      | 4:2E:95:ILE:O      | 2.49                     | 0.43              |
| 1:1A:578:A:H5'     | 1:1A:1254:A:OP1    | 2.19                     | 0.43              |
| 9:1N:12:ARG:HD2    | 9:1N:136:GLU:OE1   | 2.19                     | 0.43              |
| 1:1A:2552:2MU:O5'  | 1:1A:2552:2MU:H6   | 2.18                     | 0.43              |
| 25:13:26:LEU:O     | 25:13:35:ARG:NE    | 2.52                     | 0.43              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 5:1F:8:GLN:HE22   | 5:1F:21:ALA:HB2    | 1.83                     | 0.43              |
| 18:2W:23:LEU:HD11 | 27:25:25:LEU:HB2   | 2.01                     | 0.43              |
| 1:2A:592:G:O2'    | 30:28:4:MET:HG3    | 2.19                     | 0.43              |
| 1:1A:141:A:C6     | 1:1A:142:A:N1      | 2.87                     | 0.43              |
| 1:1A:1059:G:OP2   | 1:1A:1060:U:H3'    | 2.19                     | 0.42              |
| 1:2A:79:G:H2'     | 1:2A:80:G:C8       | 2.54                     | 0.42              |
| 1:1A:945:A:C4     | 1:1A:2448:A:C2     | 3.07                     | 0.42              |
| 1:2A:1166:C:H2'   | 1:2A:1167:U:C6     | 2.53                     | 0.42              |
| 1:2A:1501:C:O4'   | 3:2D:100:GLY:HA2   | 2.18                     | 0.42              |
| 1:1A:370:G:OP2    | 1:1A:370:G:H8      | 2.01                     | 0.42              |
| 1:1A:782:A:H5'    | 1:1A:783:A:N7      | 2.34                     | 0.42              |
| 1:2A:674:G:H1'    | 5:2F:74:ARG:HD3    | 2.01                     | 0.42              |
| 2:2B:80:U:H2'     | 2:2B:81:G:N7       | 2.33                     | 0.42              |
| 21:1Z:129:SER:HA  | 21:1Z:130:PRO:HD3  | 1.88                     | 0.42              |
| 1:1A:2375:G:N2    | 1:1A:2378:A:OP2    | 2.48                     | 0.42              |
| 1:2A:590:A:H2'    | 1:2A:591:C:O4'     | 2.19                     | 0.42              |
| 4:2E:150:VAL:HG13 | 4:2E:154:LYS:HD2   | 2.00                     | 0.42              |
| 14:2S:26:LEU:HD22 | 14:2S:87:PHE:HD1   | 1.84                     | 0.42              |
| 1:2A:2275:C:C6    | 1:2A:2275:C:H5'    | 2.54                     | 0.42              |
| 1:2A:258:G:H2'    | 1:2A:259:G:H8      | 2.92                     | 0.42              |
| 5:2F:116:ASP:OD1  | 5:2F:119:ARG:NH2   | 2.52                     | 0.42              |
| 1:2A:186:G:H2'    | 1:2A:187:G:C8      | 2.54                     | 0.42              |
| 1:2A:1641:A:H2'   | 1:2A:1642:G:O4'    | 2.19                     | 0.42              |
| 1:2A:2406:U:C2    | 11:2P:72:PRO:HG2   | 2.53                     | 0.42              |
| 14:2S:84:GLN:HA   | 14:2S:111:GLU:O    | 2.19                     | 0.42              |
| 1:1A:1833:U:O2'   | 1:1A:1969:A:N1     | 2.42                     | 0.42              |
| 5:1F:37:VAL:O     | 5:1F:41:LEU:HG     | 2.19                     | 0.42              |
| 7:2H:3:ARG:HE     | 7:2H:54:ARG:HH12   | 1.67                     | 0.42              |
| 14:2S:62:LYS:HB3  | 14:2S:97:ARG:NE    | 2.34                     | 0.42              |
| 8:1I:92:VAL:HG11  | 8:1I:144:VAL:HG11  | 2.00                     | 0.42              |
| 1:2A:2233:U:H2'   | 1:2A:2234:G:C8     | 2.54                     | 0.42              |
| 5:2F:9:ILE:HB     | 5:2F:20:LEU:HB3    | 2.02                     | 0.42              |
| 26:24:17:GLY:N    | 26:24:33:VAL:O     | 2.52                     | 0.42              |
| 6:2G:125:PHE:HB3  | 6:2G:166:ASP:OD1   | 2.19                     | 0.42              |
| 1:1A:2141:G:C4    | 1:1A:2142:C:H1'    | 2.54                     | 0.42              |
| 3:1D:145:VAL:HG11 | 3:1D:175:LEU:HD11  | 2.00                     | 0.42              |
| 13:2R:33:ARG:NH1  | 13:2R:115:GLU:OE1  | 2.41                     | 0.42              |
| 1:1A:1637:A:H4'   | 1:1A:2711:A:O2'    | 2.19                     | 0.42              |
| 21:2Z:130:PRO:HA  | 21:2Z:133:ILE:HG13 | 2.01                     | 0.42              |
| 1:2A:117:G:C6     | 1:2A:119:A:C6      | 3.07                     | 0.42              |
| 1:2A:1921:G:O2'   | 1:2A:1922:G:H5'    | 2.19                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:13:3:ARG:HD3   | 25:13:60:GLU:OE2  | 2.19                     | 0.42              |
| 1:2A:2097:C:H2'   | 1:2A:2098:U:O4'   | 2.19                     | 0.42              |
| 1:1A:1051:G:H4'   | 1:1A:2752:C:H4'   | 2.01                     | 0.42              |
| 1:2A:1433:U:H1'   | 1:2A:1561:G:N2    | 2.34                     | 0.42              |
| 1:1A:1810:A:H2'   | 1:1A:1811:G:O4'   | 2.19                     | 0.42              |
| 1:2A:2576:G:H3'   | 1:2A:2576:G:OP1   | 2.20                     | 0.42              |
| 18:2W:12:ILE:O    | 18:2W:101:SER:OG  | 2.24                     | 0.42              |
| 1:1A:1094:U:O2    | 1:1A:1097:U:H6    | 2.02                     | 0.42              |
| 20:1Y:92:ASN:CG   | 20:1Y:94:LYS:HG2  | 2.40                     | 0.42              |
| 6:2G:11:TYR:CE2   | 6:2G:16:ARG:HD3   | 2.54                     | 0.42              |
| 9:2N:32:THR:HG22  | 9:2N:37:LYS:HB2   | 2.01                     | 0.42              |
| 1:1A:973:A:H5'    | 1:1A:1188:U:H1'   | 2.01                     | 0.42              |
| 1:1A:881:G:H3'    | 1:1A:882:G:H8     | 1.83                     | 0.42              |
| 2:2B:94:C:H2'     | 2:2B:95:C:C6      | 2.55                     | 0.42              |
| 7:1H:124:GLU:HB2  | 7:1H:132:ARG:HB3  | 2.01                     | 0.42              |
| 1:2A:517:C:OP1    | 27:25:16:ARG:NH2  | 2.51                     | 0.42              |
| 1:2A:1512:U:H2'   | 1:2A:1513:C:C6    | 2.54                     | 0.42              |
| 1:2A:589:C:H2'    | 1:2A:590:A:C8     | 2.54                     | 0.42              |
| 6:1G:47:LYS:HE3   | 6:1G:47:LYS:HB2   | 1.77                     | 0.42              |
| 12:1Q:42:ILE:HD13 | 12:1Q:97:VAL:HB   | 2.00                     | 0.42              |
| 8:1I:27:ARG:HD3   | 23:11:71:TYR:CE2  | 2.54                     | 0.42              |
| 1:2A:2096:U:H2'   | 1:2A:2097:C:C6    | 2.54                     | 0.42              |
| 20:2Y:28:LYS:HE3  | 20:2Y:28:LYS:HB3  | 1.88                     | 0.42              |
| 1:2A:1160:G:C6    | 1:2A:1161:C:N3    | 2.87                     | 0.42              |
| 7:2H:109:PHE:CE2  | 7:2H:152:ARG:HG2  | 2.54                     | 0.42              |
| 3:1D:264:LYS:HA   | 3:1D:265:PRO:HD3  | 1.93                     | 0.42              |
| 1:1A:2615:U:H2'   | 1:1A:2616:C:H6    | 1.84                     | 0.42              |
| 1:2A:1588:C:H2'   | 1:2A:1589:C:C6    | 2.53                     | 0.42              |
| 1:2A:1773:A:H5''  | 61:2A:4260:HOH:O  | 2.19                     | 0.42              |
| 1:2A:2350:C:H5''  | 30:28:42:ARG:HD3  | 2.01                     | 0.42              |
| 1:2A:1002:G:C5    | 1:2A:1003:G:H8    | 3.50                     | 0.42              |
| 1:2A:952:G:C6     | 1:2A:966:G:C6     | 3.07                     | 0.42              |
| 2:2B:75:G:H1      | 21:2Z:73:GLN:HE22 | 1.66                     | 0.42              |
| 1:2A:859:G:N2     | 1:2A:917:A:OP2    | 2.41                     | 0.42              |
| 1:2A:2127:G:C6    | 1:2A:2161:C:N3    | 2.87                     | 0.42              |
| 1:2A:1252:G:N2    | 16:2U:37:GLU:OE2  | 2.50                     | 0.42              |
| 11:2P:84:ASN:OD1  | 11:2P:117:GLU:HB2 | 2.19                     | 0.42              |
| 1:1A:27:G:N2      | 1:1A:512:G:H1'    | 2.35                     | 0.42              |
| 6:2G:5:VAL:HG22   | 6:2G:8:LYS:CB     | 2.48                     | 0.42              |
| 1:1A:1799:G:O3'   | 3:1D:183:ARG:NH1  | 2.52                     | 0.42              |
| 6:1G:37:VAL:O     | 6:1G:94:LEU:N     | 2.47                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:1A:84:A:H5''     | 20:1Y:8:LYS:HG2    | 2.01                     | 0.42              |
| 1:1A:251:A:C5      | 1:1A:252:G:H1'     | 2.55                     | 0.42              |
| 3:2D:275:LYS:HA    | 3:2D:275:LYS:HD2   | 1.88                     | 0.42              |
| 6:1G:5:VAL:HG21    | 6:1G:100:TRP:HB3   | 2.02                     | 0.42              |
| 13:2R:13:HIS:CE1   | 13:2R:16:HIS:HB2   | 2.55                     | 0.42              |
| 27:25:33:CYS:HB2   | 27:25:40:LYS:HD3   | 2.00                     | 0.42              |
| 11:2P:47:ASP:OD2   | 11:2P:49:ARG:NH2   | 2.50                     | 0.42              |
| 16:1U:17:ILE:HG23  | 16:1U:39:LEU:HD12  | 2.01                     | 0.42              |
| 5:1F:135:LYS:HB2   | 5:1F:138:GLU:CD    | 2.40                     | 0.42              |
| 1:1A:1317:A:H2'    | 1:1A:1318:C:O4'    | 2.18                     | 0.42              |
| 1:1A:2787:C:H1'    | 4:1E:62:PRO:HG3    | 2.00                     | 0.42              |
| 9:1N:20:GLY:HA2    | 9:1N:61:ARG:HG2    | 2.00                     | 0.42              |
| 1:1A:1107:G:C2'    | 1:1A:1108:U:H5'    | 2.49                     | 0.42              |
| 12:2Q:101:ARG:HD2  | 12:2Q:101:ARG:HA   | 1.86                     | 0.42              |
| 1:2A:1204:A:H5'    | 1:2A:1206:G:H1'    | 2.01                     | 0.42              |
| 6:2G:12:TYR:HA     | 6:2G:16:ARG:HG2    | 2.00                     | 0.42              |
| 9:2N:28:THR:HG22   | 9:2N:29:LYS:N      | 2.34                     | 0.42              |
| 1:2A:322:A:C5      | 1:2A:340:A:C2      | 3.08                     | 0.42              |
| 1:1A:1027:A:N3     | 61:1A:4164:HOH:O   | 2.36                     | 0.42              |
| 1:2A:997:G:OP2     | 16:2U:58:ARG:NH1   | 2.53                     | 0.42              |
| 1:1A:2160:G:C6     | 1:1A:2161:C:N4     | 2.87                     | 0.42              |
| 1:2A:2793:G:N2     | 1:2A:2804:C:H1'    | 2.33                     | 0.42              |
| 30:18:6:THR:HG22   | 30:18:63:PRO:HD2   | 2.02                     | 0.42              |
| 1:2A:990:A:N6      | 1:2A:1186:G:H1'    | 2.35                     | 0.42              |
| 6:1G:16:ARG:HE     | 6:1G:31:VAL:HG11   | 1.84                     | 0.42              |
| 1:1A:2053:G:OP1    | 4:1E:144:ARG:HG2   | 2.19                     | 0.42              |
| 20:1Y:6:HIS:CD2    | 20:1Y:6:HIS:H      | 2.37                     | 0.42              |
| 58:2A:3652:HGR:C16 | 58:2A:3652:HGR:H3  | 2.49                     | 0.42              |
| 10:1O:23:ARG:HD2   | 10:1O:23:ARG:HH11  | 1.72                     | 0.42              |
| 1:2A:1583:A:H5''   | 1:2A:1584:C:OP1    | 2.19                     | 0.42              |
| 1:2A:613:G:O2'     | 1:2A:614(C):A:N1   | 2.44                     | 0.42              |
| 6:2G:53:LEU:HD23   | 6:2G:53:LEU:HA     | 1.87                     | 0.42              |
| 1:1A:2836:U:H2'    | 1:1A:2837:G:C8     | 2.55                     | 0.42              |
| 1:2A:1987:G:H2'    | 1:2A:1988:C:C6     | 2.53                     | 0.42              |
| 13:1R:97:VAL:HG22  | 13:1R:114:VAL:HG13 | 2.02                     | 0.42              |
| 1:2A:483:A:H5''    | 20:2Y:50:ARG:HD3   | 2.01                     | 0.42              |
| 2:2B:93:G:P        | 21:2Z:79:ARG:HH22  | 2.39                     | 0.42              |
| 1:1A:1085:A:O2'    | 1:1A:1104:C:O2'    | 2.36                     | 0.42              |
| 1:2A:1818:U:O2'    | 3:2D:154:LYS:O     | 2.24                     | 0.42              |
| 1:1A:278:A:H2'     | 1:1A:279:C:H6      | 1.82                     | 0.42              |
| 1:1A:2059:A:C8     | 1:1A:2503:2MA:HM23 | 2.54                     | 0.42              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:2A:2031:A:N3    | 1:2A:2455:G:O2'  | 2.45                     | 0.42              |
| 22:10:11:ARG:O    | 22:10:14:ARG:NH2 | 2.44                     | 0.42              |
| 5:2F:126:VAL:HG11 | 5:2F:142:TRP:CZ2 | 2.55                     | 0.42              |
| 1:2A:2540:C:H2'   | 1:2A:2541:A:O4'  | 2.19                     | 0.42              |
| 1:1A:957:A:N1     | 1:1A:2458:G:H4'  | 2.35                     | 0.42              |
| 1:2A:257:A:H2'    | 1:2A:258:G:O4'   | 2.19                     | 0.42              |
| 1:1A:2615:U:H2'   | 1:1A:2616:C:C6   | 2.54                     | 0.42              |
| 1:2A:2733:A:H2    | 4:2E:204:ALA:H   | 1.68                     | 0.42              |
| 1:2A:471:A:H2'    | 1:2A:472:A:O4'   | 2.20                     | 0.42              |
| 11:1P:85:LEU:HG   | 11:1P:115:LEU:O  | 2.20                     | 0.42              |
| 30:28:34:TRP:CG   | 30:28:35:GLN:N   | 2.88                     | 0.42              |
| 5:1F:150:GLY:HA2  | 5:1F:172:TRP:CD2 | 2.54                     | 0.42              |
| 1:2A:2699:C:H2'   | 1:2A:2700:C:O4'  | 2.20                     | 0.42              |
| 16:2U:36:ARG:HG2  | 16:2U:40:PHE:CZ  | 2.55                     | 0.42              |
| 1:1A:1062:G:H5''  | 1:1A:1070:A:H1'  | 2.02                     | 0.42              |
| 7:2H:4:ILE:O      | 7:2H:69:ARG:HD2  | 2.19                     | 0.42              |
| 1:2A:974:G:OP1    | 1:2A:1187:G:O2'  | 2.25                     | 0.42              |
| 1:2A:2136:C:C4    | 1:2A:2155:G:N1   | 2.83                     | 0.42              |
| 1:1A:558:G:OP1    | 9:1N:111:PRO:HD2 | 2.18                     | 0.42              |
| 1:2A:1131:G:C2    | 1:2A:1132:A:C4   | 3.08                     | 0.42              |
| 1:2A:2371:G:O6    | 61:2A:3744:HOH:O | 2.19                     | 0.42              |
| 1:2A:521:G:H2'    | 1:2A:522:G:C8    | 2.54                     | 0.42              |
| 1:2A:1653:G:N1    | 13:2R:11:ASN:OD1 | 2.51                     | 0.42              |
| 1:1A:2141:G:C5    | 1:1A:2142:C:H1'  | 2.55                     | 0.42              |
| 7:2H:149:ARG:NH1  | 7:2H:163:TYR:HA  | 2.34                     | 0.42              |
| 29:27:12:ARG:CZ   | 29:27:44:PRO:HB3 | 2.49                     | 0.42              |
| 1:1A:2619:C:H4'   | 4:1E:151:TYR:O   | 2.20                     | 0.42              |
| 1:1A:754:C:H2'    | 1:1A:755:C:C6    | 2.54                     | 0.42              |
| 1:2A:820:A:N3     | 1:2A:943:U:H4'   | 2.34                     | 0.42              |
| 1:2A:2432:A:H5''  | 61:2A:4215:HOH:O | 2.19                     | 0.42              |
| 1:2A:1696:G:N7    | 61:2A:3855:HOH:O | 2.37                     | 0.42              |
| 1:2A:1181:C:H2'   | 1:2A:1182:A:C8   | 2.54                     | 0.42              |
| 1:2A:569:U:H1'    | 1:2A:947:G:O4'   | 2.19                     | 0.42              |
| 22:20:10:THR:HG22 | 22:20:12:ASN:N   | 2.20                     | 0.42              |
| 12:1Q:101:ARG:HD2 | 12:1Q:101:ARG:HA | 1.76                     | 0.42              |
| 18:1W:58:ALA:HB1  | 18:1W:64:MET:HB2 | 2.02                     | 0.42              |
| 6:1G:82:LEU:HA    | 6:1G:82:LEU:HD23 | 1.92                     | 0.42              |
| 8:1I:58:LEU:O     | 8:1I:61:ARG:HB3  | 2.20                     | 0.42              |
| 1:2A:247:G:H4'    | 1:2A:386:G:C4    | 2.55                     | 0.42              |
| 14:2S:35:ILE:HG21 | 14:2S:66:ALA:HA  | 2.01                     | 0.42              |
| 25:23:5:LYS:HE3   | 25:23:34:GLU:OE2 | 2.19                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 19:2X:31:HIS:HA   | 19:2X:32:PRO:HD3  | 1.85                     | 0.42              |
| 9:2N:34:LEU:HD12  | 9:2N:34:LEU:HA    | 1.88                     | 0.42              |
| 1:1A:401:A:H2'    | 1:1A:402:A:O4'    | 2.20                     | 0.42              |
| 2:1B:2:C:H2'      | 2:1B:3:C:H6       | 1.85                     | 0.42              |
| 6:1G:34:LEU:HD23  | 6:1G:161:THR:HG22 | 2.02                     | 0.42              |
| 4:1E:144:ARG:HB3  | 4:1E:145:LYS:H    | 1.49                     | 0.42              |
| 1:2A:1394:U:H4'   | 1:2A:1603:A:H4'   | 2.01                     | 0.42              |
| 1:1A:625:G:H2'    | 1:1A:626:U:H6     | 2.38                     | 0.42              |
| 19:2X:43:VAL:HG21 | 19:2X:81:VAL:HG11 | 2.01                     | 0.42              |
| 28:26:23:THR:OG1  | 28:26:24:GLU:N    | 2.51                     | 0.42              |
| 16:2U:81:HIS:O    | 16:2U:84:LYS:HB3  | 2.19                     | 0.42              |
| 1:1A:1849:G:H2'   | 1:1A:1850:G:H8    | 1.85                     | 0.42              |
| 31:19:15:LYS:HB3  | 31:19:26:ILE:HG13 | 2.02                     | 0.42              |
| 1:1A:1678:G:OP2   | 1:1A:1678:G:N2    | 2.49                     | 0.42              |
| 25:13:31:LEU:HD23 | 25:13:31:LEU:HA   | 1.77                     | 0.42              |
| 1:2A:530:G:O4'    | 1:2A:530:G:N3     | 2.52                     | 0.42              |
| 1:1A:2353:G:H1'   | 22:10:34:GLY:HA3  | 2.02                     | 0.42              |
| 1:1A:271(H):G:H4' | 23:11:81:LYS:HG2  | 2.01                     | 0.42              |
| 1:1A:1108:U:H2'   | 1:1A:1109:C:O4'   | 2.20                     | 0.42              |
| 1:2A:747:U:O2     | 1:2A:2014:A:H1'   | 2.20                     | 0.42              |
| 1:1A:1035:U:H2'   | 1:1A:1036:G:C8    | 2.54                     | 0.42              |
| 1:2A:1313:U:H4'   | 1:2A:1332:G:H4'   | 2.02                     | 0.42              |
| 1:1A:2100:G:H2'   | 1:1A:2101:G:C8    | 2.54                     | 0.42              |
| 1:1A:780:G:OP1    | 3:1D:218:ARG:NH2  | 2.44                     | 0.42              |
| 1:2A:868:U:C2     | 1:2A:869:G:C8     | 3.08                     | 0.42              |
| 1:2A:2207:G:H3'   | 1:2A:2208:A:H5''  | 2.02                     | 0.42              |
| 1:2A:563:G:H21    | 16:2U:37:GLU:CD   | 2.22                     | 0.42              |
| 3:1D:70:TRP:HB3   | 3:1D:190:TYR:CE2  | 2.54                     | 0.42              |
| 7:2H:164:TYR:HB2  | 7:2H:167:GLU:HB2  | 2.01                     | 0.42              |
| 7:1H:83:TYR:CZ    | 7:1H:138:LYS:HD2  | 2.54                     | 0.42              |
| 1:1A:2206:G:H5''  | 1:1A:2207:G:C5    | 2.55                     | 0.42              |
| 6:1G:44:GLY:O     | 6:1G:47:LYS:HB2   | 2.20                     | 0.42              |
| 3:2D:4:LYS:HB3    | 3:2D:18:VAL:HG22  | 2.01                     | 0.42              |
| 1:1A:2023:G:H5'   | 1:1A:2617:C:H4'   | 2.02                     | 0.42              |
| 1:2A:2870:C:H2'   | 1:2A:2871:C:O4'   | 2.19                     | 0.42              |
| 1:1A:2773:C:H2'   | 1:1A:2774:C:C6    | 2.54                     | 0.42              |
| 7:2H:103:LEU:HB3  | 7:2H:115:VAL:HB   | 2.01                     | 0.42              |
| 1:1A:1478:G:H1'   | 1:1A:1557:C:O2'   | 2.20                     | 0.42              |
| 1:2A:2556:C:H2'   | 1:2A:2557:G:O4'   | 2.20                     | 0.42              |
| 1:1A:2353:G:H2'   | 1:1A:2354:G:O4'   | 2.20                     | 0.42              |
| 1:2A:2188:C:H2'   | 1:2A:2189:U:O4'   | 2.20                     | 0.42              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 29:27:26:GLY:O   | 29:27:30:VAL:HG23 | 2.20                     | 0.42              |
| 1:1A:1952:A:C6   | 1:1A:1953:A:N1    | 2.87                     | 0.42              |
| 16:1U:86:ALA:O   | 17:1V:49:THR:HG23 | 2.20                     | 0.42              |
| 1:2A:2514:U:H2'  | 1:2A:2515:C:C6    | 2.54                     | 0.42              |
| 1:1A:1062:G:H2'  | 1:1A:1063:G:H8    | 1.85                     | 0.42              |
| 1:1A:1175:U:O2'  | 1:1A:1176:G:O5'   | 2.35                     | 0.42              |
| 1:2A:1149:G:H2'  | 1:2A:1150:C:C6    | 2.55                     | 0.42              |
| 1:2A:7:G:H2'     | 1:2A:8:A:O4'      | 2.20                     | 0.42              |
| 1:2A:875:G:N2    | 1:2A:903:C:H1'    | 2.34                     | 0.42              |
| 19:2X:5:TYR:OH   | 24:22:30:ARG:NH1  | 2.51                     | 0.42              |
| 1:2A:1344:G:O2'  | 1:2A:1385:G:H2'   | 2.19                     | 0.42              |
| 1:1A:818:G:H4'   | 1:1A:838:C:O3'    | 2.20                     | 0.42              |
| 11:2P:45:LEU:HA  | 11:2P:45:LEU:HD23 | 1.80                     | 0.42              |
| 10:2O:66:LYS:O   | 10:2O:78:ARG:HG2  | 2.19                     | 0.42              |
| 1:1A:717:G:H2'   | 1:1A:718:A:O4'    | 2.19                     | 0.42              |
| 1:2A:2695:C:H2'  | 1:2A:2696:U:C6    | 2.54                     | 0.42              |
| 1:2A:2239:G:P    | 3:2D:244:ARG:HH12 | 2.43                     | 0.42              |
| 21:1Z:10:ARG:HD3 | 21:1Z:38:TYR:HB3  | 2.01                     | 0.42              |
| 12:1Q:85:LYS:HG2 | 22:10:7:LEU:HB3   | 2.01                     | 0.42              |
| 1:1A:256:A:H2'   | 1:1A:257:A:H8     | 1.85                     | 0.42              |
| 1:1A:1197:G:H2'  | 1:1A:1198:U:H6    | 1.85                     | 0.42              |
| 1:1A:1253:A:OP1  | 61:1A:4068:HOH:O  | 2.22                     | 0.42              |
| 1:2A:1702:G:H2'  | 1:2A:1703:G:O4'   | 2.20                     | 0.42              |
| 1:1A:592:G:O2'   | 30:18:4:MET:HG3   | 2.20                     | 0.42              |
| 5:1F:14:PRO:HD2  | 5:1F:127:GLU:OE1  | 2.20                     | 0.42              |
| 1:2A:1486:A:H2'  | 1:2A:1487:G:H8    | 1.85                     | 0.42              |
| 1:2A:2712:U:H2'  | 1:2A:2714:G:H5''  | 2.02                     | 0.42              |
| 27:15:41:PRO:HA  | 27:15:42:PRO:HD2  | 1.90                     | 0.42              |
| 1:1A:1082:U:N3   | 1:1A:1086:A:N6    | 2.20                     | 0.41              |
| 1:2A:784:A:OP1   | 1:2A:2588:G:H5''  | 2.20                     | 0.41              |
| 1:1A:2126:A:N3   | 1:1A:2127:G:H1'   | 2.35                     | 0.41              |
| 1:2A:1479:G:H1'  | 1:2A:1558:A:OP1   | 2.19                     | 0.41              |
| 1:1A:1239:G:H2'  | 1:1A:1240:U:O4'   | 2.20                     | 0.41              |
| 1:1A:2131:G:H4'  | 1:1A:2132:U:OP2   | 2.20                     | 0.41              |
| 1:1A:500:G:N2    | 1:1A:502:A:H3'    | 2.34                     | 0.41              |
| 16:2U:24:TYR:HB2 | 16:2U:29:SER:HB3  | 2.02                     | 0.41              |
| 4:2E:31:CYS:HA   | 4:2E:32:PRO:HD2   | 1.96                     | 0.41              |
| 6:2G:3:LEU:HD13  | 26:24:25:TYR:HE2  | 1.85                     | 0.41              |
| 1:2A:557:U:H2'   | 1:2A:558:G:H8     | 1.85                     | 0.41              |
| 1:2A:729:G:O2'   | 1:2A:763:G:H4'    | 2.19                     | 0.41              |
| 5:1F:53:THR:HG23 | 5:1F:55:GLY:H     | 1.85                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1A:1297:C:OP2   | 61:1A:4065:HOH:O  | 2.21                     | 0.41              |
| 1:1A:1226:A:OP1   | 17:1V:84:LYS:HE2  | 2.20                     | 0.41              |
| 1:1A:601:C:O2'    | 1:1A:605:C:H5''   | 2.19                     | 0.41              |
| 1:1A:2018:G:N3    | 16:1U:34:LYS:NZ   | 2.67                     | 0.41              |
| 5:1F:135:LYS:HB2  | 5:1F:138:GLU:CG   | 2.50                     | 0.41              |
| 1:1A:1252:G:OP1   | 16:1U:36:ARG:NH1  | 2.52                     | 0.41              |
| 61:1A:4092:HOH:O  | 19:1X:68:ARG:NH2  | 2.53                     | 0.41              |
| 6:1G:106:LEU:HA   | 6:1G:110:ALA:HB3  | 2.01                     | 0.41              |
| 20:1Y:98:VAL:HG12 | 20:1Y:105:ALA:HA  | 2.01                     | 0.41              |
| 3:2D:80:ALA:HB3   | 3:2D:94:LEU:HB3   | 2.01                     | 0.41              |
| 6:1G:53:LEU:HA    | 6:1G:53:LEU:HD23  | 1.71                     | 0.41              |
| 21:1Z:26:GLY:HA3  | 21:1Z:86:VAL:HG23 | 2.02                     | 0.41              |
| 1:2A:483:A:H1'    | 20:2Y:59:GLY:O    | 2.20                     | 0.41              |
| 1:2A:2748:A:H5'   | 7:2H:4:ILE:HD12   | 2.01                     | 0.41              |
| 1:2A:1042:G:H2'   | 1:2A:1042:G:N3    | 2.35                     | 0.41              |
| 6:2G:25:TYR:HB3   | 6:2G:30:GLU:HB2   | 2.02                     | 0.41              |
| 1:2A:195:A:H2'    | 1:2A:198:C:N4     | 2.35                     | 0.41              |
| 1:2A:244:A:C2     | 1:2A:255:A:C4     | 3.08                     | 0.41              |
| 1:1A:897:C:C2     | 1:1A:898:C:C5     | 3.09                     | 0.41              |
| 1:1A:784:A:H5'    | 1:1A:785:G:OP1    | 2.20                     | 0.41              |
| 1:1A:1185:C:H5''  | 1:1A:1186:G:OP1   | 2.20                     | 0.41              |
| 1:2A:672:C:H2'    | 1:2A:673:C:C6     | 2.55                     | 0.41              |
| 1:1A:2719:G:N2    | 1:1A:2872:G:H1    | 2.18                     | 0.41              |
| 1:1A:775:G:O5'    | 1:1A:777:A:H1'    | 2.20                     | 0.41              |
| 6:2G:44:GLY:O     | 6:2G:47:LYS:HB3   | 2.20                     | 0.41              |
| 1:2A:1515:G:H2'   | 1:2A:1516:C:O4'   | 2.21                     | 0.41              |
| 1:1A:1419:A:C8    | 1:1A:1421:G:C6    | 3.09                     | 0.41              |
| 1:2A:807:U:OP2    | 11:2P:41:ARG:NH2  | 2.53                     | 0.41              |
| 1:2A:570:G:H5''   | 61:2A:4337:HOH:O  | 2.20                     | 0.41              |
| 19:2X:59:VAL:HB   | 19:2X:76:ARG:HB2  | 2.01                     | 0.41              |
| 13:1R:28:LEU:HD12 | 13:1R:48:VAL:HG21 | 2.02                     | 0.41              |
| 1:1A:744:G:OP1    | 4:1E:132:HIS:ND1  | 2.44                     | 0.41              |
| 1:2A:2529:G:O6    | 31:29:31:LYS:NZ   | 2.53                     | 0.41              |
| 1:2A:2006:C:H6    | 1:2A:2006:C:O5'   | 2.04                     | 0.41              |
| 1:1A:2695:C:H2'   | 1:1A:2696:U:H6    | 1.85                     | 0.41              |
| 1:2A:1161:C:H2'   | 1:2A:1162:G:C8    | 2.55                     | 0.41              |
| 1:2A:2728:U:H2'   | 1:2A:2729:G:C8    | 2.55                     | 0.41              |
| 1:2A:1999:C:H2'   | 1:2A:2000:G:O4'   | 2.20                     | 0.41              |
| 1:1A:41:C:H2'     | 1:1A:42:G:O4'     | 2.20                     | 0.41              |
| 26:14:14:ILE:HA   | 26:14:31:ILE:O    | 2.19                     | 0.41              |
| 15:2T:73:GLU:OE2  | 15:2T:103:ARG:NE  | 2.48                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:1A:1095:A:C8     | 1:1A:1096:A:N7     | 2.88                     | 0.41              |
| 1:2A:2185:C:H2'    | 1:2A:2186:G:O4'    | 2.20                     | 0.41              |
| 2:2B:68:C:H2'      | 2:2B:69:G:H8       | 1.85                     | 0.41              |
| 1:2A:2139:C:N4     | 1:2A:2153:G:C6     | 2.88                     | 0.41              |
| 1:2A:1287:A:C5     | 1:2A:1288:U:C4     | 3.08                     | 0.41              |
| 1:1A:783:A:O2'     | 1:1A:785:G:OP1     | 2.29                     | 0.41              |
| 1:2A:1530:C:H1'    | 1:2A:1531:C:OP1    | 2.20                     | 0.41              |
| 1:1A:1328:G:H2'    | 1:1A:1330:C:C5     | 2.55                     | 0.41              |
| 31:29:10:ILE:HD12  | 31:29:32:HIS:HA    | 2.01                     | 0.41              |
| 1:2A:756:C:H2'     | 1:2A:757:U:O4'     | 2.61                     | 0.41              |
| 1:1A:35:G:H2'      | 1:1A:36:G:O4'      | 2.21                     | 0.41              |
| 6:1G:104:GLU:HG3   | 61:1G:5002:HOH:O   | 2.20                     | 0.41              |
| 1:2A:2639:A:C2     | 1:2A:2778:A:C8     | 3.08                     | 0.41              |
| 1:2A:2114:A:O2'    | 1:2A:2167:U:H1'    | 2.20                     | 0.41              |
| 13:2R:56:LYS:NZ    | 13:2R:90:ARG:O     | 2.53                     | 0.41              |
| 1:2A:361:G:O2'     | 1:2A:362:U:H5'     | 2.20                     | 0.41              |
| 1:2A:2059:A:C8     | 1:2A:2503:2MA:HM23 | 2.55                     | 0.41              |
| 1:2A:729:G:O5'     | 3:2D:208:LYS:NZ    | 2.52                     | 0.41              |
| 1:2A:108:U:H2'     | 1:2A:109:G:H8      | 1.86                     | 0.41              |
| 1:1A:1668:A:N1     | 1:1A:1675:C:N4     | 2.66                     | 0.41              |
| 1:2A:2360:A:H8     | 1:2A:2360:A:O5'    | 2.04                     | 0.41              |
| 1:1A:38:A:H2'      | 1:1A:39:C:C6       | 2.55                     | 0.41              |
| 19:1X:11:PRO:HB3   | 19:1X:92:LEU:HD11  | 2.02                     | 0.41              |
| 1:2A:2679:A:C2     | 1:2A:2729:G:C2     | 3.08                     | 0.41              |
| 21:2Z:100:VAL:HA   | 21:2Z:101:PRO:HD3  | 1.90                     | 0.41              |
| 10:2O:86:ILE:HG22  | 10:2O:94:ARG:HD3   | 2.02                     | 0.41              |
| 1:1A:2322:A:H2'    | 1:1A:2323:G:O4'    | 2.20                     | 0.41              |
| 17:1V:62:LEU:HD11  | 17:1V:95:LEU:HB2   | 2.03                     | 0.41              |
| 19:2X:94:GLY:H     | 19:2X:95:LEU:HA    | 1.85                     | 0.41              |
| 5:2F:170:LEU:HG    | 5:2F:172:TRP:NE1   | 2.35                     | 0.41              |
| 1:2A:2155:G:H5'    | 1:2A:2155:G:H8     | 1.84                     | 0.41              |
| 24:22:27:GLU:O     | 24:22:30:ARG:HB3   | 2.20                     | 0.41              |
| 1:1A:780:G:H1'     | 1:1A:785:G:C2      | 2.56                     | 0.41              |
| 4:1E:59:VAL:HG21   | 4:1E:74:PRO:HB3    | 2.03                     | 0.41              |
| 1:2A:1814:G:C6     | 1:2A:1815:A:C6     | 3.08                     | 0.41              |
| 1:1A:26:G:C6       | 1:1A:27:G:C6       | 3.08                     | 0.41              |
| 6:2G:5:VAL:HG22    | 6:2G:8:LYS:HE2     | 2.02                     | 0.41              |
| 9:2N:34:LEU:O      | 9:2N:49:GLY:HA3    | 2.20                     | 0.41              |
| 10:2O:7:TYR:HE2    | 10:2O:20:MET:HE3   | 1.84                     | 0.41              |
| 1:1A:272(A):U:HO2' | 1:1A:272(B):G:P    | 2.39                     | 0.41              |
| 21:2Z:33:LEU:HD21  | 21:2Z:90:VAL:HG21  | 2.01                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 16:1U:76:TYR:CE2  | 16:1U:80:ILE:HG13  | 2.56                     | 0.41              |
| 1:1A:684:G:H2'    | 1:1A:774:A:N6      | 2.35                     | 0.41              |
| 29:27:30:VAL:HG22 | 29:27:33:ARG:HH21  | 1.85                     | 0.41              |
| 1:2A:2722:G:H2'   | 1:2A:2723:C:C6     | 2.55                     | 0.41              |
| 6:1G:101:ILE:HG22 | 6:1G:105:LYS:HE2   | 2.03                     | 0.41              |
| 23:11:23:LYS:HB3  | 23:11:29:GLY:HA3   | 2.02                     | 0.41              |
| 1:1A:566:U:H5''   | 11:1P:29:LYS:HE3   | 2.01                     | 0.41              |
| 1:2A:1485:G:O6    | 61:2A:3761:HOH:O   | 2.22                     | 0.41              |
| 1:2A:2302:G:H2'   | 1:2A:2303:G:H8     | 1.85                     | 0.41              |
| 1:2A:1952:A:OP1   | 10:2O:42:SER:OG    | 2.37                     | 0.41              |
| 1:2A:1169:G:N2    | 1:2A:1181:C:C2     | 2.89                     | 0.41              |
| 1:1A:980:A:C4     | 1:1A:1136:G:O4'    | 2.73                     | 0.41              |
| 2:2B:42:C:N4      | 6:2G:91:ARG:HH12   | 2.13                     | 0.41              |
| 1:1A:376:C:H2'    | 1:1A:377:C:C6      | 2.56                     | 0.41              |
| 1:1A:875:G:H2'    | 1:1A:876:C:O4'     | 2.20                     | 0.41              |
| 1:1A:2124:G:N2    | 1:1A:2174:C:N3     | 2.59                     | 0.41              |
| 1:2A:565:C:H2'    | 1:2A:566:U:O4'     | 2.20                     | 0.41              |
| 1:2A:77:C:OP1     | 24:22:59:ARG:HD3   | 2.20                     | 0.41              |
| 1:2A:2731:G:C6    | 1:2A:2732:G:C6     | 3.09                     | 0.41              |
| 1:2A:329:G:H8     | 1:2A:329:G:OP1     | 2.04                     | 0.41              |
| 2:1B:1:U:HO2'     | 2:1B:2:C:P         | 2.42                     | 0.41              |
| 1:2A:1496:A:OP2   | 1:2A:1496:A:H8     | 2.03                     | 0.41              |
| 1:2A:271(H):G:N3  | 1:2A:271(I):G:C8   | 2.88                     | 0.41              |
| 1:1A:1010:A:N3    | 1:1A:1153:C:H1'    | 2.34                     | 0.41              |
| 1:1A:1268:A:H2'   | 1:1A:1269:A:O4'    | 2.21                     | 0.41              |
| 12:1Q:31:ASP:HA   | 12:1Q:134:ARG:HH11 | 1.84                     | 0.41              |
| 1:2A:2687:U:H2'   | 1:2A:2688:U:O4'    | 2.21                     | 0.41              |
| 1:1A:2018:G:O2'   | 16:1U:34:LYS:HE3   | 2.20                     | 0.41              |
| 1:1A:1645:G:H5''  | 1:1A:1646:C:O5'    | 2.19                     | 0.41              |
| 19:1X:88:LYS:HE3  | 19:1X:93:GLU:HG3   | 2.03                     | 0.41              |
| 1:1A:2220:G:H2'   | 1:1A:2221:G:H8     | 1.85                     | 0.41              |
| 1:1A:1067:A:H3'   | 1:1A:1067:A:N3     | 2.35                     | 0.41              |
| 1:2A:2228:G:C6    | 1:2A:2229:C:C4     | 3.08                     | 0.41              |
| 4:2E:111:ARG:HD2  | 4:2E:160:TYR:CE2   | 2.55                     | 0.41              |
| 12:2Q:133:ARG:O   | 21:2Z:81:ARG:NH1   | 2.54                     | 0.41              |
| 1:2A:2600:A:OP2   | 61:2A:3762:HOH:O   | 2.22                     | 0.41              |
| 1:1A:1410:G:H2'   | 1:1A:1411:C:C6     | 2.74                     | 0.41              |
| 1:1A:1881:C:H2'   | 1:1A:1882:C:H6     | 1.86                     | 0.41              |
| 1:1A:1086:A:H4'   | 1:1A:1103:A:H2     | 1.86                     | 0.41              |
| 1:2A:2838:G:C6    | 1:2A:2839:G:C5     | 3.08                     | 0.41              |
| 14:1S:11:LYS:O    | 14:1S:15:ARG:HG3   | 2.20                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:2A:654:A:H2     | 1:2A:655:A:C2     | 2.38                     | 0.41              |
| 3:1D:9:TYR:CD1    | 3:1D:10:THR:HG23  | 2.55                     | 0.41              |
| 1:2A:1453:U:O4    | 13:2R:67:LEU:HD21 | 2.20                     | 0.41              |
| 1:1A:45:C:OP2     | 1:1A:215:G:H2'    | 2.21                     | 0.41              |
| 1:1A:2629:A:O2'   | 1:1A:2630:G:P     | 2.78                     | 0.41              |
| 1:2A:480:A:OP2    | 20:2Y:47:LYS:HE3  | 2.20                     | 0.41              |
| 8:2I:79:ILE:O     | 8:2I:144:VAL:HA   | 2.20                     | 0.41              |
| 1:1A:1668:A:H4'   | 1:1A:1669:A:O5'   | 2.21                     | 0.41              |
| 5:2F:126:VAL:HG21 | 5:2F:129:PHE:CE1  | 2.55                     | 0.41              |
| 1:2A:2519:U:C6    | 1:2A:2542:A:N6    | 2.88                     | 0.41              |
| 1:2A:2758:A:C2    | 1:2A:2759:G:H1'   | 2.55                     | 0.41              |
| 7:2H:90:LYS:HD2   | 7:2H:163:TYR:CD2  | 2.56                     | 0.41              |
| 1:2A:627:A:H4'    | 1:2A:628:G:H5'    | 2.02                     | 0.41              |
| 1:2A:2611:U:OP2   | 1:2A:2611:U:H3'   | 2.21                     | 0.41              |
| 1:1A:2735:G:H2'   | 1:1A:2736:G:C8    | 2.55                     | 0.41              |
| 1:2A:1589:C:H2'   | 1:2A:1590:U:C6    | 2.56                     | 0.41              |
| 13:2R:12:ARG:HG2  | 13:2R:16:HIS:ND1  | 2.35                     | 0.41              |
| 1:2A:2432:A:C6    | 1:2A:2433:A:C6    | 3.09                     | 0.41              |
| 1:1A:2470:G:O6    | 1:1A:2476:A:O2'   | 2.23                     | 0.41              |
| 19:1X:27:THR:OG1  | 19:1X:80:ILE:HG12 | 2.21                     | 0.41              |
| 12:2Q:42:ILE:HG23 | 12:2Q:46:GLN:HB2  | 2.02                     | 0.41              |
| 1:1A:1161:C:O2'   | 17:1V:8:GLY:HA2   | 2.20                     | 0.41              |
| 1:1A:324:A:N6     | 1:1A:338:G:O2'    | 2.49                     | 0.41              |
| 1:1A:1176:G:H1'   | 1:1A:1177:A:C5'   | 2.49                     | 0.41              |
| 12:2Q:75:THR:HG21 | 12:2Q:87:LYS:NZ   | 2.35                     | 0.41              |
| 19:2X:52:VAL:HG12 | 19:2X:82:GLN:O    | 2.21                     | 0.41              |
| 1:1A:518:G:H4'    | 18:1W:18:ARG:NE   | 2.35                     | 0.41              |
| 21:1Z:19:ARG:NH1  | 21:1Z:84:GLU:O    | 2.54                     | 0.41              |
| 1:2A:923:C:H2'    | 1:2A:924:C:C6     | 2.56                     | 0.41              |
| 2:2B:76:G:H2'     | 2:2B:77:U:O4'     | 2.21                     | 0.41              |
| 1:1A:1292:U:H2'   | 1:1A:1293:C:H6    | 1.85                     | 0.41              |
| 1:2A:2330:G:H21   | 22:20:42:GLY:N    | 2.18                     | 0.41              |
| 1:1A:2319:G:N2    | 14:1S:3:ARG:HA    | 2.35                     | 0.41              |
| 1:1A:444:C:H4'    | 5:1F:49:ALA:HB2   | 2.03                     | 0.41              |
| 10:1O:23:ARG:HD3  | 10:1O:24:VAL:H    | 1.84                     | 0.41              |
| 19:1X:92:LEU:O    | 19:1X:94:GLY:N    | 2.54                     | 0.41              |
| 1:1A:652(U):G:H2' | 1:1A:652(V):C:C6  | 2.55                     | 0.41              |
| 1:2A:438:G:H2'    | 1:2A:440:G:H8     | 1.86                     | 0.41              |
| 1:1A:637:A:H2'    | 11:1P:117:GLU:OE1 | 2.20                     | 0.41              |
| 20:2Y:28:LYS:HG3  | 20:2Y:40:GLU:HB2  | 2.02                     | 0.41              |
| 1:2A:2740:A:C6    | 1:2A:2741:A:C6    | 3.07                     | 0.41              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:1A:754:C:H2'     | 1:1A:755:C:H6     | 1.85                     | 0.41              |
| 1:1A:259:G:H2'     | 1:1A:260:G:O4'    | 2.79                     | 0.41              |
| 18:1W:84:ARG:O     | 18:1W:96:ILE:N    | 2.53                     | 0.41              |
| 1:1A:1920:4OC:HM22 | 1:1A:1921:G:O4'   | 2.20                     | 0.41              |
| 17:1V:43:GLU:N     | 17:1V:43:GLU:OE1  | 2.53                     | 0.41              |
| 21:1Z:35:ARG:HA    | 21:1Z:35:ARG:HD2  | 1.71                     | 0.41              |
| 5:1F:140:LEU:CD1   | 5:1F:170:LEU:HD21 | 2.51                     | 0.41              |
| 25:23:26:LEU:O     | 25:23:35:ARG:NE   | 2.53                     | 0.41              |
| 4:1E:195:LEU:HD23  | 61:1E:417:HOH:O   | 2.20                     | 0.41              |
| 9:2N:43:THR:HB     | 9:2N:46:VAL:HG22  | 2.02                     | 0.41              |
| 1:2A:1203:G:OP2    | 1:2A:1204:A:O2'   | 2.26                     | 0.41              |
| 1:2A:1207:C:H2'    | 1:2A:1208:C:C6    | 2.56                     | 0.41              |
| 2:1B:101:G:H2'     | 2:1B:102:A:O4'    | 2.21                     | 0.41              |
| 1:2A:1625:C:H2'    | 1:2A:1626:G:O4'   | 2.21                     | 0.41              |
| 8:2I:77:LEU:HD13   | 8:2I:101:LEU:HD13 | 2.02                     | 0.41              |
| 3:2D:5:LYS:HB3     | 3:2D:5:LYS:HE3    | 1.96                     | 0.41              |
| 20:1Y:26:LYS:HA    | 20:1Y:26:LYS:HD2  | 1.74                     | 0.41              |
| 31:29:29:ASN:HB3   | 31:29:32:HIS:ND1  | 2.35                     | 0.41              |
| 31:29:32:HIS:O     | 31:29:34:GLN:HG3  | 2.21                     | 0.41              |
| 23:11:72:GLU:O     | 23:11:76:ARG:HG3  | 2.21                     | 0.41              |
| 1:1A:2134:A:N3     | 1:1A:2159:G:O2'   | 2.39                     | 0.41              |
| 1:2A:1512:U:H2'    | 1:2A:1513:C:H6    | 1.86                     | 0.41              |
| 23:21:83:GLU:HA    | 23:21:84:GLY:HA2  | 1.69                     | 0.41              |
| 1:1A:236:C:H2'     | 1:1A:237:C:C6     | 2.56                     | 0.41              |
| 14:2S:10:ARG:O     | 14:2S:14:VAL:HG13 | 2.21                     | 0.41              |
| 1:2A:489:G:H2'     | 1:2A:491:G:O4'    | 2.21                     | 0.41              |
| 4:2E:11:MET:HG2    | 4:2E:24:THR:HB    | 2.02                     | 0.41              |
| 1:1A:1584:C:H5'    | 56:1A:3130:MG:MG  | 1.46                     | 0.41              |
| 11:1P:43:GLY:HA3   | 61:1P:301:HOH:O   | 2.20                     | 0.41              |
| 11:1P:58:THR:HG21  | 30:18:54:GLU:HG3  | 2.02                     | 0.41              |
| 11:2P:91:PHE:O     | 11:2P:121:LYS:NZ  | 2.49                     | 0.41              |
| 1:2A:389:G:C6      | 11:2P:70:GLN:HG3  | 2.56                     | 0.41              |
| 1:1A:2576:G:H1'    | 61:1A:4543:HOH:O  | 2.21                     | 0.41              |
| 1:2A:186:G:H2'     | 1:2A:187:G:H8     | 1.86                     | 0.41              |
| 1:2A:2406:U:OP1    | 61:2A:3763:HOH:O  | 2.22                     | 0.41              |
| 1:1A:340:A:H2'     | 1:1A:341:G:O4'    | 2.21                     | 0.41              |
| 1:1A:2740:A:H2'    | 1:1A:2741:A:C8    | 2.56                     | 0.41              |
| 1:1A:537:C:H2'     | 1:1A:538:G:C8     | 2.55                     | 0.41              |
| 1:1A:1853:A:H2'    | 1:1A:1854:A:C8    | 2.55                     | 0.41              |
| 1:1A:207:A:H2'     | 1:1A:208:C:O4'    | 2.20                     | 0.41              |
| 1:2A:2001:A:H2'    | 1:2A:2002:G:C8    | 2.56                     | 0.41              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:1A:285:C:H2'     | 1:1A:286:C:C6     | 2.56                     | 0.41              |
| 11:2P:120:ALA:HB2  | 11:2P:137:LYS:HB3 | 2.02                     | 0.41              |
| 21:1Z:152:ALA:H    | 21:1Z:171:ILE:CG2 | 2.33                     | 0.41              |
| 1:2A:1308:A:H2'    | 1:2A:1309:G:O4'   | 2.21                     | 0.41              |
| 1:1A:1064:C:H2'    | 1:1A:1065:U:H5'   | 2.03                     | 0.41              |
| 4:1E:47:VAL:HG12   | 4:1E:49:LEU:HD12  | 2.02                     | 0.41              |
| 1:2A:65:C:H5'      | 19:2X:71:GLY:HA3  | 2.02                     | 0.41              |
| 1:2A:947:G:N3      | 1:2A:984:A:H2     | 2.19                     | 0.41              |
| 6:2G:64:THR:OG1    | 6:2G:66:GLN:O     | 2.39                     | 0.41              |
| 1:2A:947:G:H2'     | 1:2A:948:G:C8     | 2.56                     | 0.41              |
| 14:2S:36:TYR:HD1   | 14:2S:52:SER:HB3  | 1.86                     | 0.41              |
| 1:2A:300:A:P       | 20:2Y:86:ARG:HH21 | 2.42                     | 0.41              |
| 2:2B:115:G:O4'     | 14:2S:47:THR:HB   | 2.20                     | 0.41              |
| 1:2A:1509(A):A:H3' | 1:2A:1509(B):A:H8 | 1.86                     | 0.41              |
| 1:2A:839:U:H1'     | 1:2A:1191:G:H1'   | 2.03                     | 0.41              |
| 1:1A:1400:G:H2'    | 1:1A:1401:G:C8    | 2.56                     | 0.41              |
| 1:1A:1823:G:OP1    | 3:1D:54:ARG:NH1   | 2.54                     | 0.41              |
| 1:2A:829:A:N7      | 1:2A:2247:A:O2'   | 2.50                     | 0.41              |
| 1:2A:34:C:H2'      | 1:2A:35:G:C8      | 5.48                     | 0.41              |
| 4:2E:112:GLY:O     | 4:2E:159:HIS:HA   | 2.21                     | 0.41              |
| 18:2W:11:ARG:NH1   | 18:2W:99:ARG:O    | 2.53                     | 0.41              |
| 1:2A:83:G:N2       | 1:2A:103:A:OP2    | 2.52                     | 0.41              |
| 1:2A:2206:G:H3'    | 1:2A:2207:G:N7    | 2.36                     | 0.41              |
| 1:2A:2206:G:H3'    | 1:2A:2207:G:C8    | 2.56                     | 0.41              |
| 1:2A:277:C:H2'     | 1:2A:277:C:O2     | 2.19                     | 0.41              |
| 1:2A:661:C:H2'     | 1:2A:662:G:H8     | 1.86                     | 0.41              |
| 1:2A:2328:A:H2'    | 1:2A:2329:G:C8    | 2.56                     | 0.41              |
| 12:1Q:30:GLY:CA    | 12:1Q:107:ALA:HB2 | 2.49                     | 0.41              |
| 14:2S:95:HIS:CG    | 14:2S:96:GLY:N    | 2.89                     | 0.41              |
| 1:1A:1115:G:H2'    | 1:1A:1116:C:O4'   | 2.21                     | 0.41              |
| 8:2I:123:LEU:HA    | 8:2I:144:VAL:CG2  | 2.51                     | 0.41              |
| 1:2A:729:G:C4      | 1:2A:1775:U:C2    | 3.09                     | 0.41              |
| 1:2A:2508:G:O3'    | 1:2A:2555:U:H5'   | 2.20                     | 0.41              |
| 4:2E:52:LEU:HA     | 4:2E:53:PRO:HD2   | 1.97                     | 0.41              |
| 11:1P:120:ALA:HB1  | 11:1P:138:LEU:HA  | 2.02                     | 0.41              |
| 7:1H:149:ARG:HH12  | 7:1H:167:GLU:CD   | 2.24                     | 0.41              |
| 2:1B:14:U:O2       | 2:1B:108:U:H4'    | 2.20                     | 0.41              |
| 7:1H:24:VAL:HG21   | 7:1H:72:ILE:HG12  | 2.03                     | 0.41              |
| 7:2H:148:ILE:O     | 7:2H:162:ILE:HD13 | 2.20                     | 0.41              |
| 1:1A:2667:C:H1'    | 7:1H:109:PHE:CD1  | 2.56                     | 0.41              |
| 1:2A:1197:G:H2'    | 1:2A:1198:U:H6    | 1.86                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:2A:2612:C:OP2   | 27:25:2:ALA:N      | 2.54                     | 0.41              |
| 1:2A:746:A:O2'    | 1:2A:2611:U:O2'    | 2.33                     | 0.41              |
| 1:2A:2187:G:C6    | 1:2A:2188:C:C4     | 3.08                     | 0.41              |
| 1:1A:105:C:H2'    | 1:1A:106:C:C6      | 2.56                     | 0.41              |
| 23:21:88:LYS:O    | 23:21:92:LYS:HG3   | 2.20                     | 0.41              |
| 28:26:40:CYS:HA   | 28:26:41:PRO:HD3   | 1.87                     | 0.41              |
| 5:2F:114:VAL:HG21 | 5:2F:202:PHE:CZ    | 2.56                     | 0.41              |
| 7:1H:98:LEU:HD13  | 7:1H:125:VAL:HG23  | 2.02                     | 0.41              |
| 1:2A:1445:A:H8    | 1:2A:1460:A:C8     | 2.39                     | 0.41              |
| 23:21:78:LYS:HD2  | 23:21:78:LYS:HA    | 1.81                     | 0.41              |
| 11:1P:135:LEU:HA  | 11:1P:135:LEU:HD23 | 1.83                     | 0.41              |
| 13:2R:87:TYR:OH   | 13:2R:116:LEU:HB3  | 2.21                     | 0.41              |
| 1:2A:2510:C:C4    | 1:2A:2511:U:C4     | 3.08                     | 0.41              |
| 16:2U:108:GLU:O   | 16:2U:112:ARG:HG2  | 2.19                     | 0.41              |
| 1:2A:1996:C:H4'   | 1:2A:1997:G:OP1    | 2.21                     | 0.41              |
| 1:2A:2564:A:C6    | 1:2A:2565:A:C6     | 3.08                     | 0.41              |
| 1:1A:2853:C:H2'   | 1:1A:2854:G:C8     | 2.55                     | 0.41              |
| 3:1D:35:LYS:HB2   | 3:1D:36:PRO:HD2    | 2.02                     | 0.41              |
| 4:1E:174:ASP:OD1  | 4:1E:175:VAL:N     | 2.53                     | 0.41              |
| 11:1P:128:HIS:NE2 | 11:1P:148:LEU:HD11 | 2.36                     | 0.41              |
| 26:14:16:CYS:HB3  | 26:14:20:ASN:HB3   | 2.02                     | 0.41              |
| 3:2D:129:ASN:O    | 3:2D:192:THR:HA    | 2.21                     | 0.41              |
| 1:1A:2093:G:C6    | 1:1A:2225:A:C8     | 3.09                     | 0.41              |
| 1:1A:1045:A:H1'   | 1:1A:1047:G:N3     | 2.35                     | 0.41              |
| 1:1A:1045:A:O2'   | 1:1A:1047:G:C4     | 2.70                     | 0.41              |
| 16:2U:66:ASN:OD1  | 16:2U:70:ARG:NE    | 2.50                     | 0.41              |
| 1:2A:2313:C:C4'   | 6:2G:91:ARG:HD3    | 2.51                     | 0.41              |
| 1:2A:2151:G:C2    | 1:2A:2152:G:C5     | 3.09                     | 0.41              |
| 1:2A:1500:G:O2'   | 3:2D:100:GLY:O     | 2.27                     | 0.41              |
| 1:1A:79:G:C2      | 1:1A:90:U:O2       | 30.43                    | 0.41              |
| 1:2A:869:G:C4     | 1:2A:870:A:C8      | 3.09                     | 0.41              |
| 5:1F:89:VAL:HG12  | 5:1F:90:PHE:CD2    | 2.55                     | 0.41              |
| 1:1A:2328:A:H2'   | 1:1A:2329:G:H8     | 1.81                     | 0.41              |
| 1:2A:42:G:H2'     | 1:2A:43:A:O4'      | 2.21                     | 0.41              |
| 13:1R:33:ARG:NH2  | 27:15:57:VAL:O     | 2.51                     | 0.41              |
| 6:2G:111:LEU:HB3  | 6:2G:117:PHE:CE1   | 2.56                     | 0.41              |
| 1:2A:2742:C:H2'   | 1:2A:2743:C:C6     | 2.56                     | 0.41              |
| 3:1D:71:ASP:OD2   | 3:1D:103:ARG:NH2   | 2.48                     | 0.41              |
| 1:1A:2206:G:H5''  | 1:1A:2207:G:N7     | 2.36                     | 0.41              |
| 1:2A:1899:G:O2'   | 1:2A:1900:A:OP2    | 2.31                     | 0.41              |
| 21:2Z:82:ARG:HA   | 21:2Z:83:PRO:HD2   | 1.87                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:2A:2575:C:OP1   | 4:2E:144:ARG:HD2  | 2.21                     | 0.41              |
| 61:2A:4040:HOH:O  | 27:25:8:LYS:HB3   | 2.21                     | 0.41              |
| 20:2Y:42:VAL:HG11 | 20:2Y:67:LEU:HD11 | 2.03                     | 0.41              |
| 1:1A:2097:C:H2'   | 1:1A:2098:U:O4'   | 2.21                     | 0.41              |
| 1:2A:2712:U:OP1   | 1:2A:2714:G:H4'   | 2.21                     | 0.41              |
| 15:1T:65:LYS:HE3  | 15:1T:67:SER:HB2  | 2.03                     | 0.41              |
| 24:12:31:GLU:O    | 24:12:35:LEU:HG   | 2.21                     | 0.41              |
| 1:2A:2561:A:H2'   | 1:2A:2562:U:O4'   | 2.20                     | 0.41              |
| 10:2O:80:ASP:OD1  | 15:2T:64:ARG:NH2  | 2.53                     | 0.41              |
| 1:1A:2315:G:H2'   | 1:1A:2316:C:C6    | 2.56                     | 0.41              |
| 19:2X:84:ALA:HB3  | 19:2X:87:GLN:NE2  | 2.36                     | 0.41              |
| 23:11:2:SER:HB3   | 23:11:46:LEU:HD12 | 2.03                     | 0.41              |
| 1:1A:1042:G:C6    | 1:1A:1043:C:C4    | 3.09                     | 0.40              |
| 1:2A:840:C:H2'    | 1:2A:841:A:C8     | 2.56                     | 0.40              |
| 1:2A:1479:G:H5''  | 1:2A:1560:G:H4'   | 2.02                     | 0.40              |
| 21:2Z:144:LEU:HG  | 21:2Z:149:SER:HA  | 2.03                     | 0.40              |
| 2:1B:77:U:OP1     | 21:1Z:19:ARG:NH2  | 2.53                     | 0.40              |
| 1:2A:566:U:H2'    | 1:2A:567:A:O4'    | 2.21                     | 0.40              |
| 1:2A:755:C:H2'    | 1:2A:756:C:C6     | 2.56                     | 0.40              |
| 1:2A:566:U:O2'    | 1:2A:809:G:OP2    | 2.33                     | 0.40              |
| 1:1A:380:U:H5'    | 23:11:16:ASN:O    | 2.21                     | 0.40              |
| 1:2A:56:A:H2'     | 1:2A:57:C:O4'     | 2.21                     | 0.40              |
| 8:2I:110:ASP:HA   | 8:2I:111:PRO:HD2  | 1.87                     | 0.40              |
| 1:1A:2141:G:C5    | 1:1A:2151:G:C2    | 3.09                     | 0.40              |
| 1:1A:2561:A:H2    | 10:1O:23:ARG:NH2  | 2.19                     | 0.40              |
| 1:1A:756:C:H2'    | 1:1A:757:U:O4'    | 2.53                     | 0.40              |
| 20:2Y:13:VAL:HB   | 20:2Y:72:VAL:HG13 | 2.04                     | 0.40              |
| 1:2A:2823:A:OP1   | 4:2E:113:PHE:HB2  | 2.21                     | 0.40              |
| 1:2A:1451:C:H42   | 1:2A:1459:G:H1    | 1.69                     | 0.40              |
| 12:2Q:42:ILE:HD13 | 12:2Q:97:VAL:HG21 | 2.03                     | 0.40              |
| 25:23:6:VAL:HG22  | 25:23:56:VAL:HG22 | 2.03                     | 0.40              |
| 6:1G:56:ALA:O     | 6:1G:59:GLU:HG2   | 2.20                     | 0.40              |
| 1:1A:2298:A:H2'   | 1:1A:2299:G:O4'   | 2.21                     | 0.40              |
| 21:1Z:1:MET:HA    | 21:1Z:2:GLU:HA    | 1.72                     | 0.40              |
| 1:2A:1628:G:H2'   | 1:2A:1629:U:C6    | 2.56                     | 0.40              |
| 20:1Y:14:LEU:HB2  | 20:1Y:75:ILE:HD11 | 2.02                     | 0.40              |
| 1:2A:303:U:H2'    | 1:2A:304:G:H8     | 1.86                     | 0.40              |
| 13:1R:13:HIS:CE1  | 13:1R:16:HIS:HB2  | 2.56                     | 0.40              |
| 22:20:82:ARG:HA   | 22:20:83:PRO:HD3  | 1.73                     | 0.40              |
| 1:2A:2525:G:C2    | 1:2A:2539:C:C2    | 3.09                     | 0.40              |
| 1:1A:1063:G:C6    | 1:1A:1064:C:N4    | 2.89                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:2A:195:A:H61     | 1:2A:198:C:H3'     | 1.86                     | 0.40              |
| 1:2A:784:A:C8      | 1:2A:792:G:C5      | 3.10                     | 0.40              |
| 1:2A:664:C:H2'     | 1:2A:665:C:H6      | 1.86                     | 0.40              |
| 1:2A:834:C:H2'     | 1:2A:835:A:C8      | 2.56                     | 0.40              |
| 1:2A:82:G:N1       | 1:2A:103:A:OP2     | 2.42                     | 0.40              |
| 1:2A:2836:U:O5'    | 1:2A:2836:U:H6     | 2.04                     | 0.40              |
| 18:1W:46:PHE:O     | 18:1W:50:VAL:HG23  | 2.21                     | 0.40              |
| 1:2A:1653:G:C4     | 13:2R:9:LYS:HD2    | 2.56                     | 0.40              |
| 6:1G:11:TYR:HA     | 6:1G:15:VAL:HB     | 2.03                     | 0.40              |
| 1:2A:557:U:H2'     | 1:2A:558:G:C8      | 2.57                     | 0.40              |
| 1:1A:1266:G:O5'    | 18:1W:15:ARG:NH2   | 2.55                     | 0.40              |
| 1:2A:229:A:O5'     | 1:2A:230:U:H5'     | 2.22                     | 0.40              |
| 7:2H:15:VAL:HB     | 7:2H:29:PRO:HD3    | 2.02                     | 0.40              |
| 1:2A:2526:G:C6     | 1:2A:2527:C:C4     | 3.10                     | 0.40              |
| 11:1P:101:VAL:HG23 | 11:1P:106:LEU:O    | 2.21                     | 0.40              |
| 1:1A:2698:U:H2'    | 1:1A:2699:C:C6     | 2.57                     | 0.40              |
| 8:2I:12:LEU:HA     | 8:2I:12:LEU:HD23   | 1.93                     | 0.40              |
| 9:2N:138:LEU:HD23  | 9:2N:138:LEU:HA    | 1.88                     | 0.40              |
| 21:1Z:124:ILE:HD12 | 21:1Z:124:ILE:HA   | 1.95                     | 0.40              |
| 1:1A:1095:A:C8     | 1:1A:1096:A:C8     | 3.10                     | 0.40              |
| 1:1A:1170:G:H2'    | 1:1A:1171:G:O4'    | 2.21                     | 0.40              |
| 16:2U:58:ARG:HA    | 16:2U:61:TRP:CE3   | 2.56                     | 0.40              |
| 1:2A:899:A:HO2'    | 1:2A:900:A:H8      | 1.66                     | 0.40              |
| 1:2A:892:G:H2'     | 1:2A:893:C:H4'     | 2.02                     | 0.40              |
| 2:2B:72:G:O2'      | 2:2B:73:A:O4'      | 2.34                     | 0.40              |
| 1:1A:1204:A:H61    | 1:1A:1240:U:H2'    | 1.86                     | 0.40              |
| 12:2Q:54:MET:HE1   | 12:2Q:118:LEU:HD23 | 2.04                     | 0.40              |
| 1:2A:2684:U:H1'    | 10:2O:70:LYS:HD2   | 2.04                     | 0.40              |
| 1:2A:1713:U:H2'    | 1:2A:1714:G:C8     | 2.51                     | 0.40              |
| 1:2A:1219:G:H1     | 1:2A:1230:C:H42    | 1.70                     | 0.40              |
| 7:1H:83:TYR:CE2    | 7:1H:138:LYS:HB2   | 2.57                     | 0.40              |
| 7:1H:167:GLU:HA    | 7:1H:168:PRO:HD3   | 1.86                     | 0.40              |
| 8:2I:23:PRO:O      | 8:2I:27:ARG:HG3    | 2.21                     | 0.40              |
| 1:1A:1432:C:H2'    | 1:1A:1433:U:O4'    | 2.22                     | 0.40              |
| 1:2A:113:G:O4'     | 1:2A:354:G:H4'     | 47.40                    | 0.40              |
| 1:2A:1430:C:H2'    | 1:2A:1431:U:H6     | 1.85                     | 0.40              |
| 1:2A:1894:C:H2'    | 1:2A:1895:C:C6     | 2.56                     | 0.40              |
| 1:2A:2006:C:O2'    | 1:2A:2823:A:N3     | 2.53                     | 0.40              |
| 31:19:7:VAL:HG12   | 31:19:34:GLN:HB3   | 2.02                     | 0.40              |
| 1:1A:2837:G:H21    | 13:1R:45:ARG:HH12  | 1.67                     | 0.40              |
| 1:2A:1827:C:OP2    | 3:2D:222:ARG:HD2   | 2.21                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:1F:140:LEU:HD11 | 5:1F:170:LEU:HD11 | 2.02                     | 0.40              |
| 1:1A:1526:G:C6    | 1:1A:1527:G:C2    | 3.09                     | 0.40              |
| 1:2A:827:U:H1'    | 1:2A:2246:G:O2'   | 2.21                     | 0.40              |
| 1:2A:2493:U:H2'   | 1:2A:2494:G:O4'   | 2.21                     | 0.40              |
| 1:1A:844:C:C2'    | 1:1A:845:G:H5'    | 2.51                     | 0.40              |
| 12:2Q:120:ILE:O   | 12:2Q:123:HIS:HB2 | 2.21                     | 0.40              |
| 2:2B:59:A:H2'     | 2:2B:60:C:O4'     | 2.21                     | 0.40              |
| 1:2A:2748:A:H2'   | 1:2A:2749:A:O4'   | 2.21                     | 0.40              |
| 2:2B:43:C:O4'     | 6:2G:66:GLN:NE2   | 2.54                     | 0.40              |
| 1:2A:1400:G:H2'   | 1:2A:1401:G:C8    | 2.56                     | 0.40              |
| 23:11:52:ARG:HD2  | 23:11:55:GLY:C    | 2.42                     | 0.40              |
| 11:2P:52:GLU:O    | 11:2P:55:ARG:HG2  | 2.22                     | 0.40              |
| 8:2I:62:LYS:HE2   | 8:2I:133:HIS:HE1  | 1.87                     | 0.40              |
| 1:2A:829:A:N7     | 1:2A:2248:C:H5'   | 2.36                     | 0.40              |
| 1:2A:921:G:C6     | 1:2A:922:U:C4     | 3.10                     | 0.40              |
| 1:2A:602:G:N1     | 1:2A:655:A:OP2    | 2.48                     | 0.40              |
| 1:2A:1256:G:H1'   | 5:2F:82:ILE:HD11  | 2.03                     | 0.40              |
| 1:2A:1224:C:O2'   | 17:2V:85:LYS:HA   | 2.22                     | 0.40              |
| 10:2O:26:LYS:O    | 10:2O:30:ALA:HB2  | 2.22                     | 0.40              |
| 10:2O:77:ILE:HB   | 15:2T:74:ARG:HD3  | 2.04                     | 0.40              |
| 1:2A:2645:G:H4'   | 1:2A:2732:G:O3'   | 2.21                     | 0.40              |
| 1:2A:522:G:C2     | 1:2A:523:C:C2     | 3.08                     | 0.40              |
| 1:1A:1914:C:H2'   | 1:1A:1915:5MU:O4' | 2.21                     | 0.40              |
| 1:2A:2583:G:H2'   | 1:2A:2584:U:C6    | 2.56                     | 0.40              |
| 1:2A:676:A:H2     | 1:2A:2069:G:N3    | 2.19                     | 0.40              |
| 1:2A:1188:U:C4'   | 17:2V:79:VAL:HG22 | 2.51                     | 0.40              |
| 17:2V:52:VAL:HG21 | 17:2V:55:ALA:HB3  | 2.02                     | 0.40              |
| 12:1Q:31:ASP:HA   | 12:1Q:134:ARG:NH1 | 2.36                     | 0.40              |
| 31:19:10:ILE:HD11 | 31:19:34:GLN:HE21 | 1.86                     | 0.40              |
| 1:1A:2735:G:H2'   | 1:1A:2736:G:H8    | 1.86                     | 0.40              |
| 1:1A:1791:A:OP2   | 1:1A:1791:A:H8    | 2.05                     | 0.40              |
| 1:2A:262:A:H2'    | 1:2A:263:C:O4'    | 2.21                     | 0.40              |
| 1:2A:2577:A:OP2   | 27:25:3:LYS:NZ    | 2.48                     | 0.40              |
| 1:2A:271(S):G:C6  | 1:2A:271(T):C:C4  | 3.10                     | 0.40              |
| 21:1Z:125:LEU:C   | 21:1Z:164:ALA:HB3 | 2.42                     | 0.40              |
| 8:1I:57:ARG:HE    | 8:1I:57:ARG:HB3   | 1.72                     | 0.40              |
| 26:14:28:LYS:HA   | 26:14:29:PRO:HD3  | 1.95                     | 0.40              |
| 1:2A:2773:C:OP1   | 4:2E:166:THR:OG1  | 2.32                     | 0.40              |
| 1:2A:2518:A:OP2   | 61:2A:3765:HOH:O  | 2.22                     | 0.40              |
| 4:1E:101:ARG:HD2  | 4:1E:169:ASN:O    | 2.21                     | 0.40              |
| 6:1G:67:LYS:HD3   | 26:14:5:ILE:HB    | 2.02                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:2A:2263:C:H2'    | 1:2A:2264:C:O4'    | 2.21                     | 0.40              |
| 7:2H:13:LYS:HA     | 7:2H:14:GLY:HA2    | 1.60                     | 0.40              |
| 1:1A:1175:U:H1'    | 1:1A:1176:G:OP1    | 2.21                     | 0.40              |
| 1:2A:2184:G:O2'    | 1:2A:2185:C:H5'    | 2.22                     | 0.40              |
| 1:2A:1208:C:H2'    | 1:2A:1209:G:H5'    | 2.03                     | 0.40              |
| 1:1A:1125:G:H5'    | 31:19:37:GLY:HA2   | 2.04                     | 0.40              |
| 1:2A:839:U:H2'     | 1:2A:840:C:H6      | 1.86                     | 0.40              |
| 8:1I:124:GLY:H     | 8:1I:144:VAL:HG23  | 1.86                     | 0.40              |
| 11:2P:38:GLN:HG2   | 11:2P:45:LEU:H     | 1.87                     | 0.40              |
| 5:2F:148:LEU:HD22  | 5:2F:154:VAL:HG21  | 2.04                     | 0.40              |
| 1:1A:588:U:H1'     | 5:1F:90:PHE:CG     | 2.56                     | 0.40              |
| 1:2A:390:A:N6      | 61:2A:3962:HOH:O   | 2.51                     | 0.40              |
| 1:2A:2261:C:O2'    | 1:2A:2262:U:H5'    | 2.22                     | 0.40              |
| 1:2A:265:A:C8      | 1:2A:266:G:H1'     | 2.57                     | 0.40              |
| 15:1T:127:ALA:C    | 15:1T:129:ARG:N    | 2.69                     | 0.40              |
| 58:1A:3915:HGR:C16 | 58:1A:3915:HGR:H3  | 2.52                     | 0.40              |
| 1:2A:1581:G:C6     | 1:2A:1582:C:C4     | 3.09                     | 0.40              |
| 3:2D:13:ARG:HA     | 3:2D:13:ARG:HD3    | 1.93                     | 0.40              |
| 6:2G:173:LEU:O     | 6:2G:178:PHE:N     | 2.48                     | 0.40              |
| 5:1F:133:ASN:N     | 5:1F:138:GLU:OE1   | 2.49                     | 0.40              |
| 21:1Z:152:ALA:H    | 21:1Z:171:ILE:HG21 | 1.86                     | 0.40              |
| 1:2A:2494:G:C4     | 1:2A:2495:G:C8     | 3.10                     | 0.40              |
| 8:2I:25:TYR:O      | 8:2I:29:TYR:HB3    | 2.21                     | 0.40              |
| 1:2A:2666:C:N4     | 7:2H:108:GLY:O     | 2.47                     | 0.40              |
| 13:1R:29:LEU:HA    | 13:1R:29:LEU:HD12  | 1.87                     | 0.40              |
| 31:29:17:ILE:HA    | 31:29:17:ILE:HD12  | 1.92                     | 0.40              |
| 1:1A:2412:A:H2'    | 1:1A:2413:G:O4'    | 2.22                     | 0.40              |
| 16:2U:19:LYS:HA    | 16:2U:22:LYS:HG3   | 2.03                     | 0.40              |

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 32:1a:358:U:OP1 | 8:2I:121:LYS:NZ[2_655] | 2.11                     | 0.09              |

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 3   | 1D    | 273/276 (99%) | 259 (95%) | 13 (5%)  | 1 (0%)   | 39          | 65  |
| 3   | 2D    | 273/276 (99%) | 261 (96%) | 11 (4%)  | 1 (0%)   | 39          | 65  |
| 4   | 1E    | 202/206 (98%) | 194 (96%) | 7 (4%)   | 1 (0%)   | 34          | 60  |
| 4   | 2E    | 202/206 (98%) | 194 (96%) | 6 (3%)   | 2 (1%)   | 19          | 39  |
| 5   | 1F    | 201/210 (96%) | 195 (97%) | 5 (2%)   | 1 (0%)   | 34          | 60  |
| 5   | 2F    | 201/210 (96%) | 195 (97%) | 4 (2%)   | 2 (1%)   | 19          | 39  |
| 6   | 1G    | 179/182 (98%) | 167 (93%) | 10 (6%)  | 2 (1%)   | 17          | 36  |
| 6   | 2G    | 179/182 (98%) | 165 (92%) | 12 (7%)  | 2 (1%)   | 17          | 36  |
| 7   | 1H    | 172/180 (96%) | 162 (94%) | 9 (5%)   | 1 (1%)   | 30          | 56  |
| 7   | 2H    | 172/180 (96%) | 160 (93%) | 11 (6%)  | 1 (1%)   | 30          | 56  |
| 8   | 1I    | 144/148 (97%) | 126 (88%) | 13 (9%)  | 5 (4%)   | 4           | 6   |
| 8   | 2I    | 144/148 (97%) | 129 (90%) | 14 (10%) | 1 (1%)   | 26          | 51  |
| 9   | 1N    | 138/140 (99%) | 130 (94%) | 8 (6%)   | 0        | 100         | 100 |
| 9   | 2N    | 138/140 (99%) | 128 (93%) | 10 (7%)  | 0        | 100         | 100 |
| 10  | 1O    | 120/122 (98%) | 112 (93%) | 7 (6%)   | 1 (1%)   | 24          | 46  |
| 10  | 2O    | 120/122 (98%) | 112 (93%) | 8 (7%)   | 0        | 100         | 100 |
| 11  | 1P    | 147/150 (98%) | 139 (95%) | 7 (5%)   | 1 (1%)   | 26          | 51  |
| 11  | 2P    | 147/150 (98%) | 135 (92%) | 10 (7%)  | 2 (1%)   | 14          | 28  |
| 12  | 1Q    | 139/141 (99%) | 130 (94%) | 9 (6%)   | 0        | 100         | 100 |
| 12  | 2Q    | 139/141 (99%) | 131 (94%) | 7 (5%)   | 1 (1%)   | 26          | 51  |
| 13  | 1R    | 116/118 (98%) | 109 (94%) | 7 (6%)   | 0        | 100         | 100 |
| 13  | 2R    | 116/118 (98%) | 109 (94%) | 7 (6%)   | 0        | 100         | 100 |
| 14  | 1S    | 108/112 (96%) | 106 (98%) | 2 (2%)   | 0        | 100         | 100 |
| 14  | 2S    | 108/112 (96%) | 104 (96%) | 3 (3%)   | 1 (1%)   | 21          | 42  |
| 15  | 1T    | 129/146 (88%) | 119 (92%) | 9 (7%)   | 1 (1%)   | 24          | 46  |

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| Mol | Chain | Analysed      | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|------------|----------|----------|-------------|-----|
| 15  | 2T    | 129/146 (88%) | 121 (94%)  | 8 (6%)   | 0        | 100         | 100 |
| 16  | 1U    | 114/118 (97%) | 114 (100%) | 0        | 0        | 100         | 100 |
| 16  | 2U    | 114/118 (97%) | 114 (100%) | 0        | 0        | 100         | 100 |
| 17  | 1V    | 99/101 (98%)  | 94 (95%)   | 4 (4%)   | 1 (1%)   | 19          | 39  |
| 17  | 2V    | 99/101 (98%)  | 96 (97%)   | 2 (2%)   | 1 (1%)   | 19          | 39  |
| 18  | 1W    | 110/113 (97%) | 109 (99%)  | 1 (1%)   | 0        | 100         | 100 |
| 18  | 2W    | 110/113 (97%) | 110 (100%) | 0        | 0        | 100         | 100 |
| 19  | 1X    | 93/96 (97%)   | 89 (96%)   | 4 (4%)   | 0        | 100         | 100 |
| 19  | 2X    | 93/96 (97%)   | 88 (95%)   | 4 (4%)   | 1 (1%)   | 17          | 36  |
| 20  | 1Y    | 105/110 (96%) | 97 (92%)   | 6 (6%)   | 2 (2%)   | 10          | 19  |
| 20  | 2Y    | 105/110 (96%) | 99 (94%)   | 5 (5%)   | 1 (1%)   | 19          | 39  |
| 21  | 1Z    | 148/206 (72%) | 128 (86%)  | 16 (11%) | 4 (3%)   | 6           | 10  |
| 21  | 2Z    | 156/206 (76%) | 131 (84%)  | 22 (14%) | 3 (2%)   | 10          | 19  |
| 22  | 10    | 81/85 (95%)   | 78 (96%)   | 3 (4%)   | 0        | 100         | 100 |
| 22  | 20    | 81/85 (95%)   | 76 (94%)   | 3 (4%)   | 2 (2%)   | 7           | 12  |
| 23  | 11    | 95/98 (97%)   | 92 (97%)   | 2 (2%)   | 1 (1%)   | 17          | 36  |
| 23  | 21    | 95/98 (97%)   | 91 (96%)   | 3 (3%)   | 1 (1%)   | 17          | 36  |
| 24  | 12    | 68/72 (94%)   | 67 (98%)   | 1 (2%)   | 0        | 100         | 100 |
| 24  | 22    | 68/72 (94%)   | 66 (97%)   | 2 (3%)   | 0        | 100         | 100 |
| 25  | 13    | 57/60 (95%)   | 56 (98%)   | 1 (2%)   | 0        | 100         | 100 |
| 25  | 23    | 57/60 (95%)   | 55 (96%)   | 2 (4%)   | 0        | 100         | 100 |
| 26  | 14    | 67/71 (94%)   | 53 (79%)   | 8 (12%)  | 6 (9%)   | 1           | 1   |
| 26  | 24    | 67/71 (94%)   | 52 (78%)   | 8 (12%)  | 7 (10%)  | 1           | 0   |
| 27  | 15    | 57/60 (95%)   | 55 (96%)   | 2 (4%)   | 0        | 100         | 100 |
| 27  | 25    | 57/60 (95%)   | 56 (98%)   | 1 (2%)   | 0        | 100         | 100 |
| 28  | 16    | 51/54 (94%)   | 49 (96%)   | 2 (4%)   | 0        | 100         | 100 |
| 28  | 26    | 51/54 (94%)   | 50 (98%)   | 1 (2%)   | 0        | 100         | 100 |
| 29  | 17    | 46/49 (94%)   | 44 (96%)   | 2 (4%)   | 0        | 100         | 100 |
| 29  | 27    | 46/49 (94%)   | 44 (96%)   | 1 (2%)   | 1 (2%)   | 8           | 15  |
| 30  | 18    | 62/65 (95%)   | 61 (98%)   | 1 (2%)   | 0        | 100         | 100 |
| 30  | 28    | 62/65 (95%)   | 60 (97%)   | 2 (3%)   | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 31  | 19    | 35/37 (95%)   | 35 (100%) | 0        | 0        | 100         | 100 |
| 31  | 29    | 35/37 (95%)   | 35 (100%) | 0        | 0        | 100         | 100 |
| 33  | 1b    | 229/256 (90%) | 197 (86%) | 27 (12%) | 5 (2%)   | 8           | 15  |
| 33  | 2b    | 229/256 (90%) | 199 (87%) | 21 (9%)  | 9 (4%)   | 4           | 5   |
| 34  | 1c    | 204/239 (85%) | 183 (90%) | 19 (9%)  | 2 (1%)   | 19          | 39  |
| 34  | 2c    | 204/239 (85%) | 181 (89%) | 20 (10%) | 3 (2%)   | 13          | 26  |
| 35  | 1d    | 206/209 (99%) | 191 (93%) | 15 (7%)  | 0        | 100         | 100 |
| 35  | 2d    | 206/209 (99%) | 191 (93%) | 15 (7%)  | 0        | 100         | 100 |
| 36  | 1e    | 146/162 (90%) | 142 (97%) | 2 (1%)   | 2 (1%)   | 14          | 28  |
| 36  | 2e    | 146/162 (90%) | 141 (97%) | 5 (3%)   | 0        | 100         | 100 |
| 37  | 1f    | 98/101 (97%)  | 95 (97%)  | 3 (3%)   | 0        | 100         | 100 |
| 37  | 2f    | 98/101 (97%)  | 95 (97%)  | 3 (3%)   | 0        | 100         | 100 |
| 38  | 1g    | 153/156 (98%) | 142 (93%) | 9 (6%)   | 2 (1%)   | 15          | 30  |
| 38  | 2g    | 153/156 (98%) | 140 (92%) | 11 (7%)  | 2 (1%)   | 15          | 30  |
| 39  | 1h    | 135/138 (98%) | 131 (97%) | 4 (3%)   | 0        | 100         | 100 |
| 39  | 2h    | 135/138 (98%) | 128 (95%) | 6 (4%)   | 1 (1%)   | 26          | 51  |
| 40  | 1i    | 125/128 (98%) | 108 (86%) | 17 (14%) | 0        | 100         | 100 |
| 40  | 2i    | 125/128 (98%) | 107 (86%) | 17 (14%) | 1 (1%)   | 24          | 46  |
| 41  | 1j    | 95/105 (90%)  | 81 (85%)  | 8 (8%)   | 6 (6%)   | 2           | 2   |
| 41  | 2j    | 94/105 (90%)  | 80 (85%)  | 9 (10%)  | 5 (5%)   | 2           | 2   |
| 42  | 1k    | 112/129 (87%) | 105 (94%) | 7 (6%)   | 0        | 100         | 100 |
| 42  | 2k    | 112/129 (87%) | 105 (94%) | 7 (6%)   | 0        | 100         | 100 |
| 43  | 1l    | 119/132 (90%) | 113 (95%) | 6 (5%)   | 0        | 100         | 100 |
| 43  | 2l    | 119/132 (90%) | 112 (94%) | 7 (6%)   | 0        | 100         | 100 |
| 44  | 1m    | 121/126 (96%) | 113 (93%) | 6 (5%)   | 2 (2%)   | 11          | 22  |
| 44  | 2m    | 120/126 (95%) | 110 (92%) | 7 (6%)   | 3 (2%)   | 7           | 12  |
| 45  | 1n    | 58/61 (95%)   | 54 (93%)  | 4 (7%)   | 0        | 100         | 100 |
| 45  | 2n    | 58/61 (95%)   | 54 (93%)  | 4 (7%)   | 0        | 100         | 100 |
| 46  | 1o    | 86/89 (97%)   | 85 (99%)  | 1 (1%)   | 0        | 100         | 100 |
| 46  | 2o    | 86/89 (97%)   | 80 (93%)  | 4 (5%)   | 2 (2%)   | 8           | 14  |
| 47  | 1p    | 80/88 (91%)   | 75 (94%)  | 4 (5%)   | 1 (1%)   | 15          | 30  |

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| Mol | Chain | Analysed          | Favoured    | Allowed  | Outliers | Percentiles |     |
|-----|-------|-------------------|-------------|----------|----------|-------------|-----|
| 47  | 2p    | 80/88 (91%)       | 74 (92%)    | 5 (6%)   | 1 (1%)   | 15          | 30  |
| 48  | 1q    | 97/105 (92%)      | 90 (93%)    | 6 (6%)   | 1 (1%)   | 19          | 39  |
| 48  | 2q    | 97/105 (92%)      | 91 (94%)    | 6 (6%)   | 0        | 100         | 100 |
| 49  | 1r    | 66/88 (75%)       | 63 (96%)    | 3 (4%)   | 0        | 100         | 100 |
| 49  | 2r    | 66/88 (75%)       | 64 (97%)    | 2 (3%)   | 0        | 100         | 100 |
| 50  | 1s    | 81/93 (87%)       | 73 (90%)    | 6 (7%)   | 2 (2%)   | 7           | 12  |
| 50  | 2s    | 81/93 (87%)       | 72 (89%)    | 7 (9%)   | 2 (2%)   | 7           | 12  |
| 51  | 1t    | 94/106 (89%)      | 87 (93%)    | 2 (2%)   | 5 (5%)   | 2           | 2   |
| 51  | 2t    | 94/106 (89%)      | 87 (93%)    | 1 (1%)   | 6 (6%)   | 2           | 2   |
| 52  | 1u    | 21/27 (78%)       | 19 (90%)    | 2 (10%)  | 0        | 100         | 100 |
| 52  | 2u    | 21/27 (78%)       | 19 (90%)    | 2 (10%)  | 0        | 100         | 100 |
| All | All   | 11370/12128 (94%) | 10613 (93%) | 636 (6%) | 121 (1%) | 17          | 36  |

All (121) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | 1D    | 275 | LYS  |
| 5   | 1F    | 130 | ALA  |
| 6   | 1G    | 47  | LYS  |
| 6   | 1G    | 51  | ARG  |
| 7   | 1H    | 126 | PRO  |
| 17  | 1V    | 79  | VAL  |
| 21  | 1Z    | 159 | PRO  |
| 23  | 11    | 3   | LYS  |
| 26  | 14    | 53  | GLU  |
| 33  | 1b    | 17  | PHE  |
| 38  | 1g    | 79  | ARG  |
| 38  | 1g    | 80  | VAL  |
| 41  | 1j    | 55  | LYS  |
| 44  | 1m    | 3   | ARG  |
| 47  | 1p    | 53  | VAL  |
| 48  | 1q    | 68  | ARG  |
| 51  | 1t    | 95  | ALA  |
| 3   | 2D    | 3   | VAL  |
| 5   | 2F    | 21  | ALA  |
| 5   | 2F    | 130 | ALA  |
| 7   | 2H    | 126 | PRO  |
| 8   | 2I    | 10  | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 12  | 2Q    | 28  | ALA  |
| 17  | 2V    | 79  | VAL  |
| 26  | 24    | 53  | GLU  |
| 26  | 24    | 55  | ARG  |
| 29  | 27    | 46  | VAL  |
| 33  | 2b    | 16  | HIS  |
| 33  | 2b    | 17  | PHE  |
| 33  | 2b    | 123 | ALA  |
| 33  | 2b    | 126 | GLU  |
| 41  | 2j    | 29  | ARG  |
| 47  | 2p    | 53  | VAL  |
| 51  | 2t    | 95  | ALA  |
| 8   | 1I    | 106 | GLY  |
| 26  | 14    | 45  | GLY  |
| 26  | 14    | 47  | GLN  |
| 26  | 14    | 56  | VAL  |
| 33  | 1b    | 165 | VAL  |
| 34  | 1c    | 66  | VAL  |
| 41  | 1j    | 29  | ARG  |
| 41  | 1j    | 75  | ILE  |
| 50  | 1s    | 42  | PRO  |
| 51  | 1t    | 47  | GLY  |
| 14  | 2S    | 84  | GLN  |
| 22  | 20    | 4   | LYS  |
| 22  | 20    | 13  | GLY  |
| 26  | 24    | 45  | GLY  |
| 26  | 24    | 48  | ARG  |
| 26  | 24    | 62  | ARG  |
| 33  | 2b    | 165 | VAL  |
| 34  | 2c    | 107 | GLN  |
| 38  | 2g    | 80  | VAL  |
| 41  | 2j    | 75  | ILE  |
| 44  | 2m    | 4   | ILE  |
| 50  | 2s    | 29  | ARG  |
| 50  | 2s    | 42  | PRO  |
| 51  | 2t    | 10  | LEU  |
| 51  | 2t    | 47  | GLY  |
| 4   | 1E    | 52  | LEU  |
| 8   | 1I    | 10  | GLU  |
| 8   | 1I    | 105 | HIS  |
| 21  | 1Z    | 134 | PRO  |
| 21  | 1Z    | 152 | ALA  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 33  | 1b    | 10  | LEU  |
| 33  | 1b    | 231 | GLU  |
| 36  | 1e    | 86  | ALA  |
| 41  | 1j    | 78  | ASN  |
| 51  | 1t    | 100 | ILE  |
| 6   | 2G    | 48  | GLU  |
| 6   | 2G    | 51  | ARG  |
| 23  | 2I    | 3   | LYS  |
| 33  | 2b    | 125 | PRO  |
| 33  | 2b    | 231 | GLU  |
| 38  | 2g    | 7   | ALA  |
| 40  | 2i    | 54  | ASP  |
| 41  | 2j    | 55  | LYS  |
| 41  | 2j    | 78  | ASN  |
| 51  | 2t    | 102 | GLY  |
| 8   | 1I    | 107 | VAL  |
| 26  | 14    | 44  | THR  |
| 36  | 1e    | 85  | GLY  |
| 41  | 1j    | 77  | PRO  |
| 44  | 1m    | 67  | GLU  |
| 4   | 2E    | 52  | LEU  |
| 4   | 2E    | 73  | GLU  |
| 11  | 2P    | 38  | GLN  |
| 19  | 2X    | 2   | LYS  |
| 21  | 2Z    | 134 | PRO  |
| 21  | 2Z    | 171 | ILE  |
| 26  | 24    | 46  | GLN  |
| 26  | 24    | 49  | PHE  |
| 34  | 2c    | 3   | ASN  |
| 34  | 2c    | 108 | ASN  |
| 44  | 2m    | 67  | GLU  |
| 51  | 2t    | 9   | ASN  |
| 15  | 1T    | 128 | GLU  |
| 20  | 1Y    | 54  | LYS  |
| 26  | 14    | 62  | ARG  |
| 34  | 1c    | 3   | ASN  |
| 11  | 2P    | 45  | LEU  |
| 39  | 2h    | 73  | ASP  |
| 41  | 2j    | 77  | PRO  |
| 46  | 2o    | 88  | ARG  |
| 8   | 1I    | 11  | ASN  |
| 10  | 1O    | 29  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 21  | 1Z    | 163 | LEU  |
| 50  | 1s    | 81  | ARG  |
| 51  | 1t    | 10  | LEU  |
| 33  | 2b    | 10  | LEU  |
| 46  | 2o    | 23  | GLY  |
| 51  | 2t    | 100 | ILE  |
| 44  | 2m    | 6   | GLY  |
| 33  | 1b    | 124 | SER  |
| 11  | 1P    | 122 | PRO  |
| 51  | 1t    | 102 | GLY  |
| 21  | 2Z    | 146 | ILE  |
| 20  | 1Y    | 103 | GLY  |
| 41  | 1j    | 91  | PRO  |
| 20  | 2Y    | 103 | GLY  |
| 33  | 2b    | 234 | PRO  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed      | Rotameric | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|-------------|----|
| 3   | 1D    | 215/218 (99%) | 208 (97%) | 7 (3%)   | 45          | 73 |
| 3   | 2D    | 215/218 (99%) | 207 (96%) | 8 (4%)   | 41          | 69 |
| 4   | 1E    | 164/166 (99%) | 154 (94%) | 10 (6%)  | 23          | 46 |
| 4   | 2E    | 164/166 (99%) | 151 (92%) | 13 (8%)  | 15          | 30 |
| 5   | 1F    | 160/166 (96%) | 149 (93%) | 11 (7%)  | 19          | 38 |
| 5   | 2F    | 159/166 (96%) | 149 (94%) | 10 (6%)  | 22          | 44 |
| 6   | 1G    | 144/156 (92%) | 136 (94%) | 8 (6%)   | 26          | 50 |
| 6   | 2G    | 143/156 (92%) | 135 (94%) | 8 (6%)   | 26          | 50 |
| 7   | 1H    | 144/148 (97%) | 140 (97%) | 4 (3%)   | 51          | 78 |
| 7   | 2H    | 144/148 (97%) | 140 (97%) | 4 (3%)   | 51          | 78 |
| 8   | 1I    | 113/124 (91%) | 110 (97%) | 3 (3%)   | 52          | 79 |
| 8   | 2I    | 105/124 (85%) | 102 (97%) | 3 (3%)   | 50          | 77 |

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| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |     |
|-----|-------|----------------|-----------|----------|-------------|-----|
| 9   | 1N    | 118/119 (99%)  | 114 (97%) | 4 (3%)   | 44          | 72  |
| 9   | 2N    | 118/119 (99%)  | 115 (98%) | 3 (2%)   | 55          | 81  |
| 10  | 1O    | 100/100 (100%) | 98 (98%)  | 2 (2%)   | 63          | 85  |
| 10  | 2O    | 100/100 (100%) | 99 (99%)  | 1 (1%)   | 82          | 94  |
| 11  | 1P    | 115/116 (99%)  | 110 (96%) | 5 (4%)   | 35          | 64  |
| 11  | 2P    | 115/116 (99%)  | 113 (98%) | 2 (2%)   | 68          | 88  |
| 12  | 1Q    | 111/111 (100%) | 110 (99%) | 1 (1%)   | 84          | 95  |
| 12  | 2Q    | 111/111 (100%) | 109 (98%) | 2 (2%)   | 66          | 87  |
| 13  | 1R    | 101/101 (100%) | 90 (89%)  | 11 (11%) | 8           | 14  |
| 13  | 2R    | 101/101 (100%) | 92 (91%)  | 9 (9%)   | 12          | 23  |
| 14  | 1S    | 86/88 (98%)    | 84 (98%)  | 2 (2%)   | 58          | 83  |
| 14  | 2S    | 85/88 (97%)    | 82 (96%)  | 3 (4%)   | 43          | 71  |
| 15  | 1T    | 115/127 (91%)  | 113 (98%) | 2 (2%)   | 68          | 88  |
| 15  | 2T    | 113/127 (89%)  | 112 (99%) | 1 (1%)   | 84          | 95  |
| 16  | 1U    | 93/94 (99%)    | 90 (97%)  | 3 (3%)   | 46          | 74  |
| 16  | 2U    | 93/94 (99%)    | 92 (99%)  | 1 (1%)   | 80          | 93  |
| 17  | 1V    | 80/82 (98%)    | 73 (91%)  | 7 (9%)   | 12          | 24  |
| 17  | 2V    | 80/82 (98%)    | 76 (95%)  | 4 (5%)   | 30          | 56  |
| 18  | 1W    | 90/92 (98%)    | 86 (96%)  | 4 (4%)   | 35          | 63  |
| 18  | 2W    | 90/92 (98%)    | 87 (97%)  | 3 (3%)   | 45          | 73  |
| 19  | 1X    | 77/78 (99%)    | 75 (97%)  | 2 (3%)   | 54          | 80  |
| 19  | 2X    | 77/78 (99%)    | 75 (97%)  | 2 (3%)   | 54          | 80  |
| 20  | 1Y    | 85/91 (93%)    | 81 (95%)  | 4 (5%)   | 32          | 59  |
| 20  | 2Y    | 85/91 (93%)    | 84 (99%)  | 1 (1%)   | 78          | 92  |
| 21  | 1Z    | 135/179 (75%)  | 131 (97%) | 4 (3%)   | 48          | 76  |
| 21  | 2Z    | 137/179 (76%)  | 134 (98%) | 3 (2%)   | 60          | 83  |
| 22  | 10    | 65/67 (97%)    | 64 (98%)  | 1 (2%)   | 72          | 90  |
| 22  | 20    | 65/67 (97%)    | 65 (100%) | 0        | 100         | 100 |
| 23  | 11    | 80/83 (96%)    | 79 (99%)  | 1 (1%)   | 76          | 91  |
| 23  | 21    | 80/83 (96%)    | 80 (100%) | 0        | 100         | 100 |
| 24  | 12    | 65/67 (97%)    | 64 (98%)  | 1 (2%)   | 72          | 90  |

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| Mol | Chain | Analysed      | Rotameric  | Outliers | Percentiles |     |
|-----|-------|---------------|------------|----------|-------------|-----|
| 24  | 22    | 65/67 (97%)   | 63 (97%)   | 2 (3%)   | 47          | 76  |
| 25  | 13    | 51/52 (98%)   | 49 (96%)   | 2 (4%)   | 39          | 68  |
| 25  | 23    | 50/52 (96%)   | 48 (96%)   | 2 (4%)   | 38          | 67  |
| 26  | 14    | 59/63 (94%)   | 53 (90%)   | 6 (10%)  | 9           | 17  |
| 26  | 24    | 53/63 (84%)   | 49 (92%)   | 4 (8%)   | 17          | 33  |
| 27  | 15    | 50/52 (96%)   | 46 (92%)   | 4 (8%)   | 15          | 29  |
| 27  | 25    | 50/52 (96%)   | 47 (94%)   | 3 (6%)   | 24          | 47  |
| 28  | 16    | 51/52 (98%)   | 49 (96%)   | 2 (4%)   | 39          | 68  |
| 28  | 26    | 50/52 (96%)   | 47 (94%)   | 3 (6%)   | 24          | 47  |
| 29  | 17    | 41/42 (98%)   | 40 (98%)   | 1 (2%)   | 57          | 82  |
| 29  | 27    | 41/42 (98%)   | 40 (98%)   | 1 (2%)   | 57          | 82  |
| 30  | 18    | 54/55 (98%)   | 52 (96%)   | 2 (4%)   | 41          | 69  |
| 30  | 28    | 54/55 (98%)   | 52 (96%)   | 2 (4%)   | 41          | 69  |
| 31  | 19    | 34/34 (100%)  | 34 (100%)  | 0        | 100         | 100 |
| 31  | 29    | 34/34 (100%)  | 32 (94%)   | 2 (6%)   | 24          | 47  |
| 33  | 1b    | 192/220 (87%) | 186 (97%)  | 6 (3%)   | 47          | 76  |
| 33  | 2b    | 187/220 (85%) | 183 (98%)  | 4 (2%)   | 61          | 85  |
| 34  | 1c    | 142/188 (76%) | 139 (98%)  | 3 (2%)   | 61          | 85  |
| 34  | 2c    | 140/188 (74%) | 139 (99%)  | 1 (1%)   | 88          | 96  |
| 35  | 1d    | 169/181 (93%) | 164 (97%)  | 5 (3%)   | 48          | 76  |
| 35  | 2d    | 173/181 (96%) | 170 (98%)  | 3 (2%)   | 68          | 88  |
| 36  | 1e    | 113/123 (92%) | 110 (97%)  | 3 (3%)   | 52          | 79  |
| 36  | 2e    | 114/123 (93%) | 112 (98%)  | 2 (2%)   | 66          | 87  |
| 37  | 1f    | 84/90 (93%)   | 84 (100%)  | 0        | 100         | 100 |
| 37  | 2f    | 85/90 (94%)   | 85 (100%)  | 0        | 100         | 100 |
| 38  | 1g    | 119/127 (94%) | 119 (100%) | 0        | 100         | 100 |
| 38  | 2g    | 120/127 (94%) | 117 (98%)  | 3 (2%)   | 55          | 81  |
| 39  | 1h    | 114/119 (96%) | 112 (98%)  | 2 (2%)   | 66          | 87  |
| 39  | 2h    | 114/119 (96%) | 113 (99%)  | 1 (1%)   | 84          | 95  |
| 40  | 1i    | 90/99 (91%)   | 86 (96%)   | 4 (4%)   | 35          | 63  |
| 40  | 2i    | 89/99 (90%)   | 85 (96%)   | 4 (4%)   | 34          | 62  |

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| Mol | Chain | Analysed         | Rotameric  | Outliers | Percentiles |     |
|-----|-------|------------------|------------|----------|-------------|-----|
| 41  | 1j    | 66/92 (72%)      | 65 (98%)   | 1 (2%)   | 72          | 90  |
| 41  | 2j    | 69/92 (75%)      | 68 (99%)   | 1 (1%)   | 74          | 90  |
| 42  | 1k    | 82/99 (83%)      | 80 (98%)   | 2 (2%)   | 57          | 82  |
| 42  | 2k    | 83/99 (84%)      | 82 (99%)   | 1 (1%)   | 78          | 92  |
| 43  | 1l    | 96/108 (89%)     | 92 (96%)   | 4 (4%)   | 36          | 65  |
| 43  | 2l    | 96/108 (89%)     | 94 (98%)   | 2 (2%)   | 61          | 85  |
| 44  | 1m    | 93/101 (92%)     | 91 (98%)   | 2 (2%)   | 60          | 83  |
| 44  | 2m    | 92/101 (91%)     | 90 (98%)   | 2 (2%)   | 60          | 83  |
| 45  | 1n    | 49/50 (98%)      | 45 (92%)   | 4 (8%)   | 14          | 27  |
| 45  | 2n    | 49/50 (98%)      | 45 (92%)   | 4 (8%)   | 14          | 27  |
| 46  | 1o    | 78/80 (98%)      | 78 (100%)  | 0        | 100         | 100 |
| 46  | 2o    | 78/80 (98%)      | 75 (96%)   | 3 (4%)   | 40          | 68  |
| 47  | 1p    | 69/74 (93%)      | 65 (94%)   | 4 (6%)   | 25          | 49  |
| 47  | 2p    | 68/74 (92%)      | 64 (94%)   | 4 (6%)   | 24          | 47  |
| 48  | 1q    | 94/97 (97%)      | 93 (99%)   | 1 (1%)   | 80          | 93  |
| 48  | 2q    | 94/97 (97%)      | 92 (98%)   | 2 (2%)   | 61          | 85  |
| 49  | 1r    | 59/77 (77%)      | 56 (95%)   | 3 (5%)   | 29          | 55  |
| 49  | 2r    | 59/77 (77%)      | 55 (93%)   | 4 (7%)   | 20          | 39  |
| 50  | 1s    | 69/80 (86%)      | 69 (100%)  | 0        | 100         | 100 |
| 50  | 2s    | 67/80 (84%)      | 67 (100%)  | 0        | 100         | 100 |
| 51  | 1t    | 70/82 (85%)      | 67 (96%)   | 3 (4%)   | 35          | 64  |
| 51  | 2t    | 70/82 (85%)      | 68 (97%)   | 2 (3%)   | 50          | 77  |
| 52  | 1u    | 18/22 (82%)      | 18 (100%)  | 0        | 100         | 100 |
| 52  | 2u    | 18/22 (82%)      | 18 (100%)  | 0        | 100         | 100 |
| All | All   | 9304/10064 (92%) | 9000 (97%) | 304 (3%) | 45          | 73  |

All (304) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | 1D    | 94  | LEU  |
| 3   | 1D    | 142 | VAL  |
| 3   | 1D    | 193 | VAL  |
| 3   | 1D    | 211 | ARG  |
| 3   | 1D    | 229 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | 1D    | 242 | ARG  |
| 3   | 1D    | 257 | LEU  |
| 4   | 1E    | 9   | VAL  |
| 4   | 1E    | 21  | VAL  |
| 4   | 1E    | 24  | THR  |
| 4   | 1E    | 77  | ILE  |
| 4   | 1E    | 116 | VAL  |
| 4   | 1E    | 144 | ARG  |
| 4   | 1E    | 170 | LEU  |
| 4   | 1E    | 181 | LEU  |
| 4   | 1E    | 184 | VAL  |
| 4   | 1E    | 195 | LEU  |
| 5   | 1F    | 28  | ILE  |
| 5   | 1F    | 33  | LEU  |
| 5   | 1F    | 53  | THR  |
| 5   | 1F    | 106 | ARG  |
| 5   | 1F    | 125 | LEU  |
| 5   | 1F    | 132 | VAL  |
| 5   | 1F    | 158 | THR  |
| 5   | 1F    | 170 | LEU  |
| 5   | 1F    | 183 | VAL  |
| 5   | 1F    | 192 | LEU  |
| 5   | 1F    | 201 | VAL  |
| 6   | 1G    | 3   | LEU  |
| 6   | 1G    | 5   | VAL  |
| 6   | 1G    | 7   | LEU  |
| 6   | 1G    | 43  | LEU  |
| 6   | 1G    | 82  | LEU  |
| 6   | 1G    | 109 | VAL  |
| 6   | 1G    | 150 | ASP  |
| 6   | 1G    | 159 | VAL  |
| 7   | 1H    | 15  | VAL  |
| 7   | 1H    | 84  | SER  |
| 7   | 1H    | 129 | THR  |
| 7   | 1H    | 152 | ARG  |
| 8   | 1I    | 47  | LEU  |
| 8   | 1I    | 57  | ARG  |
| 8   | 1I    | 92  | VAL  |
| 9   | 1N    | 33  | LEU  |
| 9   | 1N    | 34  | LEU  |
| 9   | 1N    | 35  | ARG  |
| 9   | 1N    | 48  | MET  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10  | 1O    | 10  | VAL  |
| 10  | 1O    | 24  | VAL  |
| 11  | 1P    | 65  | ARG  |
| 11  | 1P    | 83  | VAL  |
| 11  | 1P    | 95  | VAL  |
| 11  | 1P    | 106 | LEU  |
| 11  | 1P    | 147 | LEU  |
| 12  | 1Q    | 109 | VAL  |
| 13  | 1R    | 18  | LEU  |
| 13  | 1R    | 24  | GLN  |
| 13  | 1R    | 28  | LEU  |
| 13  | 1R    | 29  | LEU  |
| 13  | 1R    | 33  | ARG  |
| 13  | 1R    | 36  | THR  |
| 13  | 1R    | 44  | LEU  |
| 13  | 1R    | 54  | LEU  |
| 13  | 1R    | 65  | LEU  |
| 13  | 1R    | 100 | LEU  |
| 13  | 1R    | 111 | LEU  |
| 14  | 1S    | 14  | VAL  |
| 14  | 1S    | 52  | SER  |
| 15  | 1T    | 28  | VAL  |
| 15  | 1T    | 89  | VAL  |
| 16  | 1U    | 8   | VAL  |
| 16  | 1U    | 31  | SER  |
| 16  | 1U    | 95  | LEU  |
| 17  | 1V    | 18  | LEU  |
| 17  | 1V    | 46  | VAL  |
| 17  | 1V    | 51  | VAL  |
| 17  | 1V    | 61  | VAL  |
| 17  | 1V    | 72  | VAL  |
| 17  | 1V    | 79  | VAL  |
| 17  | 1V    | 82  | ARG  |
| 18  | 1W    | 1   | MET  |
| 18  | 1W    | 23  | LEU  |
| 18  | 1W    | 67  | ASP  |
| 18  | 1W    | 107 | LEU  |
| 19  | 1X    | 35  | THR  |
| 19  | 1X    | 76  | ARG  |
| 20  | 1Y    | 1   | MET  |
| 20  | 1Y    | 43  | ASN  |
| 20  | 1Y    | 72  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 20  | 1Y    | 97  | ARG  |
| 21  | 1Z    | 86  | VAL  |
| 21  | 1Z    | 91  | LEU  |
| 21  | 1Z    | 154 | ASP  |
| 21  | 1Z    | 171 | ILE  |
| 22  | 10    | 7   | LEU  |
| 23  | 11    | 59  | THR  |
| 24  | 12    | 19  | VAL  |
| 25  | 13    | 8   | LEU  |
| 25  | 13    | 54  | VAL  |
| 26  | 14    | 34  | GLU  |
| 26  | 14    | 49  | PHE  |
| 26  | 14    | 50  | VAL  |
| 26  | 14    | 56  | VAL  |
| 26  | 14    | 58  | ARG  |
| 26  | 14    | 63  | TYR  |
| 27  | 15    | 6   | VAL  |
| 27  | 15    | 16  | ARG  |
| 27  | 15    | 29  | THR  |
| 27  | 15    | 33  | CYS  |
| 28  | 16    | 6   | ARG  |
| 28  | 16    | 48  | VAL  |
| 29  | 17    | 24  | THR  |
| 30  | 18    | 31  | HIS  |
| 30  | 18    | 32  | LEU  |
| 33  | 1b    | 8   | LYS  |
| 33  | 1b    | 21  | ARG  |
| 33  | 1b    | 24  | TRP  |
| 33  | 1b    | 35  | GLU  |
| 33  | 1b    | 189 | ASP  |
| 33  | 1b    | 196 | LEU  |
| 34  | 1c    | 28  | GLN  |
| 34  | 1c    | 70  | VAL  |
| 34  | 1c    | 115 | LEU  |
| 35  | 1d    | 31  | CYS  |
| 35  | 1d    | 115 | ARG  |
| 35  | 1d    | 135 | LEU  |
| 35  | 1d    | 158 | ILE  |
| 35  | 1d    | 200 | GLU  |
| 36  | 1e    | 12  | LEU  |
| 36  | 1e    | 31  | LEU  |
| 36  | 1e    | 41  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 39  | 1h    | 51  | VAL  |
| 39  | 1h    | 112 | LEU  |
| 40  | 1i    | 42  | ARG  |
| 40  | 1i    | 50  | LEU  |
| 40  | 1i    | 65  | VAL  |
| 40  | 1i    | 108 | VAL  |
| 41  | 1j    | 92  | THR  |
| 42  | 1k    | 31  | THR  |
| 42  | 1k    | 114 | VAL  |
| 43  | 1l    | 27  | LEU  |
| 43  | 1l    | 83  | VAL  |
| 43  | 1l    | 84  | LEU  |
| 43  | 1l    | 123 | LYS  |
| 44  | 1m    | 4   | ILE  |
| 44  | 1m    | 109 | THR  |
| 45  | 1n    | 3   | ARG  |
| 45  | 1n    | 6   | LEU  |
| 45  | 1n    | 18  | VAL  |
| 45  | 1n    | 22  | THR  |
| 47  | 1p    | 2   | VAL  |
| 47  | 1p    | 20  | VAL  |
| 47  | 1p    | 54  | GLU  |
| 47  | 1p    | 67  | THR  |
| 48  | 1q    | 78  | GLU  |
| 49  | 1r    | 26  | LEU  |
| 49  | 1r    | 31  | LEU  |
| 49  | 1r    | 47  | THR  |
| 51  | 1t    | 10  | LEU  |
| 51  | 1t    | 13  | LEU  |
| 51  | 1t    | 62  | LEU  |
| 3   | 2D    | 3   | VAL  |
| 3   | 2D    | 94  | LEU  |
| 3   | 2D    | 103 | ARG  |
| 3   | 2D    | 142 | VAL  |
| 3   | 2D    | 193 | VAL  |
| 3   | 2D    | 211 | ARG  |
| 3   | 2D    | 229 | VAL  |
| 3   | 2D    | 242 | ARG  |
| 4   | 2E    | 9   | VAL  |
| 4   | 2E    | 12  | THR  |
| 4   | 2E    | 21  | VAL  |
| 4   | 2E    | 47  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | 2E    | 52  | LEU  |
| 4   | 2E    | 75  | VAL  |
| 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    | 195 | LEU  |
| 5   | 2F    | 33  | LEU  |
| 5   | 2F    | 53  | THR  |
| 5   | 2F    | 70  | THR  |
| 5   | 2F    | 88  | VAL  |
| 5   | 2F    | 93  | LYS  |
| 5   | 2F    | 106 | ARG  |
| 5   | 2F    | 158 | THR  |
| 5   | 2F    | 170 | LEU  |
| 5   | 2F    | 183 | VAL  |
| 5   | 2F    | 192 | LEU  |
| 6   | 2G    | 3   | LEU  |
| 6   | 2G    | 21  | ARG  |
| 6   | 2G    | 43  | LEU  |
| 6   | 2G    | 49  | ASP  |
| 6   | 2G    | 60  | LEU  |
| 6   | 2G    | 79  | ASN  |
| 6   | 2G    | 140 | ILE  |
| 6   | 2G    | 159 | VAL  |
| 7   | 2H    | 63  | SER  |
| 7   | 2H    | 125 | VAL  |
| 7   | 2H    | 136 | ILE  |
| 7   | 2H    | 152 | ARG  |
| 8   | 2I    | 20  | ASP  |
| 8   | 2I    | 47  | LEU  |
| 8   | 2I    | 92  | VAL  |
| 9   | 2N    | 32  | THR  |
| 9   | 2N    | 33  | LEU  |
| 9   | 2N    | 34  | LEU  |
| 10  | 2O    | 24  | VAL  |
| 11  | 2P    | 95  | VAL  |
| 11  | 2P    | 147 | LEU  |
| 12  | 2Q    | 1   | MET  |
| 12  | 2Q    | 109 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 13  | 2R    | 18  | LEU  |
| 13  | 2R    | 24  | GLN  |
| 13  | 2R    | 29  | LEU  |
| 13  | 2R    | 33  | ARG  |
| 13  | 2R    | 44  | LEU  |
| 13  | 2R    | 60  | LEU  |
| 13  | 2R    | 65  | LEU  |
| 13  | 2R    | 79  | LEU  |
| 13  | 2R    | 100 | LEU  |
| 14  | 2S    | 8   | GLU  |
| 14  | 2S    | 14  | VAL  |
| 14  | 2S    | 52  | SER  |
| 15  | 2T    | 89  | VAL  |
| 16  | 2U    | 31  | SER  |
| 17  | 2V    | 18  | LEU  |
| 17  | 2V    | 46  | VAL  |
| 17  | 2V    | 72  | VAL  |
| 17  | 2V    | 79  | VAL  |
| 18  | 2W    | 1   | MET  |
| 18  | 2W    | 67  | ASP  |
| 18  | 2W    | 107 | LEU  |
| 19  | 2X    | 35  | THR  |
| 19  | 2X    | 65  | ARG  |
| 20  | 2Y    | 43  | ASN  |
| 21  | 2Z    | 142 | SER  |
| 21  | 2Z    | 154 | ASP  |
| 21  | 2Z    | 161 | VAL  |
| 24  | 22    | 52  | ASP  |
| 24  | 22    | 66  | GLU  |
| 25  | 23    | 8   | LEU  |
| 25  | 23    | 30  | ARG  |
| 26  | 24    | 34  | GLU  |
| 26  | 24    | 48  | ARG  |
| 26  | 24    | 50  | VAL  |
| 26  | 24    | 56  | VAL  |
| 27  | 25    | 6   | VAL  |
| 27  | 25    | 16  | ARG  |
| 27  | 25    | 35  | GLU  |
| 28  | 26    | 6   | ARG  |
| 28  | 26    | 48  | VAL  |
| 28  | 26    | 52  | VAL  |
| 29  | 27    | 1   | MET  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 30  | 28    | 31  | HIS  |
| 30  | 28    | 32  | LEU  |
| 31  | 29    | 4   | ARG  |
| 31  | 29    | 7   | VAL  |
| 33  | 2b    | 35  | GLU  |
| 33  | 2b    | 128 | GLU  |
| 33  | 2b    | 189 | ASP  |
| 33  | 2b    | 215 | LEU  |
| 34  | 2c    | 70  | VAL  |
| 35  | 2d    | 135 | LEU  |
| 35  | 2d    | 170 | VAL  |
| 35  | 2d    | 194 | LEU  |
| 36  | 2e    | 12  | LEU  |
| 36  | 2e    | 41  | VAL  |
| 38  | 2g    | 72  | ARG  |
| 38  | 2g    | 79  | ARG  |
| 38  | 2g    | 104 | LEU  |
| 39  | 2h    | 51  | VAL  |
| 40  | 2i    | 50  | LEU  |
| 40  | 2i    | 65  | VAL  |
| 40  | 2i    | 89  | ASN  |
| 40  | 2i    | 102 | LEU  |
| 41  | 2j    | 89  | ASP  |
| 42  | 2k    | 114 | VAL  |
| 43  | 2l    | 27  | LEU  |
| 43  | 2l    | 84  | LEU  |
| 44  | 2m    | 47  | ASP  |
| 44  | 2m    | 117 | VAL  |
| 45  | 2n    | 3   | ARG  |
| 45  | 2n    | 6   | LEU  |
| 45  | 2n    | 18  | VAL  |
| 45  | 2n    | 22  | THR  |
| 46  | 2o    | 7   | GLU  |
| 46  | 2o    | 21  | ASP  |
| 46  | 2o    | 39  | LEU  |
| 47  | 2p    | 2   | VAL  |
| 47  | 2p    | 5   | ARG  |
| 47  | 2p    | 20  | VAL  |
| 47  | 2p    | 62  | VAL  |
| 48  | 2q    | 9   | VAL  |
| 48  | 2q    | 63  | ARG  |
| 49  | 2r    | 26  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 49  | 2r    | 47  | THR  |
| 49  | 2r    | 76  | LEU  |
| 49  | 2r    | 85  | LEU  |
| 51  | 2t    | 62  | LEU  |
| 51  | 2t    | 89  | ARG  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (100) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | 1D    | 87  | ASN  |
| 3   | 1D    | 126 | GLN  |
| 4   | 1E    | 48  | GLN  |
| 5   | 1F    | 8   | GLN  |
| 5   | 1F    | 69  | HIS  |
| 6   | 1G    | 41  | GLN  |
| 8   | 1I    | 104 | GLN  |
| 15  | 1T    | 58  | ASN  |
| 15  | 1T    | 123 | GLN  |
| 16  | 1U    | 81  | HIS  |
| 19  | 1X    | 31  | HIS  |
| 19  | 1X    | 82  | GLN  |
| 20  | 1Y    | 43  | ASN  |
| 21  | 1Z    | 73  | GLN  |
| 22  | 10    | 3   | HIS  |
| 24  | 12    | 9   | GLN  |
| 24  | 12    | 65  | ASN  |
| 25  | 13    | 32  | GLN  |
| 33  | 1b    | 40  | HIS  |
| 34  | 1c    | 6   | HIS  |
| 34  | 1c    | 37  | GLN  |
| 34  | 1c    | 162 | GLN  |
| 35  | 1d    | 42  | GLN  |
| 35  | 1d    | 77  | ASN  |
| 35  | 1d    | 116 | GLN  |
| 35  | 1d    | 123 | HIS  |
| 35  | 1d    | 161 | ASN  |
| 37  | 1f    | 100 | ASN  |
| 38  | 1g    | 28  | ASN  |
| 38  | 1g    | 86  | GLN  |
| 40  | 1i    | 3   | GLN  |
| 40  | 1i    | 31  | GLN  |
| 40  | 1i    | 34  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 40  | 1i    | 58  | HIS  |
| 40  | 1i    | 89  | ASN  |
| 41  | 1j    | 56  | HIS  |
| 43  | 1l    | 99  | HIS  |
| 45  | 1n    | 49  | HIS  |
| 47  | 1p    | 13  | HIS  |
| 50  | 1s    | 23  | ASN  |
| 50  | 1s    | 47  | HIS  |
| 50  | 1s    | 69  | HIS  |
| 50  | 1s    | 83  | HIS  |
| 51  | 1t    | 75  | ASN  |
| 3   | 2D    | 87  | ASN  |
| 3   | 2D    | 116 | GLN  |
| 4   | 2E    | 48  | GLN  |
| 5   | 2F    | 69  | HIS  |
| 6   | 2G    | 26  | GLN  |
| 8   | 2I    | 104 | GLN  |
| 9   | 2N    | 38  | HIS  |
| 9   | 2N    | 131 | GLN  |
| 9   | 2N    | 133 | GLN  |
| 10  | 2O    | 3   | GLN  |
| 12  | 2Q    | 12  | GLN  |
| 12  | 2Q    | 13  | GLN  |
| 14  | 2S    | 38  | GLN  |
| 14  | 2S    | 68  | GLN  |
| 15  | 2T    | 58  | ASN  |
| 15  | 2T    | 123 | GLN  |
| 16  | 2U    | 81  | HIS  |
| 17  | 2V    | 64  | HIS  |
| 18  | 2W    | 60  | ASN  |
| 19  | 2X    | 31  | HIS  |
| 19  | 2X    | 82  | GLN  |
| 20  | 2Y    | 43  | ASN  |
| 21  | 2Z    | 55  | HIS  |
| 21  | 2Z    | 73  | GLN  |
| 21  | 2Z    | 132 | ASN  |
| 23  | 21    | 56  | GLN  |
| 24  | 22    | 65  | ASN  |
| 26  | 24    | 46  | GLN  |
| 31  | 29    | 20  | HIS  |
| 33  | 2b    | 40  | HIS  |
| 33  | 2b    | 95  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 34  | 2c    | 6   | HIS  |
| 34  | 2c    | 37  | GLN  |
| 34  | 2c    | 139 | GLN  |
| 34  | 2c    | 162 | GLN  |
| 35  | 2d    | 42  | GLN  |
| 35  | 2d    | 77  | ASN  |
| 35  | 2d    | 116 | GLN  |
| 35  | 2d    | 123 | HIS  |
| 35  | 2d    | 125 | HIS  |
| 35  | 2d    | 161 | ASN  |
| 36  | 2e    | 20  | GLN  |
| 36  | 2e    | 78  | HIS  |
| 37  | 2f    | 13  | ASN  |
| 37  | 2f    | 100 | ASN  |
| 38  | 2g    | 28  | ASN  |
| 39  | 2h    | 78  | GLN  |
| 40  | 2i    | 3   | GLN  |
| 40  | 2i    | 31  | GLN  |
| 40  | 2i    | 58  | HIS  |
| 40  | 2i    | 89  | ASN  |
| 42  | 2k    | 22  | HIS  |
| 46  | 2o    | 28  | GLN  |
| 47  | 2p    | 13  | HIS  |
| 50  | 2s    | 83  | HIS  |
| 51  | 2t    | 42  | GLN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1   | 1A    | 2861/2915 (98%) | 440 (15%)         | 33 (1%)         |
| 1   | 2A    | 2788/2915 (95%) | 516 (18%)         | 30 (1%)         |
| 2   | 1B    | 120/121 (99%)   | 8 (6%)            | 1 (0%)          |
| 2   | 2B    | 118/121 (97%)   | 36 (30%)          | 0               |
| 32  | 1a    | 1494/1521 (98%) | 226 (15%)         | 0               |
| 32  | 2a    | 1498/1521 (98%) | 240 (16%)         | 0               |
| 53  | 1v    | 12/27 (44%)     | 3 (25%)           | 0               |
| 53  | 2v    | 12/27 (44%)     | 3 (25%)           | 0               |
| 54  | 1w    | 70/76 (92%)     | 18 (25%)          | 0               |
| 54  | 1y    | 71/76 (93%)     | 23 (32%)          | 0               |
| 54  | 2w    | 69/76 (90%)     | 20 (28%)          | 0               |
| 54  | 2y    | 69/76 (90%)     | 17 (24%)          | 0               |

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| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 55  | 1x    | 74/77 (96%)     | 9 (12%)           | 0               |
| 55  | 2x    | 74/77 (96%)     | 8 (10%)           | 0               |
| All | All   | 9330/9626 (96%) | 1567 (16%)        | 64 (0%)         |

All (1567) RNA backbone outliers are listed below:

| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | 1A    | 10     | G    |
| 1   | 1A    | 12     | U    |
| 1   | 1A    | 13     | A    |
| 1   | 1A    | 34     | C    |
| 1   | 1A    | 45     | C    |
| 1   | 1A    | 55     | G    |
| 1   | 1A    | 58     | G    |
| 1   | 1A    | 71     | A    |
| 1   | 1A    | 74     | A    |
| 1   | 1A    | 75     | G    |
| 1   | 1A    | 83     | G    |
| 1   | 1A    | 84     | A    |
| 1   | 1A    | 95     | G    |
| 1   | 1A    | 118    | A    |
| 1   | 1A    | 119    | A    |
| 1   | 1A    | 120    | U    |
| 1   | 1A    | 182    | A    |
| 1   | 1A    | 196    | A    |
| 1   | 1A    | 199    | A    |
| 1   | 1A    | 205    | G    |
| 1   | 1A    | 214    | G    |
| 1   | 1A    | 215    | G    |
| 1   | 1A    | 216    | A    |
| 1   | 1A    | 222    | A    |
| 1   | 1A    | 223    | A    |
| 1   | 1A    | 229    | A    |
| 1   | 1A    | 232    | G    |
| 1   | 1A    | 233    | A    |
| 1   | 1A    | 248    | G    |
| 1   | 1A    | 250    | G    |
| 1   | 1A    | 267    | C    |
| 1   | 1A    | 269    | U    |
| 1   | 1A    | 271(E) | U    |
| 1   | 1A    | 271(L) | U    |
| 1   | 1A    | 271(M) | G    |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | 1A    | 271(S) | G    |
| 1   | 1A    | 272(B) | G    |
| 1   | 1A    | 272(J) | C    |
| 1   | 1A    | 275    | G    |
| 1   | 1A    | 279    | C    |
| 1   | 1A    | 282    | A    |
| 1   | 1A    | 311    | A    |
| 1   | 1A    | 329    | G    |
| 1   | 1A    | 330    | A    |
| 1   | 1A    | 352    | G    |
| 1   | 1A    | 360    | G    |
| 1   | 1A    | 362    | U    |
| 1   | 1A    | 363    | G    |
| 1   | 1A    | 363(B) | G    |
| 1   | 1A    | 370    | G    |
| 1   | 1A    | 372    | G    |
| 1   | 1A    | 380    | U    |
| 1   | 1A    | 386    | G    |
| 1   | 1A    | 390    | A    |
| 1   | 1A    | 396    | G    |
| 1   | 1A    | 405    | U    |
| 1   | 1A    | 411    | G    |
| 1   | 1A    | 428    | A    |
| 1   | 1A    | 444    | C    |
| 1   | 1A    | 448    | U    |
| 1   | 1A    | 451    | C    |
| 1   | 1A    | 455    | C    |
| 1   | 1A    | 456    | C    |
| 1   | 1A    | 457    | A    |
| 1   | 1A    | 481    | G    |
| 1   | 1A    | 504    | U    |
| 1   | 1A    | 505    | A    |
| 1   | 1A    | 508    | G    |
| 1   | 1A    | 509    | C    |
| 1   | 1A    | 512    | G    |
| 1   | 1A    | 530    | G    |
| 1   | 1A    | 531    | C    |
| 1   | 1A    | 532    | A    |
| 1   | 1A    | 533    | G    |
| 1   | 1A    | 545    | G    |
| 1   | 1A    | 549    | G    |
| 1   | 1A    | 563    | G    |

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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    | 669    | G    |
| 1   | 1A    | 686    | G    |
| 1   | 1A    | 717    | G    |
| 1   | 1A    | 730    | C    |
| 1   | 1A    | 764    | A    |
| 1   | 1A    | 776    | G    |
| 1   | 1A    | 782    | A    |
| 1   | 1A    | 784    | A    |
| 1   | 1A    | 785    | G    |
| 1   | 1A    | 792    | G    |
| 1   | 1A    | 805    | G    |
| 1   | 1A    | 812    | C    |
| 1   | 1A    | 819    | A    |
| 1   | 1A    | 827    | U    |
| 1   | 1A    | 828    | U    |
| 1   | 1A    | 830    | G    |
| 1   | 1A    | 859    | G    |
| 1   | 1A    | 866    | A    |
| 1   | 1A    | 879    | G    |
| 1   | 1A    | 880    | G    |
| 1   | 1A    | 884    | C    |
| 1   | 1A    | 885    | C    |
| 1   | 1A    | 886    | C    |
| 1   | 1A    | 887    | A    |
| 1   | 1A    | 888    | C    |
| 1   | 1A    | 889    | C    |
| 1   | 1A    | 890    | A    |
| 1   | 1A    | 892    | G    |
| 1   | 1A    | 895    | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 1A    | 896  | A    |
| 1   | 1A    | 897  | C    |
| 1   | 1A    | 899  | A    |
| 1   | 1A    | 907  | U    |
| 1   | 1A    | 910  | A    |
| 1   | 1A    | 932  | G    |
| 1   | 1A    | 938  | G    |
| 1   | 1A    | 941  | A    |
| 1   | 1A    | 945  | A    |
| 1   | 1A    | 946  | G    |
| 1   | 1A    | 953  | A    |
| 1   | 1A    | 959  | A    |
| 1   | 1A    | 961  | C    |
| 1   | 1A    | 974  | G    |
| 1   | 1A    | 975  | C    |
| 1   | 1A    | 983  | A    |
| 1   | 1A    | 996  | A    |
| 1   | 1A    | 1005 | C    |
| 1   | 1A    | 1008 | C    |
| 1   | 1A    | 1012 | U    |
| 1   | 1A    | 1013 | C    |
| 1   | 1A    | 1022 | G    |
| 1   | 1A    | 1026 | U    |
| 1   | 1A    | 1033 | U    |
| 1   | 1A    | 1041 | C    |
| 1   | 1A    | 1045 | A    |
| 1   | 1A    | 1046 | A    |
| 1   | 1A    | 1047 | G    |
| 1   | 1A    | 1048 | A    |
| 1   | 1A    | 1051 | G    |
| 1   | 1A    | 1054 | A    |
| 1   | 1A    | 1055 | G    |
| 1   | 1A    | 1058 | G    |
| 1   | 1A    | 1067 | A    |
| 1   | 1A    | 1068 | G    |
| 1   | 1A    | 1071 | G    |
| 1   | 1A    | 1073 | A    |
| 1   | 1A    | 1074 | G    |
| 1   | 1A    | 1075 | C    |
| 1   | 1A    | 1076 | C    |
| 1   | 1A    | 1077 | A    |
| 1   | 1A    | 1078 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 1A    | 1079 | C    |
| 1   | 1A    | 1080 | C    |
| 1   | 1A    | 1085 | A    |
| 1   | 1A    | 1086 | A    |
| 1   | 1A    | 1088 | A    |
| 1   | 1A    | 1089 | G    |
| 1   | 1A    | 1090 | U    |
| 1   | 1A    | 1091 | G    |
| 1   | 1A    | 1094 | U    |
| 1   | 1A    | 1097 | U    |
| 1   | 1A    | 1098 | A    |
| 1   | 1A    | 1100 | C    |
| 1   | 1A    | 1101 | U    |
| 1   | 1A    | 1105 | U    |
| 1   | 1A    | 1107 | G    |
| 1   | 1A    | 1108 | U    |
| 1   | 1A    | 1109 | C    |
| 1   | 1A    | 1110 | G    |
| 1   | 1A    | 1111 | A    |
| 1   | 1A    | 1112 | 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    | 1149 | G    |
| 1   | 1A    | 1155 | A    |
| 1   | 1A    | 1170 | G    |
| 1   | 1A    | 1171 | G    |
| 1   | 1A    | 1173 | G    |
| 1   | 1A    | 1174 | A    |
| 1   | 1A    | 1175 | U    |
| 1   | 1A    | 1176 | G    |
| 1   | 1A    | 1177 | A    |
| 1   | 1A    | 1210 | A    |
| 1   | 1A    | 1211 | U    |
| 1   | 1A    | 1220 | A    |
| 1   | 1A    | 1241 | A    |
| 1   | 1A    | 1244 | G    |
| 1   | 1A    | 1253 | A    |
| 1   | 1A    | 1256 | G    |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 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    | 1306    | C    |
| 1   | 1A    | 1313    | U    |
| 1   | 1A    | 1318    | C    |
| 1   | 1A    | 1320    | C    |
| 1   | 1A    | 1352    | U    |
| 1   | 1A    | 1359    | A    |
| 1   | 1A    | 1360    | A    |
| 1   | 1A    | 1365    | A    |
| 1   | 1A    | 1380    | G    |
| 1   | 1A    | 1384    | A    |
| 1   | 1A    | 1385    | G    |
| 1   | 1A    | 1386    | C    |
| 1   | 1A    | 1395    | A    |
| 1   | 1A    | 1403    | C    |
| 1   | 1A    | 1416    | G    |
| 1   | 1A    | 1417    | C    |
| 1   | 1A    | 1420    | U    |
| 1   | 1A    | 1421    | G    |
| 1   | 1A    | 1428    | C    |
| 1   | 1A    | 1445    | A    |
| 1   | 1A    | 1450    | G    |
| 1   | 1A    | 1455    | G    |
| 1   | 1A    | 1461    | G    |
| 1   | 1A    | 1467    | C    |
| 1   | 1A    | 1471    | A    |
| 1   | 1A    | 1482    | G    |
| 1   | 1A    | 1484    | G    |
| 1   | 1A    | 1493    | C    |
| 1   | 1A    | 1508    | A    |
| 1   | 1A    | 1509    | C    |
| 1   | 1A    | 1509(A) | A    |
| 1   | 1A    | 1509(B) | A    |
| 1   | 1A    | 1513    | C    |
| 1   | 1A    | 1514    | U    |
| 1   | 1A    | 1531    | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 1A    | 1554 | A    |
| 1   | 1A    | 1558 | A    |
| 1   | 1A    | 1566 | A    |
| 1   | 1A    | 1569 | A    |
| 1   | 1A    | 1578 | U    |
| 1   | 1A    | 1580 | A    |
| 1   | 1A    | 1581 | G    |
| 1   | 1A    | 1584 | C    |
| 1   | 1A    | 1586 | A    |
| 1   | 1A    | 1608 | A    |
| 1   | 1A    | 1609 | A    |
| 1   | 1A    | 1610 | A    |
| 1   | 1A    | 1646 | C    |
| 1   | 1A    | 1647 | G    |
| 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    | 1703 | G    |
| 1   | 1A    | 1722 | A    |
| 1   | 1A    | 1739 | U    |
| 1   | 1A    | 1746 | G    |
| 1   | 1A    | 1756 | G    |
| 1   | 1A    | 1762 | A    |
| 1   | 1A    | 1763 | G    |
| 1   | 1A    | 1764 | G    |
| 1   | 1A    | 1773 | A    |
| 1   | 1A    | 1780 | A    |
| 1   | 1A    | 1782 | C    |
| 1   | 1A    | 1791 | A    |
| 1   | 1A    | 1800 | C    |
| 1   | 1A    | 1801 | G    |
| 1   | 1A    | 1816 | G    |
| 1   | 1A    | 1817 | G    |
| 1   | 1A    | 1828 | G    |
| 1   | 1A    | 1829 | A    |
| 1   | 1A    | 1847 | A    |
| 1   | 1A    | 1861 | G    |
| 1   | 1A    | 1877 | A    |
| 1   | 1A    | 1878 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 1A    | 1900 | A    |
| 1   | 1A    | 1906 | G    |
| 1   | 1A    | 1929 | G    |
| 1   | 1A    | 1930 | G    |
| 1   | 1A    | 1937 | A    |
| 1   | 1A    | 1938 | A    |
| 1   | 1A    | 1955 | U    |
| 1   | 1A    | 1963 | U    |
| 1   | 1A    | 1967 | C    |
| 1   | 1A    | 1970 | A    |
| 1   | 1A    | 1971 | A    |
| 1   | 1A    | 1972 | A    |
| 1   | 1A    | 1993 | U    |
| 1   | 1A    | 1997 | G    |
| 1   | 1A    | 2023 | G    |
| 1   | 1A    | 2031 | A    |
| 1   | 1A    | 2032 | G    |
| 1   | 1A    | 2033 | A    |
| 1   | 1A    | 2043 | C    |
| 1   | 1A    | 2055 | C    |
| 1   | 1A    | 2056 | G    |
| 1   | 1A    | 2060 | A    |
| 1   | 1A    | 2061 | G    |
| 1   | 1A    | 2069 | G    |
| 1   | 1A    | 2093 | G    |
| 1   | 1A    | 2096 | U    |
| 1   | 1A    | 2098 | U    |
| 1   | 1A    | 2101 | G    |
| 1   | 1A    | 2110 | G    |
| 1   | 1A    | 2113 | U    |
| 1   | 1A    | 2116 | G    |
| 1   | 1A    | 2119 | A    |
| 1   | 1A    | 2121 | G    |
| 1   | 1A    | 2122 | U    |
| 1   | 1A    | 2126 | A    |
| 1   | 1A    | 2127 | G    |
| 1   | 1A    | 2131 | G    |
| 1   | 1A    | 2132 | U    |
| 1   | 1A    | 2133 | G    |
| 1   | 1A    | 2134 | A    |
| 1   | 1A    | 2135 | A    |
| 1   | 1A    | 2139 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 1A    | 2140 | C    |
| 1   | 1A    | 2142 | C    |
| 1   | 1A    | 2146 | C    |
| 1   | 1A    | 2147 | G    |
| 1   | 1A    | 2151 | G    |
| 1   | 1A    | 2156 | G    |
| 1   | 1A    | 2157 | G    |
| 1   | 1A    | 2159 | G    |
| 1   | 1A    | 2165 | G    |
| 1   | 1A    | 2166 | G    |
| 1   | 1A    | 2171 | A    |
| 1   | 1A    | 2172 | U    |
| 1   | 1A    | 2173 | A    |
| 1   | 1A    | 2178 | C    |
| 1   | 1A    | 2181 | G    |
| 1   | 1A    | 2182 | G    |
| 1   | 1A    | 2184 | G    |
| 1   | 1A    | 2188 | C    |
| 1   | 1A    | 2192 | G    |
| 1   | 1A    | 2198 | A    |
| 1   | 1A    | 2206 | G    |
| 1   | 1A    | 2207 | G    |
| 1   | 1A    | 2225 | A    |
| 1   | 1A    | 2238 | G    |
| 1   | 1A    | 2239 | G    |
| 1   | 1A    | 2268 | A    |
| 1   | 1A    | 2269 | A    |
| 1   | 1A    | 2273 | A    |
| 1   | 1A    | 2283 | C    |
| 1   | 1A    | 2287 | A    |
| 1   | 1A    | 2289 | G    |
| 1   | 1A    | 2305 | A    |
| 1   | 1A    | 2307 | G    |
| 1   | 1A    | 2308 | G    |
| 1   | 1A    | 2314 | C    |
| 1   | 1A    | 2320 | A    |
| 1   | 1A    | 2325 | G    |
| 1   | 1A    | 2334 | G    |
| 1   | 1A    | 2336 | A    |
| 1   | 1A    | 2347 | C    |
| 1   | 1A    | 2350 | C    |
| 1   | 1A    | 2361 | A    |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 1   | 1A    | 2372    | G    |
| 1   | 1A    | 2383    | G    |
| 1   | 1A    | 2385    | C    |
| 1   | 1A    | 2406    | U    |
| 1   | 1A    | 2410    | G    |
| 1   | 1A    | 2414    | G    |
| 1   | 1A    | 2425    | A    |
| 1   | 1A    | 2429    | G    |
| 1   | 1A    | 2430    | A    |
| 1   | 1A    | 2435    | A    |
| 1   | 1A    | 2439    | A    |
| 1   | 1A    | 2441    | C    |
| 1   | 1A    | 2448    | A    |
| 1   | 1A    | 2468    | G    |
| 1   | 1A    | 2476    | A    |
| 1   | 1A    | 2487    | G    |
| 1   | 1A    | 2491    | U    |
| 1   | 1A    | 2498    | C    |
| 1   | 1A    | 2502    | G    |
| 1   | 1A    | 2505    | G    |
| 1   | 1A    | 2506    | U    |
| 1   | 1A    | 2518    | A    |
| 1   | 1A    | 2529    | G    |
| 1   | 1A    | 2554    | U    |
| 1   | 1A    | 2566    | A    |
| 1   | 1A    | 2567    | G    |
| 1   | 1A    | 2572    | A    |
| 1   | 1A    | 2573    | C    |
| 1   | 1A    | 2602    | A    |
| 1   | 1A    | 2609    | U    |
| 1   | 1A    | 2611    | U    |
| 1   | 1A    | 2612    | C    |
| 1   | 1A    | 2629    | A    |
| 1   | 1A    | 2630    | G    |
| 1   | 1A    | 2637    | U    |
| 1   | 1A    | 2654    | A    |
| 1   | 1A    | 2686    | G    |
| 1   | 1A    | 2689    | U    |
| 1   | 1A    | 2690    | C    |
| 1   | 1A    | 2691    | C    |
| 1   | 1A    | 2703    | C    |
| 1   | 1A    | 2712(A) | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 1A    | 2713 | A    |
| 1   | 1A    | 2714 | G    |
| 1   | 1A    | 2721 | A    |
| 1   | 1A    | 2726 | U    |
| 1   | 1A    | 2733 | A    |
| 1   | 1A    | 2757 | A    |
| 1   | 1A    | 2758 | A    |
| 1   | 1A    | 2761 | G    |
| 1   | 1A    | 2765 | A    |
| 1   | 1A    | 2766 | G    |
| 1   | 1A    | 2778 | A    |
| 1   | 1A    | 2780 | G    |
| 1   | 1A    | 2790 | A    |
| 1   | 1A    | 2791 | C    |
| 1   | 1A    | 2793 | G    |
| 1   | 1A    | 2794 | C    |
| 1   | 1A    | 2802 | G    |
| 1   | 1A    | 2805 | G    |
| 1   | 1A    | 2808 | U    |
| 1   | 1A    | 2820 | A    |
| 1   | 1A    | 2821 | A    |
| 1   | 1A    | 2834 | G    |
| 1   | 1A    | 2835 | A    |
| 1   | 1A    | 2872 | G    |
| 1   | 1A    | 2880 | C    |
| 1   | 1A    | 2892 | A    |
| 1   | 1A    | 2894 | G    |
| 2   | 1B    | 2    | C    |
| 2   | 1B    | 25   | A    |
| 2   | 1B    | 35   | U    |
| 2   | 1B    | 45   | A    |
| 2   | 1B    | 56   | G    |
| 2   | 1B    | 67   | G    |
| 2   | 1B    | 73   | A    |
| 2   | 1B    | 110  | G    |
| 32  | 1a    | 7    | G    |
| 32  | 1a    | 9    | G    |
| 32  | 1a    | 32   | A    |
| 32  | 1a    | 39   | G    |
| 32  | 1a    | 47   | C    |
| 32  | 1a    | 48   | C    |
| 32  | 1a    | 51   | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 32  | 1a    | 54  | C    |
| 32  | 1a    | 61  | G    |
| 32  | 1a    | 78  | G    |
| 32  | 1a    | 91  | C    |
| 32  | 1a    | 96  | U    |
| 32  | 1a    | 98  | G    |
| 32  | 1a    | 101 | A    |
| 32  | 1a    | 116 | A    |
| 32  | 1a    | 121 | C    |
| 32  | 1a    | 131 | C    |
| 32  | 1a    | 146 | G    |
| 32  | 1a    | 159 | G    |
| 32  | 1a    | 163 | C    |
| 32  | 1a    | 174 | C    |
| 32  | 1a    | 180 | U    |
| 32  | 1a    | 182 | U    |
| 32  | 1a    | 195 | A    |
| 32  | 1a    | 197 | A    |
| 32  | 1a    | 202 | U    |
| 32  | 1a    | 203 | U    |
| 32  | 1a    | 204 | U    |
| 32  | 1a    | 216 | G    |
| 32  | 1a    | 217 | C    |
| 32  | 1a    | 243 | A    |
| 32  | 1a    | 247 | G    |
| 32  | 1a    | 251 | G    |
| 32  | 1a    | 258 | G    |
| 32  | 1a    | 266 | G    |
| 32  | 1a    | 267 | C    |
| 32  | 1a    | 289 | G    |
| 32  | 1a    | 321 | A    |
| 32  | 1a    | 328 | C    |
| 32  | 1a    | 332 | G    |
| 32  | 1a    | 344 | A    |
| 32  | 1a    | 352 | C    |
| 32  | 1a    | 353 | A    |
| 32  | 1a    | 354 | G    |
| 32  | 1a    | 367 | U    |
| 32  | 1a    | 372 | C    |
| 32  | 1a    | 373 | A    |
| 32  | 1a    | 384 | G    |
| 32  | 1a    | 397 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 32  | 1a    | 398 | C    |
| 32  | 1a    | 406 | G    |
| 32  | 1a    | 412 | A    |
| 32  | 1a    | 424 | G    |
| 32  | 1a    | 429 | U    |
| 32  | 1a    | 441 | A    |
| 32  | 1a    | 442 | C    |
| 32  | 1a    | 452 | A    |
| 32  | 1a    | 461 | A    |
| 32  | 1a    | 470 | 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    | 518 | C    |
| 32  | 1a    | 527 | 7MG  |
| 32  | 1a    | 531 | U    |
| 32  | 1a    | 532 | A    |
| 32  | 1a    | 533 | A    |
| 32  | 1a    | 547 | A    |
| 32  | 1a    | 559 | A    |
| 32  | 1a    | 561 | U    |
| 32  | 1a    | 562 | C    |
| 32  | 1a    | 568 | G    |
| 32  | 1a    | 572 | A    |
| 32  | 1a    | 573 | A    |
| 32  | 1a    | 576 | G    |
| 32  | 1a    | 577 | G    |
| 32  | 1a    | 596 | C    |
| 32  | 1a    | 630 | G    |
| 32  | 1a    | 653 | A    |
| 32  | 1a    | 665 | A    |
| 32  | 1a    | 673 | G    |
| 32  | 1a    | 687 | A    |
| 32  | 1a    | 688 | G    |
| 32  | 1a    | 695 | A    |
| 32  | 1a    | 702 | A    |
| 32  | 1a    | 723 | U    |
| 32  | 1a    | 731 | G    |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 32  | 1a    | 749     | C    |
| 32  | 1a    | 755     | G    |
| 32  | 1a    | 759     | A    |
| 32  | 1a    | 773     | G    |
| 32  | 1a    | 777     | A    |
| 32  | 1a    | 792     | A    |
| 32  | 1a    | 793     | U    |
| 32  | 1a    | 794     | A    |
| 32  | 1a    | 815     | A    |
| 32  | 1a    | 816     | A    |
| 32  | 1a    | 817     | C    |
| 32  | 1a    | 821     | G    |
| 32  | 1a    | 828     | A    |
| 32  | 1a    | 840     | C    |
| 32  | 1a    | 841     | U    |
| 32  | 1a    | 851     | G    |
| 32  | 1a    | 859     | A    |
| 32  | 1a    | 870     | U    |
| 32  | 1a    | 885     | G    |
| 32  | 1a    | 902     | G    |
| 32  | 1a    | 914     | A    |
| 32  | 1a    | 926     | G    |
| 32  | 1a    | 927     | G    |
| 32  | 1a    | 931     | C    |
| 32  | 1a    | 934     | C    |
| 32  | 1a    | 960     | U    |
| 32  | 1a    | 961     | U    |
| 32  | 1a    | 968     | A    |
| 32  | 1a    | 969     | A    |
| 32  | 1a    | 971     | G    |
| 32  | 1a    | 972     | C    |
| 32  | 1a    | 974     | A    |
| 32  | 1a    | 975     | A    |
| 32  | 1a    | 976     | G    |
| 32  | 1a    | 977     | A    |
| 32  | 1a    | 992     | U    |
| 32  | 1a    | 993     | G    |
| 32  | 1a    | 1001    | A    |
| 32  | 1a    | 1001(A) | G    |
| 32  | 1a    | 1003    | G    |
| 32  | 1a    | 1005    | A    |
| 32  | 1a    | 1006    | C    |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 32  | 1a    | 1009    | G    |
| 32  | 1a    | 1020    | U    |
| 32  | 1a    | 1021    | G    |
| 32  | 1a    | 1022    | G    |
| 32  | 1a    | 1023    | G    |
| 32  | 1a    | 1025    | U    |
| 32  | 1a    | 1026    | G    |
| 32  | 1a    | 1027    | C    |
| 32  | 1a    | 1028    | C    |
| 32  | 1a    | 1029    | C    |
| 32  | 1a    | 1030    | C    |
| 32  | 1a    | 1030(A) | G    |
| 32  | 1a    | 1030(C) | G    |
| 32  | 1a    | 1031    | G    |
| 32  | 1a    | 1032    | G    |
| 32  | 1a    | 1033    | G    |
| 32  | 1a    | 1039    | C    |
| 32  | 1a    | 1043    | C    |
| 32  | 1a    | 1054    | C    |
| 32  | 1a    | 1065    | U    |
| 32  | 1a    | 1066    | C    |
| 32  | 1a    | 1068    | G    |
| 32  | 1a    | 1081    | G    |
| 32  | 1a    | 1087    | G    |
| 32  | 1a    | 1094    | G    |
| 32  | 1a    | 1095    | U    |
| 32  | 1a    | 1101    | A    |
| 32  | 1a    | 1104    | G    |
| 32  | 1a    | 1108    | G    |
| 32  | 1a    | 1123    | A    |
| 32  | 1a    | 1125    | U    |
| 32  | 1a    | 1134    | G    |
| 32  | 1a    | 1135    | U    |
| 32  | 1a    | 1136    | U    |
| 32  | 1a    | 1137    | C    |
| 32  | 1a    | 1138    | G    |
| 32  | 1a    | 1139    | G    |
| 32  | 1a    | 1140    | C    |
| 32  | 1a    | 1141    | C    |
| 32  | 1a    | 1146    | A    |
| 32  | 1a    | 1152    | A    |
| 32  | 1a    | 1157    | A    |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 32         | 1a           | 1159       | U           |
| 32         | 1a           | 1183       | A           |
| 32         | 1a           | 1184       | G           |
| 32         | 1a           | 1196       | U           |
| 32         | 1a           | 1197       | G           |
| 32         | 1a           | 1202       | G           |
| 32         | 1a           | 1212       | U           |
| 32         | 1a           | 1213       | A           |
| 32         | 1a           | 1222       | G           |
| 32         | 1a           | 1227       | A           |
| 32         | 1a           | 1236       | A           |
| 32         | 1a           | 1238       | A           |
| 32         | 1a           | 1240       | U           |
| 32         | 1a           | 1241       | G           |
| 32         | 1a           | 1256       | A           |
| 32         | 1a           | 1257       | U           |
| 32         | 1a           | 1258       | G           |
| 32         | 1a           | 1260       | C           |
| 32         | 1a           | 1269       | A           |
| 32         | 1a           | 1270       | C           |
| 32         | 1a           | 1278       | U           |
| 32         | 1a           | 1279       | A           |
| 32         | 1a           | 1280       | A           |
| 32         | 1a           | 1286       | A           |
| 32         | 1a           | 1287       | A           |
| 32         | 1a           | 1299       | A           |
| 32         | 1a           | 1300       | G           |
| 32         | 1a           | 1302       | U           |
| 32         | 1a           | 1305       | G           |
| 32         | 1a           | 1320       | C           |
| 32         | 1a           | 1338       | G           |
| 32         | 1a           | 1346       | A           |
| 32         | 1a           | 1347       | G           |
| 32         | 1a           | 1363       | C           |
| 32         | 1a           | 1370       | G           |
| 32         | 1a           | 1419       | G           |
| 32         | 1a           | 1442       | G           |
| 32         | 1a           | 1442(A)    | G           |
| 32         | 1a           | 1446       | U           |
| 32         | 1a           | 1447       | A           |
| 32         | 1a           | 1452       | C           |
| 32         | 1a           | 1487       | G           |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 32  | 1a    | 1492 | A    |
| 32  | 1a    | 1494 | G    |
| 32  | 1a    | 1503 | A    |
| 32  | 1a    | 1504 | G    |
| 32  | 1a    | 1506 | U    |
| 32  | 1a    | 1517 | G    |
| 32  | 1a    | 1529 | G    |
| 32  | 1a    | 1530 | G    |
| 32  | 1a    | 1532 | U    |
| 53  | 1v    | 13   | A    |
| 53  | 1v    | 14   | A    |
| 53  | 1v    | 24   | A    |
| 54  | 1w    | 3    | C    |
| 54  | 1w    | 7    | A    |
| 54  | 1w    | 10   | G    |
| 54  | 1w    | 19   | G    |
| 54  | 1w    | 21   | A    |
| 54  | 1w    | 22   | G    |
| 54  | 1w    | 23   | A    |
| 54  | 1w    | 24   | G    |
| 54  | 1w    | 46   | 7MG  |
| 54  | 1w    | 47   | U    |
| 54  | 1w    | 48   | C    |
| 54  | 1w    | 59   | U    |
| 54  | 1w    | 62   | C    |
| 54  | 1w    | 68   | C    |
| 54  | 1w    | 72   | C    |
| 54  | 1w    | 73   | A    |
| 54  | 1w    | 75   | C    |
| 54  | 1w    | 76   | A    |
| 55  | 1x    | 6    | G    |
| 55  | 1x    | 9    | G    |
| 55  | 1x    | 19   | G    |
| 55  | 1x    | 20   | U    |
| 55  | 1x    | 21   | A    |
| 55  | 1x    | 34   | C    |
| 55  | 1x    | 42   | G    |
| 55  | 1x    | 48   | C    |
| 55  | 1x    | 67   | C    |
| 54  | 1y    | 2    | C    |
| 54  | 1y    | 5    | G    |
| 54  | 1y    | 9    | A    |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 54  | 1y    | 11     | C    |
| 54  | 1y    | 13     | C    |
| 54  | 1y    | 19     | G    |
| 54  | 1y    | 20     | U    |
| 54  | 1y    | 21     | A    |
| 54  | 1y    | 22     | G    |
| 54  | 1y    | 26     | A    |
| 54  | 1y    | 33     | U    |
| 54  | 1y    | 34     | G    |
| 54  | 1y    | 39     | PSU  |
| 54  | 1y    | 44     | G    |
| 54  | 1y    | 45     | U    |
| 54  | 1y    | 46     | 7MG  |
| 54  | 1y    | 47     | U    |
| 54  | 1y    | 48     | C    |
| 54  | 1y    | 56     | C    |
| 54  | 1y    | 57     | G    |
| 54  | 1y    | 58     | A    |
| 54  | 1y    | 65     | G    |
| 54  | 1y    | 70     | G    |
| 1   | 2A    | 12     | U    |
| 1   | 2A    | 15     | G    |
| 1   | 2A    | 35     | G    |
| 1   | 2A    | 45     | C    |
| 1   | 2A    | 55     | G    |
| 1   | 2A    | 71     | A    |
| 1   | 2A    | 74     | A    |
| 1   | 2A    | 75     | G    |
| 1   | 2A    | 79     | G    |
| 1   | 2A    | 84     | A    |
| 1   | 2A    | 90     | U    |
| 1   | 2A    | 95     | G    |
| 1   | 2A    | 96     | G    |
| 1   | 2A    | 100    | G    |
| 1   | 2A    | 102    | G    |
| 1   | 2A    | 118    | A    |
| 1   | 2A    | 119    | A    |
| 1   | 2A    | 120    | U    |
| 1   | 2A    | 131    | G    |
| 1   | 2A    | 154(A) | C    |
| 1   | 2A    | 157    | U    |
| 1   | 2A    | 181    | A    |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | 2A    | 196    | A    |
| 1   | 2A    | 198    | C    |
| 1   | 2A    | 199    | A    |
| 1   | 2A    | 205    | G    |
| 1   | 2A    | 214    | G    |
| 1   | 2A    | 215    | G    |
| 1   | 2A    | 216    | A    |
| 1   | 2A    | 219    | G    |
| 1   | 2A    | 221    | A    |
| 1   | 2A    | 222    | A    |
| 1   | 2A    | 227    | A    |
| 1   | 2A    | 228    | A    |
| 1   | 2A    | 229    | A    |
| 1   | 2A    | 232    | G    |
| 1   | 2A    | 233    | A    |
| 1   | 2A    | 248    | G    |
| 1   | 2A    | 266    | G    |
| 1   | 2A    | 271(A) | A    |
| 1   | 2A    | 271(E) | U    |
| 1   | 2A    | 271(F) | C    |
| 1   | 2A    | 271(I) | G    |
| 1   | 2A    | 271(K) | U    |
| 1   | 2A    | 271(L) | U    |
| 1   | 2A    | 271(M) | G    |
| 1   | 2A    | 271(N) | U    |
| 1   | 2A    | 272(B) | G    |
| 1   | 2A    | 277    | C    |
| 1   | 2A    | 278    | A    |
| 1   | 2A    | 294    | A    |
| 1   | 2A    | 311    | A    |
| 1   | 2A    | 327    | G    |
| 1   | 2A    | 328    | U    |
| 1   | 2A    | 329    | G    |
| 1   | 2A    | 330    | A    |
| 1   | 2A    | 333    | G    |
| 1   | 2A    | 338    | G    |
| 1   | 2A    | 342    | G    |
| 1   | 2A    | 348    | G    |
| 1   | 2A    | 352    | G    |
| 1   | 2A    | 354    | G    |
| 1   | 2A    | 362    | U    |
| 1   | 2A    | 363    | G    |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | 2A    | 363(B) | G    |
| 1   | 2A    | 370    | G    |
| 1   | 2A    | 386    | G    |
| 1   | 2A    | 396    | G    |
| 1   | 2A    | 402    | A    |
| 1   | 2A    | 405    | U    |
| 1   | 2A    | 411    | G    |
| 1   | 2A    | 412    | A    |
| 1   | 2A    | 422    | A    |
| 1   | 2A    | 435    | C    |
| 1   | 2A    | 442    | G    |
| 1   | 2A    | 443    | A    |
| 1   | 2A    | 444    | C    |
| 1   | 2A    | 454    | A    |
| 1   | 2A    | 455    | C    |
| 1   | 2A    | 457    | A    |
| 1   | 2A    | 470    | A    |
| 1   | 2A    | 481    | G    |
| 1   | 2A    | 505    | A    |
| 1   | 2A    | 508    | G    |
| 1   | 2A    | 509    | C    |
| 1   | 2A    | 517    | C    |
| 1   | 2A    | 529    | A    |
| 1   | 2A    | 530    | G    |
| 1   | 2A    | 531    | C    |
| 1   | 2A    | 532    | A    |
| 1   | 2A    | 533    | G    |
| 1   | 2A    | 545    | G    |
| 1   | 2A    | 562    | U    |
| 1   | 2A    | 563    | G    |
| 1   | 2A    | 573    | G    |
| 1   | 2A    | 574    | C    |
| 1   | 2A    | 575    | A    |
| 1   | 2A    | 587    | C    |
| 1   | 2A    | 588    | U    |
| 1   | 2A    | 592    | G    |
| 1   | 2A    | 599    | G    |
| 1   | 2A    | 603    | A    |
| 1   | 2A    | 604    | G    |
| 1   | 2A    | 607    | U    |
| 1   | 2A    | 614(B) | G    |
| 1   | 2A    | 614(C) | A    |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | 2A    | 615    | G    |
| 1   | 2A    | 616    | G    |
| 1   | 2A    | 627    | A    |
| 1   | 2A    | 634    | C    |
| 1   | 2A    | 637    | A    |
| 1   | 2A    | 645    | C    |
| 1   | 2A    | 646    | A    |
| 1   | 2A    | 647    | G    |
| 1   | 2A    | 652(B) | A    |
| 1   | 2A    | 652(C) | G    |
| 1   | 2A    | 653    | A    |
| 1   | 2A    | 661    | C    |
| 1   | 2A    | 669    | G    |
| 1   | 2A    | 686    | G    |
| 1   | 2A    | 717    | G    |
| 1   | 2A    | 722    | A    |
| 1   | 2A    | 726    | G    |
| 1   | 2A    | 730    | C    |
| 1   | 2A    | 752    | A    |
| 1   | 2A    | 753    | C    |
| 1   | 2A    | 771    | G    |
| 1   | 2A    | 775    | G    |
| 1   | 2A    | 776    | G    |
| 1   | 2A    | 782    | A    |
| 1   | 2A    | 784    | A    |
| 1   | 2A    | 785    | G    |
| 1   | 2A    | 790    | C    |
| 1   | 2A    | 792    | G    |
| 1   | 2A    | 794    | G    |
| 1   | 2A    | 805    | G    |
| 1   | 2A    | 811    | U    |
| 1   | 2A    | 812    | C    |
| 1   | 2A    | 819    | A    |
| 1   | 2A    | 827    | U    |
| 1   | 2A    | 828    | U    |
| 1   | 2A    | 847    | U    |
| 1   | 2A    | 848    | G    |
| 1   | 2A    | 857    | C    |
| 1   | 2A    | 859    | G    |
| 1   | 2A    | 864    | G    |
| 1   | 2A    | 866    | A    |
| 1   | 2A    | 867    | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 2A    | 869  | G    |
| 1   | 2A    | 874  | G    |
| 1   | 2A    | 875  | G    |
| 1   | 2A    | 878  | A    |
| 1   | 2A    | 879  | G    |
| 1   | 2A    | 880  | G    |
| 1   | 2A    | 884  | C    |
| 1   | 2A    | 886  | C    |
| 1   | 2A    | 887  | A    |
| 1   | 2A    | 888  | C    |
| 1   | 2A    | 889  | C    |
| 1   | 2A    | 893  | C    |
| 1   | 2A    | 894  | C    |
| 1   | 2A    | 896  | A    |
| 1   | 2A    | 897  | C    |
| 1   | 2A    | 900  | A    |
| 1   | 2A    | 901  | A    |
| 1   | 2A    | 910  | A    |
| 1   | 2A    | 917  | A    |
| 1   | 2A    | 923  | C    |
| 1   | 2A    | 932  | G    |
| 1   | 2A    | 933  | A    |
| 1   | 2A    | 941  | A    |
| 1   | 2A    | 943  | U    |
| 1   | 2A    | 945  | A    |
| 1   | 2A    | 946  | G    |
| 1   | 2A    | 951  | C    |
| 1   | 2A    | 952  | G    |
| 1   | 2A    | 953  | A    |
| 1   | 2A    | 957  | A    |
| 1   | 2A    | 961  | C    |
| 1   | 2A    | 974  | G    |
| 1   | 2A    | 975  | C    |
| 1   | 2A    | 983  | A    |
| 1   | 2A    | 996  | A    |
| 1   | 2A    | 1005 | C    |
| 1   | 2A    | 1012 | U    |
| 1   | 2A    | 1013 | C    |
| 1   | 2A    | 1017 | G    |
| 1   | 2A    | 1022 | G    |
| 1   | 2A    | 1026 | U    |
| 1   | 2A    | 1027 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 2A    | 1033 | U    |
| 1   | 2A    | 1036 | G    |
| 1   | 2A    | 1038 | C    |
| 1   | 2A    | 1039 | G    |
| 1   | 2A    | 1043 | C    |
| 1   | 2A    | 1114 | G    |
| 1   | 2A    | 1116 | C    |
| 1   | 2A    | 1118 | C    |
| 1   | 2A    | 1126 | A    |
| 1   | 2A    | 1130 | U    |
| 1   | 2A    | 1133 | U    |
| 1   | 2A    | 1135 | C    |
| 1   | 2A    | 1136 | G    |
| 1   | 2A    | 1137 | G    |
| 1   | 2A    | 1139 | G    |
| 1   | 2A    | 1144 | G    |
| 1   | 2A    | 1155 | A    |
| 1   | 2A    | 1166 | C    |
| 1   | 2A    | 1171 | G    |
| 1   | 2A    | 1183 | G    |
| 1   | 2A    | 1198 | U    |
| 1   | 2A    | 1205 | U    |
| 1   | 2A    | 1210 | A    |
| 1   | 2A    | 1211 | U    |
| 1   | 2A    | 1212 | G    |
| 1   | 2A    | 1220 | A    |
| 1   | 2A    | 1227 | G    |
| 1   | 2A    | 1229 | G    |
| 1   | 2A    | 1237 | A    |
| 1   | 2A    | 1250 | G    |
| 1   | 2A    | 1253 | A    |
| 1   | 2A    | 1256 | G    |
| 1   | 2A    | 1271 | G    |
| 1   | 2A    | 1272 | A    |
| 1   | 2A    | 1273 | U    |
| 1   | 2A    | 1284 | A    |
| 1   | 2A    | 1300 | U    |
| 1   | 2A    | 1301 | A    |
| 1   | 2A    | 1303 | G    |
| 1   | 2A    | 1306 | C    |
| 1   | 2A    | 1314 | C    |
| 1   | 2A    | 1318 | C    |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 1   | 2A    | 1332    | G    |
| 1   | 2A    | 1342    | A    |
| 1   | 2A    | 1345    | C    |
| 1   | 2A    | 1359    | A    |
| 1   | 2A    | 1360    | A    |
| 1   | 2A    | 1365    | A    |
| 1   | 2A    | 1368    | G    |
| 1   | 2A    | 1370    | C    |
| 1   | 2A    | 1373    | A    |
| 1   | 2A    | 1380    | G    |
| 1   | 2A    | 1384    | A    |
| 1   | 2A    | 1385    | G    |
| 1   | 2A    | 1386    | C    |
| 1   | 2A    | 1416    | G    |
| 1   | 2A    | 1417    | C    |
| 1   | 2A    | 1420    | U    |
| 1   | 2A    | 1421    | G    |
| 1   | 2A    | 1427    | A    |
| 1   | 2A    | 1428    | C    |
| 1   | 2A    | 1429    | G    |
| 1   | 2A    | 1437    | C    |
| 1   | 2A    | 1445    | A    |
| 1   | 2A    | 1449    | A    |
| 1   | 2A    | 1450    | G    |
| 1   | 2A    | 1455    | G    |
| 1   | 2A    | 1460    | A    |
| 1   | 2A    | 1467    | C    |
| 1   | 2A    | 1471    | A    |
| 1   | 2A    | 1479    | G    |
| 1   | 2A    | 1482    | G    |
| 1   | 2A    | 1490    | A    |
| 1   | 2A    | 1493    | C    |
| 1   | 2A    | 1494    | A    |
| 1   | 2A    | 1495    | A    |
| 1   | 2A    | 1496    | A    |
| 1   | 2A    | 1497    | U    |
| 1   | 2A    | 1508    | A    |
| 1   | 2A    | 1509    | C    |
| 1   | 2A    | 1509(A) | A    |
| 1   | 2A    | 1516    | C    |
| 1   | 2A    | 1525    | G    |
| 1   | 2A    | 1531    | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 2A    | 1532 | C    |
| 1   | 2A    | 1533 | G    |
| 1   | 2A    | 1541 | G    |
| 1   | 2A    | 1545 | A    |
| 1   | 2A    | 1547 | C    |
| 1   | 2A    | 1558 | A    |
| 1   | 2A    | 1566 | A    |
| 1   | 2A    | 1569 | A    |
| 1   | 2A    | 1578 | U    |
| 1   | 2A    | 1583 | A    |
| 1   | 2A    | 1584 | C    |
| 1   | 2A    | 1592 | C    |
| 1   | 2A    | 1603 | A    |
| 1   | 2A    | 1608 | A    |
| 1   | 2A    | 1609 | A    |
| 1   | 2A    | 1610 | A    |
| 1   | 2A    | 1616 | A    |
| 1   | 2A    | 1640 | C    |
| 1   | 2A    | 1648 | C    |
| 1   | 2A    | 1650 | G    |
| 1   | 2A    | 1654 | A    |
| 1   | 2A    | 1664 | A    |
| 1   | 2A    | 1674 | G    |
| 1   | 2A    | 1675 | C    |
| 1   | 2A    | 1696 | G    |
| 1   | 2A    | 1700 | A    |
| 1   | 2A    | 1701 | A    |
| 1   | 2A    | 1721 | G    |
| 1   | 2A    | 1722 | A    |
| 1   | 2A    | 1741 | A    |
| 1   | 2A    | 1746 | G    |
| 1   | 2A    | 1756 | G    |
| 1   | 2A    | 1758 | G    |
| 1   | 2A    | 1762 | A    |
| 1   | 2A    | 1763 | G    |
| 1   | 2A    | 1764 | G    |
| 1   | 2A    | 1773 | A    |
| 1   | 2A    | 1777 | U    |
| 1   | 2A    | 1780 | A    |
| 1   | 2A    | 1786 | A    |
| 1   | 2A    | 1791 | A    |
| 1   | 2A    | 1800 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 2A    | 1801 | G    |
| 1   | 2A    | 1812 | A    |
| 1   | 2A    | 1816 | G    |
| 1   | 2A    | 1829 | A    |
| 1   | 2A    | 1835 | G    |
| 1   | 2A    | 1847 | A    |
| 1   | 2A    | 1848 | A    |
| 1   | 2A    | 1858 | G    |
| 1   | 2A    | 1877 | A    |
| 1   | 2A    | 1878 | G    |
| 1   | 2A    | 1900 | A    |
| 1   | 2A    | 1906 | G    |
| 1   | 2A    | 1913 | A    |
| 1   | 2A    | 1914 | C    |
| 1   | 2A    | 1929 | G    |
| 1   | 2A    | 1930 | G    |
| 1   | 2A    | 1931 | U    |
| 1   | 2A    | 1936 | A    |
| 1   | 2A    | 1937 | A    |
| 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    | 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    | 2050 | C    |
| 1   | 2A    | 2055 | C    |
| 1   | 2A    | 2056 | G    |
| 1   | 2A    | 2060 | A    |
| 1   | 2A    | 2061 | G    |
| 1   | 2A    | 2062 | A    |
| 1   | 2A    | 2069 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 2A    | 2093 | G    |
| 1   | 2A    | 2105 | C    |
| 1   | 2A    | 2108 | C    |
| 1   | 2A    | 2110 | G    |
| 1   | 2A    | 2111 | C    |
| 1   | 2A    | 2112 | G    |
| 1   | 2A    | 2116 | G    |
| 1   | 2A    | 2119 | A    |
| 1   | 2A    | 2122 | U    |
| 1   | 2A    | 2124 | G    |
| 1   | 2A    | 2126 | A    |
| 1   | 2A    | 2127 | G    |
| 1   | 2A    | 2129 | C    |
| 1   | 2A    | 2131 | G    |
| 1   | 2A    | 2132 | U    |
| 1   | 2A    | 2133 | G    |
| 1   | 2A    | 2134 | A    |
| 1   | 2A    | 2135 | A    |
| 1   | 2A    | 2136 | C    |
| 1   | 2A    | 2137 | C    |
| 1   | 2A    | 2139 | C    |
| 1   | 2A    | 2141 | G    |
| 1   | 2A    | 2142 | C    |
| 1   | 2A    | 2146 | C    |
| 1   | 2A    | 2150 | U    |
| 1   | 2A    | 2153 | G    |
| 1   | 2A    | 2155 | G    |
| 1   | 2A    | 2157 | G    |
| 1   | 2A    | 2158 | A    |
| 1   | 2A    | 2163 | C    |
| 1   | 2A    | 2165 | G    |
| 1   | 2A    | 2166 | G    |
| 1   | 2A    | 2167 | U    |
| 1   | 2A    | 2168 | G    |
| 1   | 2A    | 2171 | A    |
| 1   | 2A    | 2172 | U    |
| 1   | 2A    | 2173 | A    |
| 1   | 2A    | 2174 | C    |
| 1   | 2A    | 2178 | C    |
| 1   | 2A    | 2181 | G    |
| 1   | 2A    | 2185 | C    |
| 1   | 2A    | 2192 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 2A    | 2198 | A    |
| 1   | 2A    | 2200 | C    |
| 1   | 2A    | 2206 | G    |
| 1   | 2A    | 2207 | G    |
| 1   | 2A    | 2208 | A    |
| 1   | 2A    | 2218 | U    |
| 1   | 2A    | 2225 | A    |
| 1   | 2A    | 2239 | G    |
| 1   | 2A    | 2248 | C    |
| 1   | 2A    | 2267 | A    |
| 1   | 2A    | 2268 | A    |
| 1   | 2A    | 2272 | U    |
| 1   | 2A    | 2275 | C    |
| 1   | 2A    | 2279 | G    |
| 1   | 2A    | 2282 | G    |
| 1   | 2A    | 2283 | C    |
| 1   | 2A    | 2287 | A    |
| 1   | 2A    | 2305 | A    |
| 1   | 2A    | 2308 | G    |
| 1   | 2A    | 2310 | A    |
| 1   | 2A    | 2311 | A    |
| 1   | 2A    | 2312 | U    |
| 1   | 2A    | 2319 | G    |
| 1   | 2A    | 2320 | A    |
| 1   | 2A    | 2325 | G    |
| 1   | 2A    | 2327 | A    |
| 1   | 2A    | 2334 | G    |
| 1   | 2A    | 2336 | A    |
| 1   | 2A    | 2347 | C    |
| 1   | 2A    | 2350 | C    |
| 1   | 2A    | 2354 | G    |
| 1   | 2A    | 2376 | A    |
| 1   | 2A    | 2377 | A    |
| 1   | 2A    | 2383 | G    |
| 1   | 2A    | 2385 | C    |
| 1   | 2A    | 2388 | A    |
| 1   | 2A    | 2400 | G    |
| 1   | 2A    | 2402 | C    |
| 1   | 2A    | 2403 | C    |
| 1   | 2A    | 2406 | U    |
| 1   | 2A    | 2425 | A    |
| 1   | 2A    | 2429 | G    |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 1   | 2A    | 2430    | A    |
| 1   | 2A    | 2435    | A    |
| 1   | 2A    | 2439    | A    |
| 1   | 2A    | 2441    | C    |
| 1   | 2A    | 2448    | A    |
| 1   | 2A    | 2465    | C    |
| 1   | 2A    | 2469    | A    |
| 1   | 2A    | 2474    | C    |
| 1   | 2A    | 2476    | A    |
| 1   | 2A    | 2484    | G    |
| 1   | 2A    | 2487    | G    |
| 1   | 2A    | 2489    | G    |
| 1   | 2A    | 2490    | G    |
| 1   | 2A    | 2491    | U    |
| 1   | 2A    | 2494    | G    |
| 1   | 2A    | 2502    | G    |
| 1   | 2A    | 2504    | U    |
| 1   | 2A    | 2505    | G    |
| 1   | 2A    | 2506    | U    |
| 1   | 2A    | 2518    | A    |
| 1   | 2A    | 2520    | C    |
| 1   | 2A    | 2525    | G    |
| 1   | 2A    | 2528    | U    |
| 1   | 2A    | 2532    | G    |
| 1   | 2A    | 2554    | U    |
| 1   | 2A    | 2566    | A    |
| 1   | 2A    | 2567    | G    |
| 1   | 2A    | 2573    | C    |
| 1   | 2A    | 2602    | A    |
| 1   | 2A    | 2611    | U    |
| 1   | 2A    | 2612    | C    |
| 1   | 2A    | 2615    | U    |
| 1   | 2A    | 2629    | A    |
| 1   | 2A    | 2630    | G    |
| 1   | 2A    | 2661    | G    |
| 1   | 2A    | 2663    | G    |
| 1   | 2A    | 2669    | G    |
| 1   | 2A    | 2673    | G    |
| 1   | 2A    | 2674    | G    |
| 1   | 2A    | 2689    | U    |
| 1   | 2A    | 2690    | C    |
| 1   | 2A    | 2712(A) | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 2A    | 2713 | A    |
| 1   | 2A    | 2714 | G    |
| 1   | 2A    | 2726 | U    |
| 1   | 2A    | 2733 | A    |
| 1   | 2A    | 2744 | G    |
| 1   | 2A    | 2745 | C    |
| 1   | 2A    | 2751 | G    |
| 1   | 2A    | 2757 | A    |
| 1   | 2A    | 2759 | G    |
| 1   | 2A    | 2761 | G    |
| 1   | 2A    | 2764 | A    |
| 1   | 2A    | 2765 | A    |
| 1   | 2A    | 2778 | A    |
| 1   | 2A    | 2779 | U    |
| 1   | 2A    | 2793 | G    |
| 1   | 2A    | 2794 | C    |
| 1   | 2A    | 2804 | C    |
| 1   | 2A    | 2808 | U    |
| 1   | 2A    | 2818 | G    |
| 1   | 2A    | 2820 | A    |
| 1   | 2A    | 2821 | A    |
| 1   | 2A    | 2833 | G    |
| 1   | 2A    | 2835 | A    |
| 1   | 2A    | 2849 | U    |
| 1   | 2A    | 2872 | G    |
| 1   | 2A    | 2875 | C    |
| 1   | 2A    | 2879 | C    |
| 1   | 2A    | 2880 | C    |
| 1   | 2A    | 2893 | G    |
| 1   | 2A    | 2894 | G    |
| 1   | 2A    | 2895 | U    |
| 1   | 2A    | 2897 | U    |
| 2   | 2B    | 2    | C    |
| 2   | 2B    | 7    | G    |
| 2   | 2B    | 8    | U    |
| 2   | 2B    | 9    | G    |
| 2   | 2B    | 13   | A    |
| 2   | 2B    | 17   | C    |
| 2   | 2B    | 20   | C    |
| 2   | 2B    | 24   | G    |
| 2   | 2B    | 25   | A    |
| 2   | 2B    | 30   | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | 2B    | 32  | C    |
| 2   | 2B    | 34  | U    |
| 2   | 2B    | 35  | U    |
| 2   | 2B    | 42  | C    |
| 2   | 2B    | 45  | A    |
| 2   | 2B    | 46  | A    |
| 2   | 2B    | 52  | A    |
| 2   | 2B    | 53  | A    |
| 2   | 2B    | 56  | G    |
| 2   | 2B    | 57  | A    |
| 2   | 2B    | 65  | C    |
| 2   | 2B    | 66  | A    |
| 2   | 2B    | 67  | G    |
| 2   | 2B    | 73  | A    |
| 2   | 2B    | 74  | U    |
| 2   | 2B    | 75  | G    |
| 2   | 2B    | 83  | G    |
| 2   | 2B    | 85  | G    |
| 2   | 2B    | 88  | C    |
| 2   | 2B    | 91  | C    |
| 2   | 2B    | 94  | C    |
| 2   | 2B    | 101 | G    |
| 2   | 2B    | 106 | G    |
| 2   | 2B    | 108 | U    |
| 2   | 2B    | 110 | G    |
| 2   | 2B    | 116 | G    |
| 32  | 2a    | 7   | G    |
| 32  | 2a    | 9   | G    |
| 32  | 2a    | 32  | A    |
| 32  | 2a    | 39  | G    |
| 32  | 2a    | 47  | C    |
| 32  | 2a    | 48  | C    |
| 32  | 2a    | 51  | A    |
| 32  | 2a    | 52  | G    |
| 32  | 2a    | 66  | G    |
| 32  | 2a    | 78  | G    |
| 32  | 2a    | 80  | G    |
| 32  | 2a    | 88  | A    |
| 32  | 2a    | 89  | C    |
| 32  | 2a    | 90  | U    |
| 32  | 2a    | 96  | U    |
| 32  | 2a    | 98  | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 32  | 2a    | 101 | A    |
| 32  | 2a    | 116 | A    |
| 32  | 2a    | 121 | C    |
| 32  | 2a    | 131 | C    |
| 32  | 2a    | 146 | G    |
| 32  | 2a    | 159 | G    |
| 32  | 2a    | 163 | C    |
| 32  | 2a    | 174 | C    |
| 32  | 2a    | 180 | U    |
| 32  | 2a    | 182 | U    |
| 32  | 2a    | 195 | A    |
| 32  | 2a    | 197 | A    |
| 32  | 2a    | 201 | C    |
| 32  | 2a    | 203 | U    |
| 32  | 2a    | 204 | U    |
| 32  | 2a    | 216 | G    |
| 32  | 2a    | 217 | C    |
| 32  | 2a    | 243 | A    |
| 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    | 321 | A    |
| 32  | 2a    | 328 | C    |
| 32  | 2a    | 332 | G    |
| 32  | 2a    | 344 | A    |
| 32  | 2a    | 352 | C    |
| 32  | 2a    | 353 | A    |
| 32  | 2a    | 354 | G    |
| 32  | 2a    | 367 | U    |
| 32  | 2a    | 372 | C    |
| 32  | 2a    | 373 | A    |
| 32  | 2a    | 384 | G    |
| 32  | 2a    | 397 | A    |
| 32  | 2a    | 398 | C    |
| 32  | 2a    | 406 | G    |
| 32  | 2a    | 412 | A    |
| 32  | 2a    | 424 | G    |
| 32  | 2a    | 429 | U    |
| 32  | 2a    | 441 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 32  | 2a    | 442 | C    |
| 32  | 2a    | 452 | A    |
| 32  | 2a    | 461 | A    |
| 32  | 2a    | 470 | C    |
| 32  | 2a    | 474 | G    |
| 32  | 2a    | 485 | G    |
| 32  | 2a    | 496 | A    |
| 32  | 2a    | 498 | U    |
| 32  | 2a    | 505 | G    |
| 32  | 2a    | 509 | A    |
| 32  | 2a    | 510 | A    |
| 32  | 2a    | 511 | C    |
| 32  | 2a    | 518 | C    |
| 32  | 2a    | 531 | U    |
| 32  | 2a    | 532 | A    |
| 32  | 2a    | 533 | A    |
| 32  | 2a    | 547 | A    |
| 32  | 2a    | 559 | A    |
| 32  | 2a    | 560 | U    |
| 32  | 2a    | 561 | U    |
| 32  | 2a    | 562 | C    |
| 32  | 2a    | 568 | G    |
| 32  | 2a    | 572 | A    |
| 32  | 2a    | 573 | A    |
| 32  | 2a    | 576 | G    |
| 32  | 2a    | 577 | G    |
| 32  | 2a    | 596 | C    |
| 32  | 2a    | 630 | G    |
| 32  | 2a    | 653 | A    |
| 32  | 2a    | 665 | A    |
| 32  | 2a    | 673 | G    |
| 32  | 2a    | 687 | A    |
| 32  | 2a    | 688 | G    |
| 32  | 2a    | 695 | A    |
| 32  | 2a    | 702 | A    |
| 32  | 2a    | 723 | U    |
| 32  | 2a    | 731 | G    |
| 32  | 2a    | 749 | C    |
| 32  | 2a    | 755 | G    |
| 32  | 2a    | 759 | A    |
| 32  | 2a    | 773 | G    |
| 32  | 2a    | 777 | A    |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 32  | 2a    | 792     | A    |
| 32  | 2a    | 793     | U    |
| 32  | 2a    | 794     | A    |
| 32  | 2a    | 815     | A    |
| 32  | 2a    | 816     | A    |
| 32  | 2a    | 817     | C    |
| 32  | 2a    | 821     | G    |
| 32  | 2a    | 828     | A    |
| 32  | 2a    | 840     | C    |
| 32  | 2a    | 841     | U    |
| 32  | 2a    | 851     | G    |
| 32  | 2a    | 859     | A    |
| 32  | 2a    | 870     | U    |
| 32  | 2a    | 885     | G    |
| 32  | 2a    | 902     | G    |
| 32  | 2a    | 914     | A    |
| 32  | 2a    | 916     | G    |
| 32  | 2a    | 926     | G    |
| 32  | 2a    | 927     | G    |
| 32  | 2a    | 931     | C    |
| 32  | 2a    | 934     | C    |
| 32  | 2a    | 960     | U    |
| 32  | 2a    | 961     | U    |
| 32  | 2a    | 968     | A    |
| 32  | 2a    | 969     | A    |
| 32  | 2a    | 971     | G    |
| 32  | 2a    | 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    | 1000    | U    |
| 32  | 2a    | 1001    | A    |
| 32  | 2a    | 1001(A) | G    |
| 32  | 2a    | 1002    | G    |
| 32  | 2a    | 1004    | A    |
| 32  | 2a    | 1005    | A    |
| 32  | 2a    | 1006    | C    |
| 32  | 2a    | 1009    | G    |
| 32  | 2a    | 1020    | U    |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 32  | 2a    | 1021    | G    |
| 32  | 2a    | 1022    | G    |
| 32  | 2a    | 1023    | G    |
| 32  | 2a    | 1025    | U    |
| 32  | 2a    | 1026    | G    |
| 32  | 2a    | 1027    | C    |
| 32  | 2a    | 1030    | C    |
| 32  | 2a    | 1030(A) | G    |
| 32  | 2a    | 1030(B) | C    |
| 32  | 2a    | 1030(C) | G    |
| 32  | 2a    | 1031    | G    |
| 32  | 2a    | 1032    | G    |
| 32  | 2a    | 1033    | G    |
| 32  | 2a    | 1039    | C    |
| 32  | 2a    | 1043    | C    |
| 32  | 2a    | 1054    | C    |
| 32  | 2a    | 1065    | U    |
| 32  | 2a    | 1066    | C    |
| 32  | 2a    | 1068    | G    |
| 32  | 2a    | 1077    | G    |
| 32  | 2a    | 1081    | G    |
| 32  | 2a    | 1087    | G    |
| 32  | 2a    | 1094    | G    |
| 32  | 2a    | 1095    | U    |
| 32  | 2a    | 1101    | A    |
| 32  | 2a    | 1104    | G    |
| 32  | 2a    | 1108    | G    |
| 32  | 2a    | 1117    | G    |
| 32  | 2a    | 1125    | U    |
| 32  | 2a    | 1129    | C    |
| 32  | 2a    | 1130    | A    |
| 32  | 2a    | 1135    | U    |
| 32  | 2a    | 1136    | U    |
| 32  | 2a    | 1137    | C    |
| 32  | 2a    | 1138    | G    |
| 32  | 2a    | 1139    | G    |
| 32  | 2a    | 1140    | C    |
| 32  | 2a    | 1141    | C    |
| 32  | 2a    | 1146    | A    |
| 32  | 2a    | 1147    | C    |
| 32  | 2a    | 1152    | A    |
| 32  | 2a    | 1157    | A    |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 32  | 2a    | 1159    | U    |
| 32  | 2a    | 1182    | G    |
| 32  | 2a    | 1183    | A    |
| 32  | 2a    | 1184    | G    |
| 32  | 2a    | 1196    | U    |
| 32  | 2a    | 1197    | G    |
| 32  | 2a    | 1202    | G    |
| 32  | 2a    | 1211    | U    |
| 32  | 2a    | 1212    | U    |
| 32  | 2a    | 1213    | A    |
| 32  | 2a    | 1222    | G    |
| 32  | 2a    | 1227    | A    |
| 32  | 2a    | 1236    | A    |
| 32  | 2a    | 1238    | A    |
| 32  | 2a    | 1240    | U    |
| 32  | 2a    | 1241    | G    |
| 32  | 2a    | 1256    | A    |
| 32  | 2a    | 1257    | U    |
| 32  | 2a    | 1258    | G    |
| 32  | 2a    | 1260    | C    |
| 32  | 2a    | 1269    | A    |
| 32  | 2a    | 1270    | C    |
| 32  | 2a    | 1278    | U    |
| 32  | 2a    | 1279    | A    |
| 32  | 2a    | 1280    | A    |
| 32  | 2a    | 1287    | A    |
| 32  | 2a    | 1300    | G    |
| 32  | 2a    | 1305    | G    |
| 32  | 2a    | 1320    | C    |
| 32  | 2a    | 1338    | G    |
| 32  | 2a    | 1346    | A    |
| 32  | 2a    | 1347    | G    |
| 32  | 2a    | 1363    | C    |
| 32  | 2a    | 1368    | G    |
| 32  | 2a    | 1370    | G    |
| 32  | 2a    | 1400    | 5MC  |
| 32  | 2a    | 1401    | G    |
| 32  | 2a    | 1419    | G    |
| 32  | 2a    | 1442    | G    |
| 32  | 2a    | 1442(A) | G    |
| 32  | 2a    | 1446    | U    |
| 32  | 2a    | 1447    | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 32  | 2a    | 1452 | C    |
| 32  | 2a    | 1456 | G    |
| 32  | 2a    | 1487 | G    |
| 32  | 2a    | 1492 | A    |
| 32  | 2a    | 1494 | G    |
| 32  | 2a    | 1503 | A    |
| 32  | 2a    | 1504 | G    |
| 32  | 2a    | 1506 | U    |
| 32  | 2a    | 1517 | G    |
| 32  | 2a    | 1520 | G    |
| 32  | 2a    | 1529 | G    |
| 32  | 2a    | 1530 | G    |
| 32  | 2a    | 1531 | A    |
| 32  | 2a    | 1532 | U    |
| 53  | 2v    | 13   | A    |
| 53  | 2v    | 14   | A    |
| 53  | 2v    | 24   | A    |
| 54  | 2w    | 3    | C    |
| 54  | 2w    | 4    | C    |
| 54  | 2w    | 7    | A    |
| 54  | 2w    | 8    | 4SU  |
| 54  | 2w    | 9    | A    |
| 54  | 2w    | 10   | G    |
| 54  | 2w    | 19   | G    |
| 54  | 2w    | 21   | A    |
| 54  | 2w    | 22   | G    |
| 54  | 2w    | 24   | G    |
| 54  | 2w    | 46   | 7MG  |
| 54  | 2w    | 48   | C    |
| 54  | 2w    | 59   | U    |
| 54  | 2w    | 62   | C    |
| 54  | 2w    | 68   | C    |
| 54  | 2w    | 71   | G    |
| 54  | 2w    | 72   | C    |
| 54  | 2w    | 73   | A    |
| 54  | 2w    | 75   | C    |
| 54  | 2w    | 76   | A    |
| 55  | 2x    | 19   | G    |
| 55  | 2x    | 21   | A    |
| 55  | 2x    | 42   | G    |
| 55  | 2x    | 47   | U    |
| 55  | 2x    | 48   | C    |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 55         | 2x           | 56         | C           |
| 55         | 2x           | 67         | C           |
| 55         | 2x           | 68         | C           |
| 54         | 2y           | 2          | C           |
| 54         | 2y           | 9          | A           |
| 54         | 2y           | 13         | C           |
| 54         | 2y           | 19         | G           |
| 54         | 2y           | 22         | G           |
| 54         | 2y           | 33         | U           |
| 54         | 2y           | 34         | G           |
| 54         | 2y           | 39         | PSU         |
| 54         | 2y           | 44         | G           |
| 54         | 2y           | 46         | 7MG         |
| 54         | 2y           | 47         | U           |
| 54         | 2y           | 52         | G           |
| 54         | 2y           | 56         | C           |
| 54         | 2y           | 57         | G           |
| 54         | 2y           | 58         | A           |
| 54         | 2y           | 65         | G           |
| 54         | 2y           | 70         | G           |

All (64) RNA pucker outliers are listed below:

| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 1          | 1A           | 90         | U           |
| 1          | 1A           | 196        | A           |
| 1          | 1A           | 266        | G           |
| 1          | 1A           | 271(K)     | U           |
| 1          | 1A           | 278        | A           |
| 1          | 1A           | 548        | A           |
| 1          | 1A           | 746        | A           |
| 1          | 1A           | 764        | A           |
| 1          | 1A           | 839        | U           |
| 1          | 1A           | 896        | A           |
| 1          | 1A           | 974        | G           |
| 1          | 1A           | 1047       | G           |
| 1          | 1A           | 1065       | U           |
| 1          | 1A           | 1067       | A           |
| 1          | 1A           | 1089       | G           |
| 1          | 1A           | 1174       | A           |
| 1          | 1A           | 1175       | U           |
| 1          | 1A           | 1176       | G           |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | 1A    | 1210   | A    |
| 1   | 1A    | 1275   | A    |
| 1   | 1A    | 1379   | A    |
| 1   | 1A    | 1442   | G    |
| 1   | 1A    | 1508   | A    |
| 1   | 1A    | 1608   | A    |
| 1   | 1A    | 1653   | G    |
| 1   | 1A    | 1992   | G    |
| 1   | 1A    | 2131   | G    |
| 1   | 1A    | 2181   | G    |
| 1   | 1A    | 2183   | C    |
| 1   | 1A    | 2430   | A    |
| 1   | 1A    | 2629   | A    |
| 1   | 1A    | 2689   | U    |
| 1   | 1A    | 2756   | U    |
| 2   | 1B    | 1      | U    |
| 1   | 2A    | 196    | A    |
| 1   | 2A    | 228    | A    |
| 1   | 2A    | 266    | G    |
| 1   | 2A    | 271(K) | U    |
| 1   | 2A    | 271(M) | G    |
| 1   | 2A    | 277    | C    |
| 1   | 2A    | 528    | A    |
| 1   | 2A    | 530    | G    |
| 1   | 2A    | 587    | C    |
| 1   | 2A    | 752    | A    |
| 1   | 2A    | 839    | U    |
| 1   | 2A    | 856    | C    |
| 1   | 2A    | 893    | C    |
| 1   | 2A    | 900    | A    |
| 1   | 2A    | 1026   | U    |
| 1   | 2A    | 1210   | A    |
| 1   | 2A    | 1300   | U    |
| 1   | 2A    | 1379   | A    |
| 1   | 2A    | 1420   | U    |
| 1   | 2A    | 1442   | G    |
| 1   | 2A    | 1493   | C    |
| 1   | 2A    | 1530   | C    |
| 1   | 2A    | 1653   | G    |
| 1   | 2A    | 1913   | A    |
| 1   | 2A    | 1992   | G    |
| 1   | 2A    | 2126   | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 2A    | 2156 | G    |
| 1   | 2A    | 2406 | U    |
| 1   | 2A    | 2689 | U    |
| 1   | 2A    | 2756 | U    |

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

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

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

| Mol | Type | Chain | Res  | Link    | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|------|---------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |      |         | Counts       | RMSZ | # $ Z  > 2$ | Counts      | RMSZ | # $ Z  > 2$ |
| 1   | PSU  | 1A    | 1911 | 1       | 15,21,22     | 1.37 | 1 (6%)      | 16,30,33    | 2.33 | 4 (25%)     |
| 1   | 5MU  | 1A    | 1915 | 1       | 13,22,23     | 0.60 | 0           | 16,32,35    | 2.46 | 2 (12%)     |
| 1   | PSU  | 1A    | 1917 | 1       | 15,21,22     | 1.37 | 2 (13%)     | 16,30,33    | 2.27 | 4 (25%)     |
| 1   | 4OC  | 1A    | 1920 | 1       | 15,22,24     | 0.60 | 0           | 20,31,35    | 1.32 | 3 (15%)     |
| 1   | 5MU  | 1A    | 1939 | 1,56    | 13,22,23     | 0.59 | 0           | 16,32,35    | 2.37 | 2 (12%)     |
| 1   | 5MC  | 1A    | 1942 | 1       | 14,22,23     | 1.19 | 1 (7%)      | 17,32,35    | 1.13 | 1 (5%)      |
| 1   | 5MC  | 1A    | 1962 | 1       | 14,22,23     | 1.36 | 1 (7%)      | 17,32,35    | 0.85 | 1 (5%)      |
| 1   | OMG  | 1A    | 2251 | 1,55,56 | 18,26,27     | 1.19 | 2 (11%)     | 21,38,41    | 2.13 | 4 (19%)     |
| 1   | 2MA  | 1A    | 2503 | 1,56    | 17,25,26     | 1.49 | 3 (17%)     | 18,37,40    | 2.92 | 1 (5%)      |
| 1   | 2MU  | 1A    | 2552 | 1,56    | 14,22,24     | 0.85 | 1 (7%)      | 19,31,36    | 1.53 | 1 (5%)      |
| 1   | PSU  | 1A    | 2605 | 1       | 15,21,22     | 1.46 | 2 (13%)     | 16,30,33    | 2.32 | 4 (25%)     |
| 32  | 2MG  | 1a    | 1207 | 32      | 18,26,27     | 1.19 | 2 (11%)     | 21,38,41    | 2.50 | 7 (33%)     |
| 32  | 5MC  | 1a    | 1400 | 32      | 14,22,23     | 1.44 | 1 (7%)      | 17,32,35    | 0.82 | 1 (5%)      |
| 32  | 4OC  | 1a    | 1402 | 32      | 15,23,24     | 0.59 | 0           | 21,32,35    | 1.87 | 3 (14%)     |
| 32  | 5MC  | 1a    | 1404 | 32      | 14,22,23     | 1.32 | 1 (7%)      | 17,32,35    | 0.96 | 1 (5%)      |
| 32  | 5MC  | 1a    | 1407 | 32      | 14,22,23     | 1.28 | 1 (7%)      | 17,32,35    | 0.97 | 1 (5%)      |
| 32  | UR3  | 1a    | 1498 | 32      | 13,22,23     | 0.81 | 1 (7%)      | 18,32,35    | 0.84 | 1 (5%)      |
| 32  | MA6  | 1a    | 1518 | 32      | 18,26,27     | 0.96 | 1 (5%)      | 15,38,41    | 2.47 | 4 (26%)     |
| 32  | MA6  | 1a    | 1519 | 32      | 18,26,27     | 0.97 | 1 (5%)      | 15,38,41    | 2.53 | 3 (20%)     |

| Mol | Type | Chain | Res  | Link    | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|---------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |         | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 32  | PSU  | 1a    | 516  | 32,56   | 15,21,22     | 1.28 | 2 (13%)  | 16,30,33    | 2.14 | 3 (18%)  |
| 32  | 7MG  | 1a    | 527  | 32,56   | 20,26,27     | 1.46 | 2 (10%)  | 23,39,42    | 3.23 | 5 (21%)  |
| 32  | M2G  | 1a    | 966  | 32      | 18,27,28     | 1.35 | 3 (16%)  | 22,40,43    | 1.78 | 4 (18%)  |
| 32  | 5MC  | 1a    | 967  | 32      | 14,22,23     | 1.34 | 1 (7%)   | 17,32,35    | 0.83 | 1 (5%)   |
| 43  | 0TD  | 1l    | 92   | 43      | 4,9,10       | 3.14 | 1 (25%)  | 4,11,13     | 9.84 | 1 (25%)  |
| 54  | PSU  | 1w    | 32   | 54      | 15,21,22     | 1.16 | 1 (6%)   | 16,30,33    | 2.20 | 3 (18%)  |
| 54  | MIA  | 1w    | 37   | 54      | 22,31,32     | 1.71 | 2 (9%)   | 26,44,47    | 1.25 | 4 (15%)  |
| 54  | PSU  | 1w    | 39   | 54      | 15,21,22     | 1.33 | 1 (6%)   | 16,30,33    | 2.31 | 4 (25%)  |
| 54  | 7MG  | 1w    | 46   | 54      | 20,26,27     | 1.33 | 2 (10%)  | 23,39,42    | 3.22 | 6 (26%)  |
| 54  | 5MU  | 1w    | 54   | 54      | 13,22,23     | 0.62 | 0        | 16,32,35    | 2.79 | 2 (12%)  |
| 54  | PSU  | 1w    | 55   | 54      | 15,21,22     | 1.19 | 1 (6%)   | 16,30,33    | 2.50 | 4 (25%)  |
| 54  | 4SU  | 1w    | 8    | 54      | 12,21,22     | 0.64 | 0        | 15,30,33    | 1.14 | 1 (6%)   |
| 55  | 5MC  | 1x    | 32   | 55      | 14,22,23     | 1.34 | 1 (7%)   | 17,32,35    | 0.92 | 1 (5%)   |
| 55  | 5MU  | 1x    | 54   | 55,56   | 13,22,23     | 0.60 | 0        | 16,32,35    | 2.84 | 2 (12%)  |
| 55  | PSU  | 1x    | 55   | 55      | 15,21,22     | 1.60 | 1 (6%)   | 16,30,33    | 2.36 | 4 (25%)  |
| 55  | M3O  | 1x    | 76   | 55,56   | 27,34,35     | 1.28 | 3 (11%)  | 28,47,50    | 2.61 | 5 (17%)  |
| 55  | 4SU  | 1x    | 8    | 55      | 12,21,22     | 1.03 | 1 (8%)   | 15,30,33    | 1.44 | 1 (6%)   |
| 54  | PSU  | 1y    | 32   | 54      | 15,21,22     | 1.13 | 1 (6%)   | 16,30,33    | 2.20 | 3 (18%)  |
| 54  | MIA  | 1y    | 37   | 54      | 17,24,32     | 1.16 | 2 (11%)  | 16,35,47    | 1.91 | 1 (6%)   |
| 54  | PSU  | 1y    | 39   | 54      | 15,21,22     | 1.32 | 2 (13%)  | 16,30,33    | 2.20 | 3 (18%)  |
| 54  | 7MG  | 1y    | 46   | 54      | 20,26,27     | 1.58 | 2 (10%)  | 23,39,42    | 3.30 | 6 (26%)  |
| 54  | 5MU  | 1y    | 54   | 54      | 13,22,23     | 0.48 | 0        | 16,32,35    | 3.32 | 2 (12%)  |
| 54  | PSU  | 1y    | 55   | 54      | 15,21,22     | 1.23 | 1 (6%)   | 16,30,33    | 2.21 | 3 (18%)  |
| 54  | 4SU  | 1y    | 8    | 54      | 12,21,22     | 0.74 | 1 (8%)   | 15,30,33    | 1.04 | 1 (6%)   |
| 1   | PSU  | 2A    | 1911 | 1       | 15,21,22     | 1.37 | 1 (6%)   | 16,30,33    | 2.25 | 4 (25%)  |
| 1   | 5MU  | 2A    | 1915 | 1       | 13,22,23     | 0.59 | 0        | 16,32,35    | 2.55 | 2 (12%)  |
| 1   | PSU  | 2A    | 1917 | 1       | 15,21,22     | 1.28 | 1 (6%)   | 16,30,33    | 2.39 | 4 (25%)  |
| 1   | 4OC  | 2A    | 1920 | 1       | 15,22,24     | 0.55 | 0        | 20,31,35    | 1.29 | 1 (5%)   |
| 1   | 5MU  | 2A    | 1939 | 1,56    | 13,22,23     | 0.67 | 0        | 16,32,35    | 2.23 | 2 (12%)  |
| 1   | 5MC  | 2A    | 1942 | 1       | 14,22,23     | 1.30 | 1 (7%)   | 17,32,35    | 1.02 | 1 (5%)   |
| 1   | 5MC  | 2A    | 1962 | 1,56    | 14,22,23     | 1.27 | 1 (7%)   | 17,32,35    | 0.98 | 1 (5%)   |
| 1   | OMG  | 2A    | 2251 | 1,55,56 | 18,26,27     | 1.16 | 2 (11%)  | 21,38,41    | 1.84 | 4 (19%)  |
| 1   | 2MA  | 2A    | 2503 | 1,56    | 17,25,26     | 1.47 | 3 (17%)  | 18,37,40    | 2.56 | 2 (11%)  |
| 1   | 2MU  | 2A    | 2552 | 1,56    | 14,22,24     | 0.83 | 0        | 19,31,36    | 1.60 | 1 (5%)   |
| 1   | PSU  | 2A    | 2605 | 1       | 15,21,22     | 1.33 | 1 (6%)   | 16,30,33    | 1.96 | 4 (25%)  |

| Mol | Type | Chain | Res  | Link  | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|-------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 32  | 2MG  | 2a    | 1207 | 32    | 18,26,27     | 1.19 | 2 (11%)  | 21,38,41    | 2.31 | 7 (33%)  |
| 32  | 5MC  | 2a    | 1400 | 32    | 14,22,23     | 1.29 | 1 (7%)   | 17,32,35    | 0.96 | 1 (5%)   |
| 32  | 4OC  | 2a    | 1402 | 32    | 15,23,24     | 0.56 | 0        | 21,32,35    | 1.93 | 3 (14%)  |
| 32  | 5MC  | 2a    | 1404 | 32    | 14,22,23     | 1.36 | 1 (7%)   | 17,32,35    | 0.92 | 1 (5%)   |
| 32  | 5MC  | 2a    | 1407 | 32    | 14,22,23     | 1.30 | 1 (7%)   | 17,32,35    | 1.01 | 1 (5%)   |
| 32  | UR3  | 2a    | 1498 | 32    | 13,22,23     | 0.74 | 1 (7%)   | 18,32,35    | 0.79 | 1 (5%)   |
| 32  | MA6  | 2a    | 1518 | 32    | 18,26,27     | 0.94 | 1 (5%)   | 15,38,41    | 2.45 | 4 (26%)  |
| 32  | MA6  | 2a    | 1519 | 32    | 18,26,27     | 0.98 | 1 (5%)   | 15,38,41    | 2.23 | 2 (13%)  |
| 32  | PSU  | 2a    | 516  | 32    | 15,21,22     | 1.24 | 1 (6%)   | 16,30,33    | 2.17 | 3 (18%)  |
| 32  | 7MG  | 2a    | 527  | 32,56 | 20,26,27     | 1.50 | 2 (10%)  | 23,39,42    | 3.09 | 5 (21%)  |
| 32  | M2G  | 2a    | 966  | 32    | 18,27,28     | 1.44 | 3 (16%)  | 22,40,43    | 1.87 | 3 (13%)  |
| 32  | 5MC  | 2a    | 967  | 32,56 | 14,22,23     | 1.33 | 1 (7%)   | 17,32,35    | 0.87 | 1 (5%)   |
| 43  | 0TD  | 2l    | 92   | 43    | 4,9,10       | 3.07 | 1 (25%)  | 4,11,13     | 5.88 | 1 (25%)  |
| 54  | PSU  | 2w    | 32   | 54    | 15,21,22     | 1.30 | 1 (6%)   | 16,30,33    | 2.34 | 4 (25%)  |
| 54  | MIA  | 2w    | 37   | 54    | 17,24,32     | 1.14 | 2 (11%)  | 16,35,47    | 1.89 | 1 (6%)   |
| 54  | PSU  | 2w    | 39   | 54    | 15,21,22     | 1.26 | 1 (6%)   | 16,30,33    | 2.47 | 3 (18%)  |
| 54  | 7MG  | 2w    | 46   | 54    | 20,26,27     | 1.50 | 2 (10%)  | 23,39,42    | 2.86 | 4 (17%)  |
| 54  | 5MU  | 2w    | 54   | 54    | 13,22,23     | 0.64 | 0        | 16,32,35    | 2.99 | 2 (12%)  |
| 54  | PSU  | 2w    | 55   | 54    | 15,21,22     | 1.13 | 1 (6%)   | 16,30,33    | 2.44 | 4 (25%)  |
| 54  | 4SU  | 2w    | 8    | 54,56 | 12,21,22     | 0.72 | 0        | 15,30,33    | 1.24 | 1 (6%)   |
| 55  | 5MC  | 2x    | 32   | 55    | 14,22,23     | 1.28 | 1 (7%)   | 17,32,35    | 0.91 | 1 (5%)   |
| 55  | 5MU  | 2x    | 54   | 55    | 13,22,23     | 0.62 | 0        | 16,32,35    | 2.53 | 2 (12%)  |
| 55  | PSU  | 2x    | 55   | 55    | 15,21,22     | 1.33 | 1 (6%)   | 16,30,33    | 2.19 | 3 (18%)  |
| 55  | M3O  | 2x    | 76   | 55,56 | 27,34,35     | 1.22 | 2 (7%)   | 28,47,50    | 2.85 | 6 (21%)  |
| 55  | 4SU  | 2x    | 8    | 55    | 12,21,22     | 0.79 | 1 (8%)   | 15,30,33    | 1.56 | 1 (6%)   |
| 54  | PSU  | 2y    | 32   | 54    | 15,21,22     | 1.15 | 1 (6%)   | 16,30,33    | 2.23 | 3 (18%)  |
| 54  | MIA  | 2y    | 37   | 54    | 17,24,32     | 1.22 | 2 (11%)  | 16,35,47    | 1.90 | 1 (6%)   |
| 54  | PSU  | 2y    | 39   | 54    | 15,21,22     | 1.37 | 1 (6%)   | 16,30,33    | 1.94 | 5 (31%)  |
| 54  | 7MG  | 2y    | 46   | 54    | 20,26,27     | 1.55 | 2 (10%)  | 23,39,42    | 3.14 | 8 (34%)  |
| 54  | 5MU  | 2y    | 54   | 54    | 13,22,23     | 0.59 | 0        | 16,32,35    | 2.81 | 2 (12%)  |
| 54  | PSU  | 2y    | 55   | 54    | 15,21,22     | 1.32 | 1 (6%)   | 16,30,33    | 2.20 | 4 (25%)  |
| 54  | 4SU  | 2y    | 8    | 54    | 12,21,22     | 0.70 | 0        | 15,30,33    | 1.11 | 1 (6%)   |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical



component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res  | Link    | Chirals | Torsions   | Rings   |
|-----|------|-------|------|---------|---------|------------|---------|
| 1   | PSU  | 1A    | 1911 | 1       | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | 5MU  | 1A    | 1915 | 1       | -       | 0/3/25/26  | 0/2/2/2 |
| 1   | PSU  | 1A    | 1917 | 1       | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | 4OC  | 1A    | 1920 | 1       | -       | 0/5/27/30  | 0/2/2/2 |
| 1   | 5MU  | 1A    | 1939 | 1,56    | -       | 0/3/25/26  | 0/2/2/2 |
| 1   | 5MC  | 1A    | 1942 | 1       | -       | 0/3/25/26  | 0/2/2/2 |
| 1   | 5MC  | 1A    | 1962 | 1       | -       | 0/3/25/26  | 0/2/2/2 |
| 1   | OMG  | 1A    | 2251 | 1,55,56 | -       | 0/5/27/28  | 0/3/3/3 |
| 1   | 2MA  | 1A    | 2503 | 1,56    | -       | 0/3/25/26  | 0/3/3/3 |
| 1   | 2MU  | 1A    | 2552 | 1,56    | -       | 0/5/27/28  | 0/2/2/2 |
| 1   | PSU  | 1A    | 2605 | 1       | -       | 0/7/25/26  | 0/2/2/2 |
| 32  | 2MG  | 1a    | 1207 | 32      | -       | 0/5/27/28  | 0/3/3/3 |
| 32  | 5MC  | 1a    | 1400 | 32      | -       | 0/3/25/26  | 0/2/2/2 |
| 32  | 4OC  | 1a    | 1402 | 32      | -       | 0/7/29/30  | 0/2/2/2 |
| 32  | 5MC  | 1a    | 1404 | 32      | -       | 0/3/25/26  | 0/2/2/2 |
| 32  | 5MC  | 1a    | 1407 | 32      | -       | 0/3/25/26  | 0/2/2/2 |
| 32  | UR3  | 1a    | 1498 | 32      | -       | 0/3/25/26  | 0/2/2/2 |
| 32  | MA6  | 1a    | 1518 | 32      | -       | 0/7/29/30  | 0/3/3/3 |
| 32  | MA6  | 1a    | 1519 | 32      | -       | 0/7/29/30  | 0/3/3/3 |
| 32  | PSU  | 1a    | 516  | 32,56   | -       | 0/7/25/26  | 0/2/2/2 |
| 32  | 7MG  | 1a    | 527  | 32,56   | -       | 0/7/37/38  | 0/3/3/3 |
| 32  | M2G  | 1a    | 966  | 32      | -       | 0/7/29/30  | 0/3/3/3 |
| 32  | 5MC  | 1a    | 967  | 32      | -       | 0/3/25/26  | 0/2/2/2 |
| 43  | 0TD  | 1l    | 92   | 43      | -       | 0/2/12/14  | 0/0/0/0 |
| 54  | PSU  | 1w    | 32   | 54      | -       | 0/7/25/26  | 0/2/2/2 |
| 54  | MIA  | 1w    | 37   | 54      | -       | 0/11/33/34 | 0/3/3/3 |
| 54  | PSU  | 1w    | 39   | 54      | -       | 0/7/25/26  | 0/2/2/2 |
| 54  | 7MG  | 1w    | 46   | 54      | -       | 0/7/37/38  | 0/3/3/3 |
| 54  | 5MU  | 1w    | 54   | 54      | -       | 0/3/25/26  | 0/2/2/2 |
| 54  | PSU  | 1w    | 55   | 54      | -       | 0/7/25/26  | 0/2/2/2 |
| 54  | 4SU  | 1w    | 8    | 54      | -       | 0/3/25/26  | 0/2/2/2 |
| 55  | 5MC  | 1x    | 32   | 55      | -       | 0/3/25/26  | 0/2/2/2 |
| 55  | 5MU  | 1x    | 54   | 55,56   | -       | 0/3/25/26  | 0/2/2/2 |
| 55  | PSU  | 1x    | 55   | 55      | -       | 0/7/25/26  | 0/2/2/2 |
| 55  | M3O  | 1x    | 76   | 55,56   | -       | 1/18/40/41 | 0/3/3/3 |
| 55  | 4SU  | 1x    | 8    | 55      | -       | 0/3/25/26  | 0/2/2/2 |
| 54  | PSU  | 1y    | 32   | 54      | -       | 0/7/25/26  | 0/2/2/2 |
| 54  | MIA  | 1y    | 37   | 54      | -       | 0/3/25/34  | 0/3/3/3 |
| 54  | PSU  | 1y    | 39   | 54      | -       | 0/7/25/26  | 0/2/2/2 |
| 54  | 7MG  | 1y    | 46   | 54      | -       | 0/7/37/38  | 0/3/3/3 |
| 54  | 5MU  | 1y    | 54   | 54      | -       | 0/3/25/26  | 0/2/2/2 |

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| Mol | Type | Chain | Res  | Link    | Chirals | Torsions   | Rings   |
|-----|------|-------|------|---------|---------|------------|---------|
| 54  | PSU  | 1y    | 55   | 54      | -       | 0/7/25/26  | 0/2/2/2 |
| 54  | 4SU  | 1y    | 8    | 54      | -       | 0/3/25/26  | 0/2/2/2 |
| 1   | PSU  | 2A    | 1911 | 1       | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | 5MU  | 2A    | 1915 | 1       | -       | 0/3/25/26  | 0/2/2/2 |
| 1   | PSU  | 2A    | 1917 | 1       | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | 4OC  | 2A    | 1920 | 1       | -       | 0/5/27/30  | 0/2/2/2 |
| 1   | 5MU  | 2A    | 1939 | 1,56    | -       | 0/3/25/26  | 0/2/2/2 |
| 1   | 5MC  | 2A    | 1942 | 1       | -       | 0/3/25/26  | 0/2/2/2 |
| 1   | 5MC  | 2A    | 1962 | 1,56    | -       | 0/3/25/26  | 0/2/2/2 |
| 1   | OMG  | 2A    | 2251 | 1,55,56 | -       | 0/5/27/28  | 0/3/3/3 |
| 1   | 2MA  | 2A    | 2503 | 1,56    | -       | 0/3/25/26  | 0/3/3/3 |
| 1   | 2MU  | 2A    | 2552 | 1,56    | -       | 0/5/27/28  | 0/2/2/2 |
| 1   | PSU  | 2A    | 2605 | 1       | -       | 0/7/25/26  | 0/2/2/2 |
| 32  | 2MG  | 2a    | 1207 | 32      | -       | 0/5/27/28  | 0/3/3/3 |
| 32  | 5MC  | 2a    | 1400 | 32      | -       | 0/3/25/26  | 0/2/2/2 |
| 32  | 4OC  | 2a    | 1402 | 32      | -       | 0/7/29/30  | 0/2/2/2 |
| 32  | 5MC  | 2a    | 1404 | 32      | -       | 0/3/25/26  | 0/2/2/2 |
| 32  | 5MC  | 2a    | 1407 | 32      | -       | 0/3/25/26  | 0/2/2/2 |
| 32  | UR3  | 2a    | 1498 | 32      | -       | 0/3/25/26  | 0/2/2/2 |
| 32  | MA6  | 2a    | 1518 | 32      | -       | 0/7/29/30  | 0/3/3/3 |
| 32  | MA6  | 2a    | 1519 | 32      | -       | 0/7/29/30  | 0/3/3/3 |
| 32  | PSU  | 2a    | 516  | 32      | -       | 0/7/25/26  | 0/2/2/2 |
| 32  | 7MG  | 2a    | 527  | 32,56   | -       | 0/7/37/38  | 0/3/3/3 |
| 32  | M2G  | 2a    | 966  | 32      | -       | 0/7/29/30  | 0/3/3/3 |
| 32  | 5MC  | 2a    | 967  | 32,56   | -       | 0/3/25/26  | 0/2/2/2 |
| 43  | 0TD  | 2l    | 92   | 43      | -       | 0/2/12/14  | 0/0/0/0 |
| 54  | PSU  | 2w    | 32   | 54      | -       | 0/7/25/26  | 0/2/2/2 |
| 54  | MIA  | 2w    | 37   | 54      | -       | 0/3/25/34  | 0/3/3/3 |
| 54  | PSU  | 2w    | 39   | 54      | -       | 0/7/25/26  | 0/2/2/2 |
| 54  | 7MG  | 2w    | 46   | 54      | -       | 0/7/37/38  | 0/3/3/3 |
| 54  | 5MU  | 2w    | 54   | 54      | -       | 0/3/25/26  | 0/2/2/2 |
| 54  | PSU  | 2w    | 55   | 54      | -       | 0/7/25/26  | 0/2/2/2 |
| 54  | 4SU  | 2w    | 8    | 54,56   | -       | 0/3/25/26  | 0/2/2/2 |
| 55  | 5MC  | 2x    | 32   | 55      | -       | 0/3/25/26  | 0/2/2/2 |
| 55  | 5MU  | 2x    | 54   | 55      | -       | 0/3/25/26  | 0/2/2/2 |
| 55  | PSU  | 2x    | 55   | 55      | -       | 0/7/25/26  | 0/2/2/2 |
| 55  | M3O  | 2x    | 76   | 55,56   | -       | 1/18/40/41 | 0/3/3/3 |
| 55  | 4SU  | 2x    | 8    | 55      | -       | 0/3/25/26  | 0/2/2/2 |
| 54  | PSU  | 2y    | 32   | 54      | -       | 0/7/25/26  | 0/2/2/2 |
| 54  | MIA  | 2y    | 37   | 54      | -       | 0/3/25/34  | 0/3/3/3 |
| 54  | PSU  | 2y    | 39   | 54      | -       | 0/7/25/26  | 0/2/2/2 |
| 54  | 7MG  | 2y    | 46   | 54      | -       | 0/7/37/38  | 0/3/3/3 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 54  | 5MU  | 2y    | 54  | 54   | -       | 0/3/25/26 | 0/2/2/2 |
| 54  | PSU  | 2y    | 55  | 54   | -       | 0/7/25/26 | 0/2/2/2 |
| 54  | 4SU  | 2y    | 8   | 54   | -       | 0/3/25/26 | 0/2/2/2 |

All (97) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 54  | 1w    | 37   | MIA  | C2-S10  | -6.67 | 1.70        | 1.75     |
| 43  | 2l    | 92   | 0TD  | CB-SB   | -5.91 | 1.69        | 1.84     |
| 43  | 1l    | 92   | 0TD  | CB-SB   | -5.88 | 1.69        | 1.84     |
| 55  | 1x    | 55   | PSU  | C5-C1'  | -5.18 | 1.47        | 1.52     |
| 1   | 1A    | 2605 | PSU  | C5-C1'  | -4.44 | 1.48        | 1.52     |
| 1   | 2A    | 1911 | PSU  | C5-C1'  | -4.21 | 1.48        | 1.52     |
| 1   | 2A    | 2605 | PSU  | C5-C1'  | -4.17 | 1.48        | 1.52     |
| 55  | 2x    | 55   | PSU  | C5-C1'  | -4.16 | 1.48        | 1.52     |
| 1   | 1A    | 1911 | PSU  | C5-C1'  | -4.10 | 1.48        | 1.52     |
| 1   | 1A    | 1917 | PSU  | C5-C1'  | -4.00 | 1.48        | 1.52     |
| 54  | 2y    | 55   | PSU  | C5-C1'  | -3.98 | 1.48        | 1.52     |
| 54  | 2w    | 32   | PSU  | C5-C1'  | -3.94 | 1.48        | 1.52     |
| 54  | 1w    | 39   | PSU  | C5-C1'  | -3.92 | 1.48        | 1.52     |
| 1   | 2A    | 1917 | PSU  | C5-C1'  | -3.85 | 1.48        | 1.52     |
| 54  | 2y    | 39   | PSU  | C5-C1'  | -3.75 | 1.49        | 1.52     |
| 32  | 2a    | 516  | PSU  | C5-C1'  | -3.64 | 1.49        | 1.52     |
| 54  | 2w    | 39   | PSU  | C5-C1'  | -3.62 | 1.49        | 1.52     |
| 32  | 1a    | 516  | PSU  | C5-C1'  | -3.56 | 1.49        | 1.52     |
| 54  | 1y    | 39   | PSU  | C5-C1'  | -3.54 | 1.49        | 1.52     |
| 54  | 1y    | 55   | PSU  | C5-C1'  | -3.48 | 1.49        | 1.52     |
| 54  | 1w    | 32   | PSU  | C5-C1'  | -3.30 | 1.49        | 1.52     |
| 55  | 1x    | 8    | 4SU  | C2-N3   | -3.30 | 1.31        | 1.38     |
| 54  | 1w    | 55   | PSU  | C5-C1'  | -3.29 | 1.49        | 1.52     |
| 55  | 1x    | 76   | M3O  | C5-N7   | -3.27 | 1.27        | 1.39     |
| 55  | 2x    | 76   | M3O  | C5-C4   | -3.20 | 1.33        | 1.40     |
| 54  | 2y    | 32   | PSU  | C5-C1'  | -3.14 | 1.49        | 1.52     |
| 55  | 1x    | 76   | M3O  | C5-C4   | -3.10 | 1.33        | 1.40     |
| 54  | 2w    | 55   | PSU  | C5-C1'  | -3.09 | 1.49        | 1.52     |
| 54  | 1y    | 32   | PSU  | C5-C1'  | -3.02 | 1.49        | 1.52     |
| 55  | 2x    | 8    | 4SU  | C2-N3   | -2.45 | 1.33        | 1.38     |
| 54  | 1y    | 39   | PSU  | O4'-C1' | -2.34 | 1.40        | 1.44     |
| 1   | 1A    | 2605 | PSU  | C2-N3   | -2.26 | 1.33        | 1.38     |
| 1   | 1A    | 2552 | 2MU  | C2-N3   | -2.05 | 1.33        | 1.38     |
| 1   | 1A    | 1917 | PSU  | C2-N3   | -2.04 | 1.33        | 1.38     |
| 32  | 1a    | 516  | PSU  | O4'-C1' | -2.02 | 1.41        | 1.44     |

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| Mol | Chain | Res  | Type | Atoms              | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------------------|-------|-------------|----------|
| 54  | 1y    | 8    | 4SU  | C2-N3              | -2.01 | 1.34        | 1.38     |
| 32  | 2a    | 1498 | UR3  | C4-N3              | 2.01  | 1.41        | 1.38     |
| 54  | 2w    | 37   | MIA  | C2-N3              | 2.33  | 1.36        | 1.32     |
| 32  | 1a    | 1498 | UR3  | C4-N3              | 2.38  | 1.41        | 1.38     |
| 54  | 1y    | 37   | MIA  | C2-N3              | 2.46  | 1.36        | 1.32     |
| 54  | 2y    | 37   | MIA  | C2-N3              | 2.48  | 1.36        | 1.32     |
| 1   | 2A    | 2503 | 2MA  | C5-C4              | 2.72  | 1.46        | 1.40     |
| 1   | 1A    | 2503 | 2MA  | C5-C4              | 2.76  | 1.46        | 1.40     |
| 32  | 1a    | 966  | M2G  | C2-N2              | 2.93  | 1.39        | 1.34     |
| 32  | 1a    | 1207 | 2MG  | C5-C4              | 2.94  | 1.47        | 1.40     |
| 32  | 1a    | 1519 | MA6  | C5-C4              | 2.97  | 1.47        | 1.40     |
| 32  | 1a    | 1518 | MA6  | C5-C4              | 3.00  | 1.47        | 1.40     |
| 32  | 2a    | 1207 | 2MG  | C5-C4              | 3.02  | 1.47        | 1.40     |
| 1   | 1A    | 2251 | OMG  | C5-C4              | 3.08  | 1.47        | 1.40     |
| 54  | 1w    | 37   | MIA  | C5-C4              | 3.08  | 1.47        | 1.40     |
| 32  | 1a    | 966  | M2G  | C5-C4              | 3.09  | 1.47        | 1.40     |
| 1   | 2A    | 2251 | OMG  | C5-C4              | 3.12  | 1.47        | 1.40     |
| 54  | 2w    | 46   | 7MG  | C5-C4              | 3.12  | 1.47        | 1.39     |
| 32  | 2a    | 966  | M2G  | C5-C4              | 3.15  | 1.47        | 1.40     |
| 32  | 2a    | 1518 | MA6  | C5-C4              | 3.16  | 1.47        | 1.40     |
| 54  | 1w    | 46   | 7MG  | C5-C4              | 3.20  | 1.47        | 1.39     |
| 54  | 2y    | 46   | 7MG  | C5-C4              | 3.23  | 1.47        | 1.39     |
| 32  | 2a    | 1519 | MA6  | C5-C4              | 3.26  | 1.47        | 1.40     |
| 32  | 2a    | 966  | M2G  | C2-N2              | 3.29  | 1.40        | 1.34     |
| 32  | 2a    | 527  | 7MG  | C5-C4              | 3.32  | 1.47        | 1.39     |
| 54  | 2w    | 37   | MIA  | C5-C4              | 3.32  | 1.48        | 1.40     |
| 54  | 1y    | 37   | MIA  | C5-C4              | 3.33  | 1.48        | 1.40     |
| 1   | 2A    | 2251 | OMG  | C6-C5              | 3.35  | 1.48        | 1.41     |
| 32  | 1a    | 527  | 7MG  | C5-C4              | 3.42  | 1.48        | 1.39     |
| 54  | 1y    | 46   | 7MG  | C5-C4              | 3.48  | 1.48        | 1.39     |
| 54  | 2y    | 37   | MIA  | C5-C4              | 3.50  | 1.48        | 1.40     |
| 1   | 1A    | 2251 | OMG  | C6-C5              | 3.50  | 1.48        | 1.41     |
| 1   | 2A    | 2503 | 2MA  | C6-N6              | 3.59  | 1.35        | 1.29     |
| 32  | 1a    | 966  | M2G  | C6-C5              | 3.60  | 1.48        | 1.41     |
| 55  | 1x    | 76   | M3O  | O3 <sup>1</sup> -C | 3.61  | 1.42        | 1.34     |
| 1   | 1A    | 2503 | 2MA  | C6-N6              | 3.64  | 1.35        | 1.29     |
| 32  | 1a    | 1207 | 2MG  | C6-C5              | 3.64  | 1.48        | 1.41     |
| 1   | 2A    | 2503 | 2MA  | C6-C5              | 3.65  | 1.47        | 1.40     |
| 32  | 2a    | 1207 | 2MG  | C6-C5              | 3.67  | 1.48        | 1.41     |
| 32  | 2a    | 966  | M2G  | C6-C5              | 3.75  | 1.48        | 1.41     |
| 1   | 1A    | 2503 | 2MA  | C6-C5              | 3.77  | 1.47        | 1.40     |
| 55  | 2x    | 76   | M3O  | O3 <sup>1</sup> -C | 3.90  | 1.43        | 1.34     |

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| Mol | Chain | Res  | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 1   | 1A    | 1942 | 5MC  | C5-C4 | 4.09 | 1.47        | 1.41     |
| 54  | 1w    | 46   | 7MG  | C6-C5 | 4.12 | 1.47        | 1.41     |
| 1   | 2A    | 1962 | 5MC  | C5-C4 | 4.37 | 1.48        | 1.41     |
| 32  | 2a    | 1400 | 5MC  | C5-C4 | 4.38 | 1.48        | 1.41     |
| 32  | 1a    | 1407 | 5MC  | C5-C4 | 4.38 | 1.48        | 1.41     |
| 55  | 2x    | 32   | 5MC  | C5-C4 | 4.46 | 1.48        | 1.41     |
| 32  | 2a    | 1407 | 5MC  | C5-C4 | 4.51 | 1.48        | 1.41     |
| 32  | 1a    | 527  | 7MG  | C6-C5 | 4.58 | 1.47        | 1.41     |
| 1   | 2A    | 1942 | 5MC  | C5-C4 | 4.59 | 1.48        | 1.41     |
| 32  | 1a    | 1404 | 5MC  | C5-C4 | 4.65 | 1.48        | 1.41     |
| 32  | 2a    | 967  | 5MC  | C5-C4 | 4.69 | 1.48        | 1.41     |
| 32  | 2a    | 527  | 7MG  | C6-C5 | 4.71 | 1.48        | 1.41     |
| 32  | 1a    | 967  | 5MC  | C5-C4 | 4.74 | 1.48        | 1.41     |
| 55  | 1x    | 32   | 5MC  | C5-C4 | 4.75 | 1.48        | 1.41     |
| 1   | 1A    | 1962 | 5MC  | C5-C4 | 4.79 | 1.48        | 1.41     |
| 32  | 2a    | 1404 | 5MC  | C5-C4 | 4.82 | 1.48        | 1.41     |
| 54  | 2y    | 46   | 7MG  | C6-C5 | 4.97 | 1.48        | 1.41     |
| 54  | 1y    | 46   | 7MG  | C6-C5 | 5.00 | 1.48        | 1.41     |
| 54  | 2w    | 46   | 7MG  | C6-C5 | 5.01 | 1.48        | 1.41     |
| 32  | 1a    | 1400 | 5MC  | C5-C4 | 5.05 | 1.49        | 1.41     |

All (233) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms     | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|--------|-------------|----------|
| 55  | 1x    | 76   | M3O  | N3-C2-N1  | -11.68 | 119.69      | 128.87   |
| 43  | 2l    | 92   | 0TD  | CSB-SB-CB | -11.61 | 79.73       | 101.44   |
| 55  | 2x    | 76   | M3O  | N3-C2-N1  | -11.43 | 119.89      | 128.87   |
| 54  | 1y    | 46   | 7MG  | C5-C4-N3  | -8.96  | 117.61      | 126.74   |
| 32  | 1a    | 527  | 7MG  | C5-C4-N3  | -8.82  | 117.75      | 126.74   |
| 54  | 1y    | 54   | 5MU  | C5-C4-N3  | -8.72  | 118.03      | 125.35   |
| 32  | 2a    | 527  | 7MG  | C5-C4-N3  | -8.21  | 118.37      | 126.74   |
| 54  | 1w    | 54   | 5MU  | C5-C4-N3  | -8.08  | 118.57      | 125.35   |
| 54  | 2w    | 54   | 5MU  | C5-C4-N3  | -7.93  | 118.70      | 125.35   |
| 54  | 2w    | 46   | 7MG  | C5-C4-N3  | -7.86  | 118.73      | 126.74   |
| 55  | 1x    | 54   | 5MU  | C5-C4-N3  | -7.77  | 118.82      | 125.35   |
| 54  | 2y    | 54   | 5MU  | C5-C4-N3  | -7.52  | 119.03      | 125.35   |
| 32  | 1a    | 1518 | MA6  | N3-C2-N1  | -7.46  | 123.01      | 128.87   |
| 1   | 2A    | 1915 | 5MU  | C5-C4-N3  | -7.44  | 119.11      | 125.35   |
| 54  | 2y    | 46   | 7MG  | C5-C4-N3  | -7.38  | 119.22      | 126.74   |
| 32  | 1a    | 1519 | MA6  | N3-C2-N1  | -7.32  | 123.12      | 128.87   |
| 55  | 2x    | 54   | 5MU  | C5-C4-N3  | -7.30  | 119.22      | 125.35   |
| 32  | 2a    | 1518 | MA6  | N3-C2-N1  | -7.23  | 123.19      | 128.87   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 54  | 1y    | 37   | MIA  | N3-C2-N1   | -7.13 | 123.27      | 128.87   |
| 54  | 2y    | 37   | MIA  | N3-C2-N1   | -6.94 | 123.42      | 128.87   |
| 54  | 2w    | 37   | MIA  | N3-C2-N1   | -6.93 | 123.43      | 128.87   |
| 1   | 1A    | 1915 | 5MU  | C5-C4-N3   | -6.89 | 119.56      | 125.35   |
| 1   | 2A    | 1939 | 5MU  | C5-C4-N3   | -6.79 | 119.65      | 125.35   |
| 54  | 1w    | 46   | 7MG  | C5-C4-N3   | -6.73 | 119.89      | 126.74   |
| 1   | 1A    | 1939 | 5MU  | C5-C4-N3   | -6.68 | 119.74      | 125.35   |
| 32  | 2a    | 1519 | MA6  | N3-C2-N1   | -6.67 | 123.63      | 128.87   |
| 54  | 1w    | 46   | 7MG  | C5-C6-N1   | -5.82 | 114.73      | 123.39   |
| 55  | 2x    | 8    | 4SU  | C5-C4-N3   | -5.43 | 117.80      | 123.56   |
| 32  | 1a    | 527  | 7MG  | C5-C6-N1   | -5.17 | 115.70      | 123.39   |
| 32  | 2a    | 1402 | 4OC  | CM4-N4-C4  | -5.12 | 118.56      | 122.87   |
| 54  | 1y    | 46   | 7MG  | C5-C6-N1   | -5.11 | 115.79      | 123.39   |
| 55  | 1x    | 8    | 4SU  | C5-C4-N3   | -5.08 | 118.17      | 123.56   |
| 54  | 2y    | 46   | 7MG  | C5-C6-N1   | -5.06 | 115.85      | 123.39   |
| 54  | 1w    | 55   | PSU  | C5-C1'-C2' | -5.00 | 106.94      | 115.44   |
| 32  | 2a    | 527  | 7MG  | C5-C6-N1   | -4.94 | 116.04      | 123.39   |
| 32  | 1a    | 1207 | 2MG  | C5-C6-N1   | -4.87 | 117.16      | 123.52   |
| 54  | 2w    | 46   | 7MG  | C5-C6-N1   | -4.81 | 116.23      | 123.39   |
| 32  | 2a    | 1207 | 2MG  | C5-C6-N1   | -4.77 | 117.29      | 123.52   |
| 32  | 1a    | 966  | M2G  | C5-C6-N1   | -4.71 | 117.37      | 123.52   |
| 55  | 2x    | 76   | M3O  | C3'-O3'-C  | -4.62 | 110.44      | 118.06   |
| 54  | 2w    | 55   | PSU  | C5-C1'-C2' | -4.45 | 107.88      | 115.44   |
| 1   | 1A    | 2251 | OMG  | C5-C6-N1   | -4.43 | 117.73      | 123.52   |
| 55  | 1x    | 76   | M3O  | C3'-O3'-C  | -4.34 | 110.90      | 118.06   |
| 32  | 2a    | 966  | M2G  | C5-C6-N1   | -4.34 | 117.85      | 123.52   |
| 32  | 1a    | 1402 | 4OC  | CM4-N4-C4  | -4.26 | 119.28      | 122.87   |
| 1   | 2A    | 2605 | PSU  | C5-C6-N1   | -4.19 | 118.54      | 124.38   |
| 1   | 1A    | 2605 | PSU  | C5-C6-N1   | -4.10 | 118.66      | 124.38   |
| 1   | 2A    | 1917 | PSU  | C5-C1'-C2' | -4.03 | 108.59      | 115.44   |
| 1   | 1A    | 2251 | OMG  | N3-C2-N1   | -4.03 | 122.08      | 127.56   |
| 54  | 2w    | 8    | 4SU  | C5-C4-N3   | -3.97 | 119.36      | 123.56   |
| 54  | 2w    | 32   | PSU  | C5-C1'-C2' | -3.96 | 108.70      | 115.44   |
| 1   | 2A    | 2251 | OMG  | C5-C6-N1   | -3.94 | 118.37      | 123.52   |
| 54  | 2w    | 32   | PSU  | C5-C6-N1   | -3.85 | 119.01      | 124.38   |
| 32  | 2a    | 1207 | 2MG  | C1'-N9-C4  | -3.84 | 122.52      | 126.81   |
| 1   | 2A    | 1917 | PSU  | C5-C6-N1   | -3.81 | 119.06      | 124.38   |
| 1   | 1A    | 1917 | PSU  | C5-C1'-C2' | -3.76 | 109.06      | 115.44   |
| 1   | 1A    | 1911 | PSU  | C5-C6-N1   | -3.69 | 119.23      | 124.38   |
| 1   | 1A    | 1911 | PSU  | C5-C1'-C2' | -3.65 | 109.23      | 115.44   |
| 55  | 1x    | 55   | PSU  | C5-C1'-C2' | -3.64 | 109.25      | 115.44   |
| 54  | 1w    | 8    | 4SU  | C5-C4-N3   | -3.64 | 119.71      | 123.56   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 54  | 1w    | 46   | 7MG  | C8-N9-C1'  | -3.63 | 111.53      | 122.43   |
| 55  | 1x    | 55   | PSU  | C5-C6-N1   | -3.63 | 119.32      | 124.38   |
| 1   | 1A    | 1917 | PSU  | C5-C6-N1   | -3.61 | 119.34      | 124.38   |
| 32  | 1a    | 1207 | 2MG  | C6-C5-C4   | -3.59 | 116.75      | 120.86   |
| 55  | 2x    | 55   | PSU  | C5-C6-N1   | -3.55 | 119.43      | 124.38   |
| 32  | 2a    | 1207 | 2MG  | C6-C5-C4   | -3.53 | 116.83      | 120.86   |
| 32  | 2a    | 516  | PSU  | C5-C6-N1   | -3.52 | 119.47      | 124.38   |
| 54  | 2y    | 55   | PSU  | C5-C6-N1   | -3.52 | 119.48      | 124.38   |
| 32  | 1a    | 516  | PSU  | C5-C6-N1   | -3.46 | 119.56      | 124.38   |
| 54  | 1w    | 39   | PSU  | C5-C6-N1   | -3.45 | 119.57      | 124.38   |
| 32  | 1a    | 1207 | 2MG  | C1'-N9-C4  | -3.44 | 122.97      | 126.81   |
| 1   | 1A    | 2251 | OMG  | C6-C5-C4   | -3.44 | 116.93      | 120.86   |
| 1   | 2A    | 2251 | OMG  | N3-C2-N1   | -3.41 | 122.92      | 127.56   |
| 54  | 1w    | 32   | PSU  | C5-C6-N1   | -3.40 | 119.64      | 124.38   |
| 54  | 2w    | 55   | PSU  | C5-C6-N1   | -3.38 | 119.67      | 124.38   |
| 1   | 2A    | 2503 | 2MA  | C1'-N9-C4  | -3.34 | 123.08      | 126.81   |
| 54  | 1y    | 8    | 4SU  | C5-C4-N3   | -3.33 | 120.03      | 123.56   |
| 32  | 1a    | 1519 | MA6  | C1'-N9-C4  | -3.32 | 123.11      | 126.81   |
| 54  | 1w    | 37   | MIA  | C12-N6-C6  | -3.27 | 119.67      | 123.46   |
| 1   | 1A    | 2605 | PSU  | C5-C1'-C2' | -3.22 | 109.97      | 115.44   |
| 54  | 2y    | 8    | 4SU  | C5-C4-N3   | -3.19 | 120.18      | 123.56   |
| 1   | 2A    | 1911 | PSU  | C5-C6-N1   | -3.18 | 119.95      | 124.38   |
| 54  | 1y    | 32   | PSU  | C5-C6-N1   | -3.17 | 119.96      | 124.38   |
| 32  | 2a    | 966  | M2G  | C6-C5-C4   | -3.16 | 117.25      | 120.86   |
| 54  | 2y    | 32   | PSU  | C5-C6-N1   | -3.14 | 120.00      | 124.38   |
| 54  | 1w    | 39   | PSU  | C5-C1'-C2' | -3.14 | 110.11      | 115.44   |
| 55  | 1x    | 76   | M3O  | OCN-CN-N   | -3.07 | 120.11      | 124.80   |
| 1   | 2A    | 2251 | OMG  | C6-C5-C4   | -3.04 | 117.38      | 120.86   |
| 54  | 1y    | 46   | 7MG  | C8-N9-C1'  | -3.02 | 113.37      | 122.43   |
| 54  | 2w    | 39   | PSU  | C5-C6-N1   | -3.02 | 120.17      | 124.38   |
| 55  | 2x    | 76   | M3O  | OCN-CN-N   | -2.98 | 120.23      | 124.80   |
| 32  | 1a    | 966  | M2G  | C6-C5-C4   | -2.96 | 117.47      | 120.86   |
| 54  | 2y    | 39   | PSU  | C5-C6-N1   | -2.95 | 120.27      | 124.38   |
| 32  | 1a    | 527  | 7MG  | C8-N9-C1'  | -2.93 | 113.64      | 122.43   |
| 54  | 2y    | 39   | PSU  | C5-C1'-C2' | -2.91 | 110.50      | 115.44   |
| 32  | 2a    | 1207 | 2MG  | CM2-N2-C2  | -2.86 | 119.81      | 123.03   |
| 32  | 1a    | 966  | M2G  | CM2-N2-C2  | -2.76 | 118.56      | 121.34   |
| 54  | 2y    | 55   | PSU  | C5-C1'-C2' | -2.74 | 110.79      | 115.44   |
| 1   | 2A    | 1911 | PSU  | C5-C1'-C2' | -2.67 | 110.91      | 115.44   |
| 32  | 1a    | 1207 | 2MG  | CM2-N2-C2  | -2.64 | 120.07      | 123.03   |
| 54  | 1w    | 55   | PSU  | C5-C6-N1   | -2.62 | 120.73      | 124.38   |
| 54  | 1w    | 37   | MIA  | C5-C6-N1   | -2.60 | 117.94      | 120.58   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 54  | 1w    | 46   | 7MG  | C5-C4-N9    | -2.56 | 102.11      | 106.25   |
| 32  | 1a    | 1207 | 2MG  | N3-C2-N1    | -2.52 | 122.41      | 126.19   |
| 54  | 1y    | 39   | PSU  | C5-C6-N1    | -2.48 | 120.92      | 124.38   |
| 1   | 2A    | 2605 | PSU  | C5-C1'-C2'  | -2.48 | 111.23      | 115.44   |
| 32  | 2a    | 1518 | MA6  | C10-N6-C9   | -2.40 | 108.11      | 115.96   |
| 32  | 2a    | 527  | 7MG  | C8-N9-C1'   | -2.40 | 115.22      | 122.43   |
| 54  | 1w    | 37   | MIA  | N3-C2-N1    | -2.29 | 122.62      | 126.84   |
| 54  | 1y    | 55   | PSU  | C5-C6-N1    | -2.28 | 121.20      | 124.38   |
| 54  | 2y    | 46   | 7MG  | C8-N9-C1'   | -2.25 | 115.67      | 122.43   |
| 55  | 1x    | 76   | M3O  | O3'-C-O     | -2.24 | 119.53      | 123.88   |
| 55  | 2x    | 76   | M3O  | O3'-C-O     | -2.18 | 119.65      | 123.88   |
| 32  | 2a    | 1518 | MA6  | C1'-N9-C4   | -2.18 | 124.38      | 126.81   |
| 32  | 1a    | 1518 | MA6  | C1'-N9-C4   | -2.17 | 124.39      | 126.81   |
| 54  | 2y    | 46   | 7MG  | N1-C2-N3    | -2.13 | 122.03      | 125.51   |
| 32  | 1a    | 1518 | MA6  | C10-N6-C9   | -2.09 | 109.13      | 115.96   |
| 1   | 1A    | 1920 | 4OC  | CM2-O2'-C2' | -2.05 | 108.84      | 114.58   |
| 54  | 1y    | 46   | 7MG  | C2-N3-C4    | 2.04  | 120.31      | 114.50   |
| 32  | 2a    | 1498 | UR3  | C3U-N3-C4   | 2.07  | 121.10      | 118.21   |
| 54  | 2y    | 46   | 7MG  | C2-N3-C4    | 2.08  | 120.42      | 114.50   |
| 54  | 2y    | 46   | 7MG  | N2-C2-N1    | 2.09  | 120.64      | 117.20   |
| 54  | 2y    | 39   | PSU  | O4'-C1'-C2' | 2.19  | 107.06      | 104.69   |
| 54  | 1w    | 55   | PSU  | O4'-C1'-C2' | 2.20  | 107.06      | 104.69   |
| 54  | 2y    | 39   | PSU  | C4-C5-C1'   | 2.20  | 124.92      | 121.22   |
| 1   | 1A    | 1920 | 4OC  | N4-C4-N3    | 2.20  | 120.34      | 116.50   |
| 32  | 1a    | 1400 | 5MC  | N4-C4-N3    | 2.24  | 120.20      | 116.92   |
| 32  | 2a    | 1207 | 2MG  | N2-C2-N1    | 2.25  | 119.55      | 116.94   |
| 32  | 1a    | 967  | 5MC  | N4-C4-N3    | 2.28  | 120.27      | 116.92   |
| 54  | 2w    | 55   | PSU  | O4'-C1'-C2' | 2.31  | 107.19      | 104.69   |
| 32  | 2a    | 967  | 5MC  | N4-C4-N3    | 2.32  | 120.32      | 116.92   |
| 32  | 2a    | 1404 | 5MC  | N4-C4-N3    | 2.36  | 120.37      | 116.92   |
| 32  | 1a    | 1498 | UR3  | C3U-N3-C4   | 2.37  | 121.53      | 118.21   |
| 1   | 2A    | 2605 | PSU  | O4'-C1'-C2' | 2.38  | 107.26      | 104.69   |
| 54  | 2w    | 32   | PSU  | O4'-C1'-C2' | 2.38  | 107.27      | 104.69   |
| 55  | 2x    | 32   | 5MC  | N4-C4-N3    | 2.43  | 120.49      | 116.92   |
| 1   | 1A    | 1962 | 5MC  | N4-C4-N3    | 2.45  | 120.51      | 116.92   |
| 1   | 1A    | 2605 | PSU  | O4'-C1'-C2' | 2.48  | 107.37      | 104.69   |
| 55  | 1x    | 32   | 5MC  | N4-C4-N3    | 2.48  | 120.56      | 116.92   |
| 1   | 2A    | 1942 | 5MC  | N4-C4-N3    | 2.49  | 120.57      | 116.92   |
| 54  | 1y    | 39   | PSU  | O4'-C1'-C2' | 2.51  | 107.41      | 104.69   |
| 32  | 1a    | 1404 | 5MC  | N4-C4-N3    | 2.52  | 120.61      | 116.92   |
| 54  | 1y    | 32   | PSU  | O4'-C1'-C2' | 2.54  | 107.44      | 104.69   |
| 32  | 1a    | 1407 | 5MC  | N4-C4-N3    | 2.55  | 120.65      | 116.92   |

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| Mol | Chain | Res  | Type | Atoms       | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|------|-------------|----------|
| 1   | 1A    | 1911 | PSU  | O4'-C1'-C2' | 2.67 | 107.57      | 104.69   |
| 1   | 2A    | 1917 | PSU  | O4'-C1'-C2' | 2.68 | 107.59      | 104.69   |
| 54  | 1w    | 39   | PSU  | O4'-C1'-C2' | 2.70 | 107.61      | 104.69   |
| 54  | 1w    | 32   | PSU  | O4'-C1'-C2' | 2.71 | 107.62      | 104.69   |
| 55  | 1x    | 76   | M3O  | O3'-C-CA    | 2.71 | 119.58      | 111.75   |
| 54  | 2y    | 55   | PSU  | O4'-C1'-C2' | 2.73 | 107.64      | 104.69   |
| 54  | 1y    | 55   | PSU  | O4'-C1'-C2' | 2.73 | 107.64      | 104.69   |
| 54  | 2w    | 39   | PSU  | O4'-C1'-C2' | 2.75 | 107.66      | 104.69   |
| 1   | 1A    | 1917 | PSU  | O4'-C1'-C2' | 2.75 | 107.66      | 104.69   |
| 54  | 2y    | 32   | PSU  | O4'-C1'-C2' | 2.77 | 107.69      | 104.69   |
| 32  | 2a    | 1407 | 5MC  | N4-C4-N3    | 2.78 | 121.00      | 116.92   |
| 55  | 1x    | 55   | PSU  | O4'-C1'-C2' | 2.78 | 107.70      | 104.69   |
| 55  | 2x    | 55   | PSU  | O4'-C1'-C2' | 2.81 | 107.73      | 104.69   |
| 55  | 2x    | 76   | M3O  | O3'-C-CA    | 2.81 | 119.88      | 111.75   |
| 1   | 2A    | 1911 | PSU  | O4'-C1'-C2' | 2.86 | 107.79      | 104.69   |
| 32  | 2a    | 1400 | 5MC  | N4-C4-N3    | 2.89 | 121.16      | 116.92   |
| 1   | 2A    | 1962 | 5MC  | N4-C4-N3    | 3.19 | 121.59      | 116.92   |
| 54  | 1w    | 37   | MIA  | C2-N1-C6    | 3.23 | 122.02      | 113.13   |
| 1   | 1A    | 1942 | 5MC  | N4-C4-N3    | 3.25 | 121.68      | 116.92   |
| 32  | 2a    | 516  | PSU  | O4'-C1'-C2' | 3.30 | 108.26      | 104.69   |
| 32  | 1a    | 516  | PSU  | O4'-C1'-C2' | 3.30 | 108.26      | 104.69   |
| 32  | 1a    | 1402 | 4OC  | C2-N3-C4    | 3.90 | 120.39      | 115.43   |
| 32  | 2a    | 1402 | 4OC  | C2-N3-C4    | 4.11 | 120.66      | 115.43   |
| 1   | 1A    | 1920 | 4OC  | C6-C5-C4    | 4.13 | 119.05      | 117.44   |
| 32  | 2a    | 1207 | 2MG  | C2-N3-C4    | 4.35 | 119.76      | 114.99   |
| 32  | 1a    | 966  | M2G  | C2-N3-C4    | 4.52 | 119.95      | 114.99   |
| 1   | 2A    | 1920 | 4OC  | C6-C5-C4    | 4.57 | 119.23      | 117.44   |
| 32  | 1a    | 1519 | MA6  | C2-N1-C6    | 4.66 | 122.64      | 111.64   |
| 32  | 2a    | 1519 | MA6  | C2-N1-C6    | 4.68 | 122.68      | 111.64   |
| 32  | 1a    | 1518 | MA6  | C2-N1-C6    | 4.74 | 122.83      | 111.64   |
| 1   | 2A    | 2605 | PSU  | C4-N3-C2    | 4.75 | 119.12      | 115.16   |
| 32  | 2a    | 1207 | 2MG  | C6-N1-C2    | 4.88 | 122.23      | 115.24   |
| 32  | 2a    | 1518 | MA6  | C2-N1-C6    | 4.90 | 123.19      | 111.64   |
| 32  | 1a    | 1207 | 2MG  | C2-N3-C4    | 4.97 | 120.44      | 114.99   |
| 32  | 2a    | 1402 | 4OC  | C6-C5-C4    | 5.04 | 119.40      | 117.42   |
| 54  | 2w    | 46   | 7MG  | C6-N1-C2    | 5.05 | 121.80      | 115.88   |
| 54  | 2y    | 39   | PSU  | C4-N3-C2    | 5.28 | 119.56      | 115.16   |
| 1   | 2A    | 1939 | 5MU  | C4-N3-C2    | 5.30 | 119.58      | 115.16   |
| 32  | 2a    | 966  | M2G  | C2-N3-C4    | 5.41 | 120.92      | 114.99   |
| 1   | 2A    | 2251 | OMG  | C6-N1-C2    | 5.43 | 122.25      | 115.88   |
| 32  | 1a    | 527  | 7MG  | C6-N1-C2    | 5.66 | 122.52      | 115.88   |
| 32  | 1a    | 1402 | 4OC  | C6-C5-C4    | 5.71 | 119.66      | 117.42   |

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| Mol | Chain | Res  | Type | Atoms      | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|------|-------------|----------|
| 32  | 1a    | 1207 | 2MG  | C6-N1-C2   | 5.83 | 123.59      | 115.24   |
| 32  | 2a    | 527  | 7MG  | C6-N1-C2   | 5.87 | 122.76      | 115.88   |
| 1   | 1A    | 2552 | 2MU  | C4-N3-C2   | 5.97 | 120.49      | 114.21   |
| 1   | 2A    | 2552 | 2MU  | C4-N3-C2   | 6.14 | 120.67      | 114.21   |
| 54  | 1y    | 46   | 7MG  | C6-N1-C2   | 6.23 | 123.19      | 115.88   |
| 55  | 2x    | 54   | 5MU  | C4-N3-C2   | 6.25 | 120.37      | 115.16   |
| 1   | 1A    | 1939 | 5MU  | C4-N3-C2   | 6.26 | 120.38      | 115.16   |
| 1   | 1A    | 2251 | OMG  | C6-N1-C2   | 6.31 | 123.27      | 115.88   |
| 1   | 1A    | 1915 | 5MU  | C4-N3-C2   | 6.48 | 120.56      | 115.16   |
| 55  | 2x    | 76   | M3O  | O4'-C1'-N9 | 6.53 | 120.44      | 108.11   |
| 1   | 1A    | 1917 | PSU  | C4-N3-C2   | 6.59 | 120.66      | 115.16   |
| 1   | 2A    | 1915 | 5MU  | C4-N3-C2   | 6.61 | 120.67      | 115.16   |
| 1   | 1A    | 2605 | PSU  | C4-N3-C2   | 6.69 | 120.74      | 115.16   |
| 54  | 2y    | 55   | PSU  | C4-N3-C2   | 6.71 | 120.76      | 115.16   |
| 54  | 2w    | 32   | PSU  | C4-N3-C2   | 6.73 | 120.78      | 115.16   |
| 32  | 1a    | 516  | PSU  | C4-N3-C2   | 6.74 | 120.78      | 115.16   |
| 32  | 2a    | 516  | PSU  | C4-N3-C2   | 6.83 | 120.86      | 115.16   |
| 1   | 1A    | 1911 | PSU  | C4-N3-C2   | 6.84 | 120.86      | 115.16   |
| 55  | 2x    | 55   | PSU  | C4-N3-C2   | 6.96 | 120.97      | 115.16   |
| 1   | 2A    | 1917 | PSU  | C4-N3-C2   | 7.00 | 121.00      | 115.16   |
| 54  | 1w    | 32   | PSU  | C4-N3-C2   | 7.04 | 121.03      | 115.16   |
| 54  | 2y    | 46   | 7MG  | C6-N1-C2   | 7.05 | 124.14      | 115.88   |
| 54  | 2w    | 55   | PSU  | C4-N3-C2   | 7.11 | 121.09      | 115.16   |
| 55  | 1x    | 55   | PSU  | C4-N3-C2   | 7.13 | 121.11      | 115.16   |
| 54  | 1w    | 39   | PSU  | C4-N3-C2   | 7.17 | 121.14      | 115.16   |
| 1   | 2A    | 1911 | PSU  | C4-N3-C2   | 7.19 | 121.16      | 115.16   |
| 54  | 1y    | 32   | PSU  | C4-N3-C2   | 7.28 | 121.23      | 115.16   |
| 54  | 1w    | 54   | 5MU  | C4-N3-C2   | 7.29 | 121.24      | 115.16   |
| 54  | 2y    | 32   | PSU  | C4-N3-C2   | 7.39 | 121.32      | 115.16   |
| 54  | 1w    | 55   | PSU  | C4-N3-C2   | 7.40 | 121.33      | 115.16   |
| 54  | 1y    | 55   | PSU  | C4-N3-C2   | 7.44 | 121.36      | 115.16   |
| 54  | 1y    | 39   | PSU  | C4-N3-C2   | 7.51 | 121.42      | 115.16   |
| 54  | 1w    | 46   | 7MG  | C6-N1-C2   | 7.54 | 124.71      | 115.88   |
| 54  | 2w    | 46   | 7MG  | N3-C4-N9   | 7.73 | 136.98      | 126.98   |
| 55  | 1x    | 54   | 5MU  | C4-N3-C2   | 7.88 | 121.74      | 115.16   |
| 54  | 2y    | 54   | 5MU  | C4-N3-C2   | 7.97 | 121.81      | 115.16   |
| 54  | 2y    | 46   | 7MG  | N3-C4-N9   | 8.21 | 137.60      | 126.98   |
| 54  | 2w    | 54   | 5MU  | C4-N3-C2   | 8.50 | 122.25      | 115.16   |
| 54  | 1w    | 46   | 7MG  | N3-C4-N9   | 8.52 | 138.00      | 126.98   |
| 54  | 2w    | 39   | PSU  | C4-N3-C2   | 8.63 | 122.36      | 115.16   |
| 32  | 2a    | 527  | 7MG  | N3-C4-N9   | 8.68 | 138.21      | 126.98   |
| 54  | 1y    | 46   | 7MG  | N3-C4-N9   | 9.11 | 138.76      | 126.98   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 32  | 1a    | 527  | 7MG  | N3-C4-N9  | 9.16  | 138.82      | 126.98   |
| 54  | 1y    | 54   | 5MU  | C4-N3-C2  | 9.77  | 123.31      | 115.16   |
| 1   | 2A    | 2503 | 2MA  | C2-N3-C4  | 9.91  | 120.06      | 115.29   |
| 1   | 1A    | 2503 | 2MA  | C2-N3-C4  | 12.01 | 121.08      | 115.29   |
| 43  | 1l    | 92   | 0TD  | CSB-SB-CB | 19.59 | 138.07      | 101.44   |

There are no chirality outliers.

All (2) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 55  | 1x    | 76  | M3O  | OCN-CN-N-CA |
| 55  | 2x    | 76  | M3O  | OCN-CN-N-CA |

There are no ring outliers.

8 monomers are involved in 10 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 1   | 1A    | 1915 | 5MU  | 1       | 0            |
| 1   | 1A    | 1920 | 4OC  | 1       | 0            |
| 1   | 1A    | 2503 | 2MA  | 1       | 0            |
| 1   | 1A    | 2552 | 2MU  | 1       | 0            |
| 1   | 2A    | 1942 | 5MC  | 1       | 0            |
| 1   | 2A    | 2251 | OMG  | 1       | 0            |
| 1   | 2A    | 2503 | 2MA  | 2       | 0            |
| 1   | 2A    | 2552 | 2MU  | 2       | 0            |

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 2319 ligands modelled in this entry, 2315 are monoatomic - leaving 4 for Mogul analysis.

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

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 58  | HGR  | 1A    | 3915 | 56   | 38,39,39     | 2.34 | 8 (21%)  | 44,58,58    | 1.84 | 12 (27%) |
| 60  | SF4  | 1d    | 501  | 35   | 0,12,12      | 0.00 | -        | 0,24,24     | 0.00 | -        |
| 58  | HGR  | 2A    | 3652 | -    | 38,39,39     | 2.33 | 8 (21%)  | 44,58,58    | 1.77 | 11 (25%) |
| 60  | SF4  | 2d    | 301  | 35   | 0,12,12      | 0.00 | -        | 0,24,24     | 0.00 | -        |

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   |
|-----|------|-------|------|------|---------|------------|---------|
| 58  | HGR  | 1A    | 3915 | 56   | -       | 0/20/79/79 | 0/4/4/4 |
| 60  | SF4  | 1d    | 501  | 35   | -       | 0/0/48/48  | 0/6/5/5 |
| 58  | HGR  | 2A    | 3652 | -    | -       | 0/20/79/79 | 0/4/4/4 |
| 60  | SF4  | 2d    | 301  | 35   | -       | 0/0/48/48  | 0/6/5/5 |

All (16) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 58  | 2A    | 3652 | HGR  | C5-C4   | -5.62 | 1.39        | 1.49     |
| 58  | 1A    | 3915 | HGR  | C5-C6   | -5.55 | 1.39        | 1.50     |
| 58  | 1A    | 3915 | HGR  | C5-C4   | -5.52 | 1.39        | 1.49     |
| 58  | 2A    | 3652 | HGR  | C5-C6   | -5.49 | 1.39        | 1.50     |
| 58  | 1A    | 3915 | HGR  | C3-C2   | -4.55 | 1.39        | 1.48     |
| 58  | 2A    | 3652 | HGR  | C3-C2   | -4.53 | 1.39        | 1.48     |
| 58  | 1A    | 3915 | HGR  | C1-C2   | -2.14 | 1.39        | 1.44     |
| 58  | 2A    | 3652 | HGR  | C1-C2   | -2.08 | 1.39        | 1.44     |
| 58  | 2A    | 3652 | HGR  | O8-C23  | 2.04  | 1.45        | 1.41     |
| 58  | 1A    | 3915 | HGR  | O8-C23  | 2.28  | 1.45        | 1.41     |
| 58  | 2A    | 3652 | HGR  | C1-C6   | 3.12  | 1.39        | 1.35     |
| 58  | 1A    | 3915 | HGR  | C1-C6   | 3.14  | 1.39        | 1.35     |
| 58  | 2A    | 3652 | HGR  | O4-C2   | 4.26  | 1.36        | 1.24     |
| 58  | 1A    | 3915 | HGR  | O4-C2   | 4.55  | 1.36        | 1.24     |
| 58  | 1A    | 3915 | HGR  | C12-C14 | 7.78  | 1.54        | 1.33     |
| 58  | 2A    | 3652 | HGR  | C12-C14 | 8.18  | 1.55        | 1.33     |

All (23) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 58  | 1A    | 3915 | HGR  | C12-C6-C1 | -4.66 | 114.97      | 119.27   |
| 58  | 2A    | 3652 | HGR  | C10-C9-C8 | -4.50 | 96.50       | 102.46   |
| 58  | 1A    | 3915 | HGR  | C10-C9-C8 | -3.60 | 97.70       | 102.46   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 58  | 1A    | 3915 | HGR  | O8-C18-C22 | -3.43 | 98.05       | 105.97   |
| 58  | 2A    | 3652 | HGR  | C12-C6-C1  | -3.35 | 116.18      | 119.27   |
| 58  | 1A    | 3915 | HGR  | O9-C22-C18 | -3.16 | 98.67       | 105.97   |
| 58  | 2A    | 3652 | HGR  | C5-C6-C1   | -3.01 | 118.19      | 120.38   |
| 58  | 2A    | 3652 | HGR  | C9-C8-C7   | -3.00 | 97.96       | 101.60   |
| 58  | 2A    | 3652 | HGR  | O9-C22-C18 | -2.91 | 99.26       | 105.97   |
| 58  | 1A    | 3915 | HGR  | C5-C6-C1   | -2.89 | 118.27      | 120.38   |
| 58  | 2A    | 3652 | HGR  | O8-C18-C22 | -2.63 | 99.89       | 105.97   |
| 58  | 2A    | 3652 | HGR  | O4-C2-C3   | -2.43 | 116.77      | 121.17   |
| 58  | 1A    | 3915 | HGR  | C4-C3-C2   | -2.41 | 118.92      | 122.09   |
| 58  | 2A    | 3652 | HGR  | C10-O3-C3  | -2.40 | 111.67      | 115.16   |
| 58  | 1A    | 3915 | HGR  | O1-C10-C9  | -2.22 | 101.77      | 104.83   |
| 58  | 1A    | 3915 | HGR  | C10-O3-C3  | -2.13 | 112.06      | 115.16   |
| 58  | 1A    | 3915 | HGR  | C9-C8-C7   | -2.01 | 99.16       | 101.60   |
| 58  | 1A    | 3915 | HGR  | C1-C2-C3   | 2.02  | 120.28      | 115.81   |
| 58  | 2A    | 3652 | HGR  | C1-C2-C3   | 2.13  | 120.52      | 115.81   |
| 58  | 2A    | 3652 | HGR  | O3-C3-C2   | 2.75  | 116.53      | 112.33   |
| 58  | 1A    | 3915 | HGR  | O3-C3-C2   | 2.94  | 116.82      | 112.33   |
| 58  | 2A    | 3652 | HGR  | C5-C6-C12  | 4.55  | 125.47      | 120.24   |
| 58  | 1A    | 3915 | HGR  | C5-C6-C12  | 5.55  | 126.62      | 120.24   |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 58  | 1A    | 3915 | HGR  | 2       | 0            |
| 58  | 2A    | 3652 | HGR  | 4       | 0            |

## 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    | 2860/2915 (98%) | 0.56   | 46 (1%) 74 69 | 22, 42, 90, 106       | 0     |
| 1   | 2A    | 2789/2915 (95%) | 0.05   | 51 (1%) 71 66 | 26, 45, 87, 104       | 0     |
| 2   | 1B    | 120/121 (99%)   | 0.36   | 0 100 100     | 37, 58, 69, 86        | 0     |
| 2   | 2B    | 120/121 (99%)   | -0.02  | 2 (1%) 73 68  | 44, 65, 74, 87        | 0     |
| 3   | 1D    | 275/276 (99%)   | 0.83   | 10 (3%) 46 38 | 21, 41, 58, 73        | 0     |
| 3   | 2D    | 275/276 (99%)   | 0.51   | 9 (3%) 50 43  | 25, 42, 61, 72        | 0     |
| 4   | 1E    | 204/206 (99%)   | 0.63   | 2 (0%) 84 81  | 22, 46, 65, 78        | 0     |
| 4   | 2E    | 204/206 (99%)   | 0.40   | 4 (1%) 68 63  | 25, 49, 66, 79        | 0     |
| 5   | 1F    | 203/210 (96%)   | 0.55   | 3 (1%) 76 71  | 21, 50, 72, 83        | 0     |
| 5   | 2F    | 203/210 (96%)   | 0.41   | 6 (2%) 54 47  | 24, 54, 74, 85        | 0     |
| 6   | 1G    | 181/182 (99%)   | 0.67   | 9 (4%) 32 26  | 49, 66, 77, 91        | 0     |
| 6   | 2G    | 181/182 (99%)   | 1.04   | 34 (18%) 2 1  | 53, 69, 80, 93        | 0     |
| 7   | 1H    | 174/180 (96%)   | 0.63   | 3 (1%) 73 68  | 47, 63, 73, 81        | 0     |
| 7   | 2H    | 174/180 (96%)   | 0.97   | 25 (14%) 3 2  | 53, 67, 76, 82        | 0     |
| 8   | 1I    | 146/148 (98%)   | 0.13   | 1 (0%) 89 87  | 44, 72, 81, 85        | 0     |
| 8   | 2I    | 146/148 (98%)   | 0.04   | 1 (0%) 89 87  | 47, 72, 81, 84        | 0     |
| 9   | 1N    | 140/140 (100%)  | 0.42   | 0 100 100     | 23, 37, 59, 69        | 0     |
| 9   | 2N    | 140/140 (100%)  | 1.31   | 30 (21%) 1 0  | 37, 64, 76, 84        | 0     |
| 10  | 1O    | 122/122 (100%)  | 0.68   | 4 (3%) 50 43  | 26, 39, 58, 66        | 0     |
| 10  | 2O    | 122/122 (100%)  | 0.95   | 15 (12%) 5 3  | 39, 56, 68, 78        | 0     |
| 11  | 1P    | 149/150 (99%)   | 0.66   | 4 (2%) 58 51  | 22, 52, 71, 81        | 0     |
| 11  | 2P    | 149/150 (99%)   | 0.28   | 4 (2%) 58 51  | 27, 55, 77, 82        | 0     |
| 12  | 1Q    | 141/141 (100%)  | 0.95   | 9 (6%) 23 17  | 32, 49, 63, 76        | 0     |
| 12  | 2Q    | 141/141 (100%)  | 1.80   | 53 (37%) 0 0  | 36, 53, 66, 77        | 0     |

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| Mol | Chain | Analysed       | <RSRZ> | #RSRZ>2      | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|----------------|--------|--------------|-----------------------|-------|
| 13  | 1R    | 118/118 (100%) | 0.66   | 3 (2%) 61 54 | 28, 39, 54, 64        | 0     |
| 13  | 2R    | 118/118 (100%) | 0.33   | 1 (0%) 87 85 | 31, 41, 57, 64        | 0     |
| 14  | 1S    | 110/112 (98%)  | 0.60   | 1 (0%) 85 83 | 46, 58, 70, 74        | 0     |
| 14  | 2S    | 110/112 (98%)  | 0.50   | 9 (8%) 14 10 | 51, 61, 73, 77        | 0     |
| 15  | 1T    | 131/146 (89%)  | 0.64   | 2 (1%) 76 71 | 39, 51, 69, 75        | 0     |
| 15  | 2T    | 131/146 (89%)  | 0.31   | 1 (0%) 87 85 | 41, 53, 70, 74        | 0     |
| 16  | 1U    | 116/118 (98%)  | 0.67   | 4 (3%) 49 41 | 26, 39, 57, 71        | 0     |
| 16  | 2U    | 116/118 (98%)  | 0.48   | 4 (3%) 49 41 | 29, 45, 63, 72        | 0     |
| 17  | 1V    | 101/101 (100%) | 0.46   | 0 100 100    | 26, 49, 66, 70        | 0     |
| 17  | 2V    | 101/101 (100%) | 0.49   | 4 (3%) 42 34 | 30, 54, 69, 73        | 0     |
| 18  | 1W    | 112/113 (99%)  | 0.53   | 0 100 100    | 26, 36, 55, 83        | 0     |
| 18  | 2W    | 112/113 (99%)  | 0.50   | 2 (1%) 71 66 | 29, 39, 59, 86        | 0     |
| 19  | 1X    | 95/96 (98%)    | 0.63   | 0 100 100    | 30, 43, 63, 80        | 0     |
| 19  | 2X    | 95/96 (98%)    | 0.45   | 5 (5%) 30 23 | 34, 47, 65, 80        | 0     |
| 20  | 1Y    | 107/110 (97%)  | 0.47   | 0 100 100    | 44, 55, 71, 79        | 0     |
| 20  | 2Y    | 107/110 (97%)  | 0.80   | 12 (11%) 7 4 | 49, 59, 73, 81        | 0     |
| 21  | 1Z    | 154/206 (74%)  | 1.01   | 27 (17%) 2 1 | 37, 61, 82, 94        | 0     |
| 21  | 2Z    | 160/206 (77%)  | 1.69   | 56 (35%) 0 0 | 65, 80, 91, 97        | 0     |
| 22  | 10    | 83/85 (97%)    | 1.02   | 7 (8%) 14 9  | 24, 36, 65, 88        | 0     |
| 22  | 20    | 83/85 (97%)    | 1.28   | 13 (15%) 3 1 | 48, 64, 80, 89        | 0     |
| 23  | 11    | 97/98 (98%)    | 0.57   | 4 (4%) 41 33 | 23, 43, 67, 74        | 0     |
| 23  | 21    | 97/98 (98%)    | 0.54   | 5 (5%) 31 24 | 35, 55, 72, 76        | 0     |
| 24  | 12    | 70/72 (97%)    | 0.40   | 0 100 100    | 41, 56, 65, 68        | 0     |
| 24  | 22    | 70/72 (97%)    | -0.02  | 0 100 100    | 45, 59, 68, 78        | 0     |
| 25  | 13    | 59/60 (98%)    | 0.45   | 0 100 100    | 28, 44, 65, 72        | 0     |
| 25  | 23    | 59/60 (98%)    | 1.51   | 15 (25%) 1 0 | 36, 49, 69, 76        | 0     |
| 26  | 14    | 69/71 (97%)    | 0.35   | 1 (1%) 78 74 | 49, 71, 85, 89        | 0     |
| 26  | 24    | 69/71 (97%)    | 1.26   | 16 (23%) 1 0 | 72, 83, 93, 97        | 0     |
| 27  | 15    | 59/60 (98%)    | 0.47   | 2 (3%) 49 41 | 17, 28, 46, 72        | 0     |
| 27  | 25    | 59/60 (98%)    | 0.44   | 1 (1%) 73 68 | 32, 49, 63, 72        | 0     |
| 28  | 16    | 53/54 (98%)    | 0.56   | 1 (1%) 70 64 | 33, 47, 60, 64        | 0     |

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| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 28  | 26    | 53/54 (98%)     | 0.55   | 6 (11%) 7 4   | 35, 51, 61, 67        | 0     |
| 29  | 17    | 48/49 (97%)     | 0.68   | 4 (8%) 14 9   | 16, 25, 49, 72        | 0     |
| 29  | 27    | 48/49 (97%)     | 0.71   | 4 (8%) 14 9   | 31, 38, 63, 69        | 0     |
| 30  | 18    | 64/65 (98%)     | 0.63   | 0 100 100     | 32, 40, 49, 60        | 0     |
| 30  | 28    | 64/65 (98%)     | 0.49   | 0 100 100     | 36, 44, 52, 61        | 0     |
| 31  | 19    | 37/37 (100%)    | 1.01   | 4 (10%) 8 4   | 36, 47, 61, 70        | 0     |
| 31  | 29    | 37/37 (100%)    | 1.33   | 11 (29%) 1 0  | 42, 52, 64, 74        | 0     |
| 32  | 1a    | 1488/1521 (97%) | 0.21   | 19 (1%) 79 75 | 39, 70, 90, 105       | 0     |
| 32  | 2a    | 1491/1521 (98%) | 0.02   | 21 (1%) 78 74 | 42, 72, 91, 104       | 0     |
| 33  | 1b    | 231/256 (90%)   | 0.15   | 1 (0%) 93 91  | 67, 79, 88, 92        | 0     |
| 33  | 2b    | 231/256 (90%)   | 0.85   | 32 (13%) 4 2  | 67, 81, 88, 93        | 0     |
| 34  | 1c    | 206/239 (86%)   | 0.85   | 21 (10%) 9 5  | 66, 76, 83, 92        | 0     |
| 34  | 2c    | 206/239 (86%)   | 1.54   | 66 (32%) 1 0  | 69, 78, 85, 92        | 0     |
| 35  | 1d    | 208/209 (99%)   | 0.95   | 29 (13%) 4 2  | 57, 71, 79, 84        | 0     |
| 35  | 2d    | 208/209 (99%)   | 1.51   | 62 (29%) 1 0  | 58, 71, 79, 84        | 0     |
| 36  | 1e    | 148/162 (91%)   | 0.76   | 8 (5%) 29 22  | 48, 63, 73, 83        | 0     |
| 36  | 2e    | 148/162 (91%)   | 1.34   | 38 (25%) 1 0  | 67, 78, 85, 90        | 0     |
| 37  | 1f    | 100/101 (99%)   | 0.71   | 8 (8%) 15 10  | 46, 65, 74, 76        | 0     |
| 37  | 2f    | 100/101 (99%)   | 0.26   | 1 (1%) 84 81  | 55, 70, 79, 87        | 0     |
| 38  | 1g    | 155/156 (99%)   | 0.80   | 18 (11%) 6 4  | 61, 72, 81, 88        | 0     |
| 38  | 2g    | 155/156 (99%)   | 0.66   | 19 (12%) 5 3  | 64, 74, 82, 87        | 0     |
| 39  | 1h    | 137/138 (99%)   | 0.29   | 5 (3%) 46 38  | 52, 64, 73, 86        | 0     |
| 39  | 2h    | 137/138 (99%)   | 1.05   | 25 (18%) 2 1  | 60, 77, 84, 89        | 0     |
| 40  | 1i    | 127/128 (99%)   | 0.44   | 8 (6%) 23 17  | 59, 77, 85, 88        | 0     |
| 40  | 2i    | 127/128 (99%)   | 1.27   | 30 (23%) 1 0  | 64, 79, 86, 89        | 0     |
| 41  | 1j    | 97/105 (92%)    | 0.45   | 5 (5%) 31 24  | 56, 75, 85, 92        | 0     |
| 41  | 2j    | 96/105 (91%)    | 1.47   | 31 (32%) 1 0  | 68, 85, 92, 94        | 0     |
| 42  | 1k    | 114/129 (88%)   | 1.56   | 35 (30%) 1 0  | 37, 64, 73, 77        | 0     |
| 42  | 2k    | 114/129 (88%)   | 1.18   | 18 (15%) 3 1  | 44, 73, 81, 85        | 0     |
| 43  | 1l    | 121/132 (91%)   | 0.56   | 5 (4%) 41 33  | 41, 55, 68, 75        | 0     |
| 43  | 2l    | 121/132 (91%)   | 1.34   | 33 (27%) 1 0  | 50, 70, 79, 83        | 0     |

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| Mol | Chain | Analysed          | <RSRZ> | #RSRZ>2         | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-------------------|--------|-----------------|-----------------------|-------|
| 44  | 1m    | 123/126 (97%)     | 0.92   | 13 (10%) 8 5    | 58, 73, 81, 84        | 0     |
| 44  | 2m    | 122/126 (96%)     | 1.47   | 35 (28%) 1 0    | 63, 76, 82, 85        | 0     |
| 45  | 1n    | 60/61 (98%)       | 1.05   | 6 (10%) 9 6     | 55, 64, 74, 80        | 0     |
| 45  | 2n    | 60/61 (98%)       | 3.63   | 49 (81%) 0 0    | 73, 85, 90, 94        | 0     |
| 46  | 1o    | 88/89 (98%)       | 0.96   | 13 (14%) 3 2    | 52, 66, 76, 83        | 0     |
| 46  | 2o    | 88/89 (98%)       | 0.22   | 2 (2%) 64 57    | 56, 68, 78, 85        | 0     |
| 47  | 1p    | 82/88 (93%)       | 0.73   | 6 (7%) 18 12    | 56, 68, 76, 81        | 0     |
| 47  | 2p    | 82/88 (93%)       | 0.80   | 5 (6%) 25 18    | 58, 68, 76, 82        | 0     |
| 48  | 1q    | 99/105 (94%)      | 0.65   | 4 (4%) 42 34    | 59, 68, 76, 78        | 0     |
| 48  | 2q    | 99/105 (94%)      | 0.90   | 17 (17%) 2 1    | 60, 69, 77, 80        | 0     |
| 49  | 1r    | 68/88 (77%)       | 0.84   | 8 (11%) 6 4     | 57, 67, 76, 82        | 0     |
| 49  | 2r    | 68/88 (77%)       | 0.33   | 4 (5%) 26 19    | 57, 68, 77, 83        | 0     |
| 50  | 1s    | 83/93 (89%)       | 0.67   | 5 (6%) 25 18    | 64, 76, 84, 91        | 0     |
| 50  | 2s    | 83/93 (89%)       | 2.09   | 42 (50%) 0 0    | 67, 79, 86, 93        | 0     |
| 51  | 1t    | 96/106 (90%)      | 0.45   | 2 (2%) 67 61    | 56, 67, 77, 81        | 0     |
| 51  | 2t    | 96/106 (90%)      | 0.27   | 2 (2%) 67 61    | 56, 68, 78, 80        | 0     |
| 52  | 1u    | 23/27 (85%)       | 0.90   | 4 (17%) 2 1     | 62, 70, 74, 75        | 0     |
| 52  | 2u    | 23/27 (85%)       | 1.22   | 6 (26%) 1 0     | 65, 72, 76, 76        | 0     |
| 53  | 1v    | 14/27 (51%)       | 2.03   | 7 (50%) 0 0     | 55, 73, 97, 105       | 0     |
| 53  | 2v    | 13/27 (48%)       | 2.08   | 5 (38%) 0 0     | 60, 75, 89, 98        | 0     |
| 54  | 1w    | 68/76 (89%)       | 1.71   | 23 (33%) 0 0    | 67, 86, 97, 105       | 0     |
| 54  | 1y    | 67/76 (88%)       | 1.22   | 11 (16%) 2 1    | 40, 91, 97, 99        | 0     |
| 54  | 2w    | 67/76 (88%)       | 3.48   | 47 (70%) 0 0    | 73, 88, 97, 99        | 0     |
| 54  | 2y    | 66/76 (86%)       | 1.16   | 11 (16%) 2 1    | 43, 93, 97, 99        | 0     |
| 55  | 1x    | 71/77 (92%)       | 0.35   | 2 (2%) 56 49    | 27, 56, 81, 85        | 0     |
| 55  | 2x    | 71/77 (92%)       | 0.63   | 5 (7%) 19 13    | 44, 77, 88, 94        | 0     |
| All | All   | 20877/21754 (95%) | 0.56   | 1422 (6%) 20 15 | 16, 61, 86, 106       | 0     |

All (1422) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 45  | 2n    | 38  | GLY  | 13.6 |
| 54  | 2w    | 74  | C    | 12.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 22  | 10    | 6   | GLY  | 10.9 |
| 54  | 2w    | 73  | A    | 10.4 |
| 22  | 20    | 7   | LEU  | 10.4 |
| 44  | 2m    | 124 | PRO  | 9.8  |
| 54  | 2w    | 76  | A    | 9.5  |
| 45  | 2n    | 39  | LEU  | 9.2  |
| 44  | 1m    | 124 | PRO  | 8.7  |
| 45  | 2n    | 25  | VAL  | 8.6  |
| 44  | 2m    | 123 | ALA  | 8.6  |
| 22  | 10    | 4   | LYS  | 8.5  |
| 50  | 2s    | 31  | ILE  | 8.4  |
| 44  | 2m    | 60  | VAL  | 8.2  |
| 21  | 2Z    | 144 | LEU  | 8.1  |
| 38  | 2g    | 82  | GLY  | 8.1  |
| 54  | 2w    | 72  | C    | 8.0  |
| 22  | 10    | 5   | LYS  | 7.9  |
| 22  | 10    | 7   | LEU  | 7.8  |
| 21  | 2Z    | 156 | LYS  | 7.7  |
| 54  | 2w    | 75  | C    | 7.6  |
| 26  | 24    | 51  | ASP  | 7.6  |
| 44  | 1m    | 2   | ALA  | 7.4  |
| 44  | 2m    | 6   | GLY  | 7.3  |
| 38  | 1g    | 83  | ALA  | 7.3  |
| 38  | 1g    | 79  | ARG  | 7.3  |
| 22  | 10    | 3   | HIS  | 7.2  |
| 54  | 2w    | 45  | U    | 7.1  |
| 54  | 1w    | 44  | G    | 7.0  |
| 22  | 20    | 2   | ALA  | 7.0  |
| 21  | 1Z    | 1   | MET  | 7.0  |
| 54  | 1w    | 74  | C    | 6.9  |
| 54  | 2w    | 71  | G    | 6.9  |
| 41  | 2j    | 47  | PHE  | 6.7  |
| 41  | 2j    | 10  | GLY  | 6.7  |
| 22  | 20    | 4   | LYS  | 6.6  |
| 18  | 2W    | 112 | GLY  | 6.6  |
| 54  | 2w    | 44  | G    | 6.5  |
| 22  | 20    | 5   | LYS  | 6.5  |
| 33  | 2b    | 165 | VAL  | 6.5  |
| 54  | 2y    | 36  | A    | 6.5  |
| 22  | 10    | 2   | ALA  | 6.4  |
| 54  | 1w    | 75  | C    | 6.4  |
| 22  | 20    | 3   | HIS  | 6.4  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 38  | 1g    | 82   | GLY  | 6.3  |
| 3   | 2D    | 2    | ALA  | 6.2  |
| 54  | 1y    | 35   | A    | 6.2  |
| 53  | 2v    | 24   | A    | 6.1  |
| 22  | 20    | 6    | GLY  | 6.1  |
| 54  | 1w    | 76   | A    | 6.1  |
| 35  | 2d    | 168  | ARG  | 6.1  |
| 50  | 2s    | 79   | THR  | 6.1  |
| 38  | 1g    | 80   | VAL  | 6.0  |
| 21  | 2Z    | 140  | ASP  | 6.0  |
| 54  | 1w    | 73   | A    | 6.0  |
| 45  | 2n    | 50   | LYS  | 6.0  |
| 34  | 2c    | 158  | GLY  | 6.0  |
| 32  | 2a    | 1034 | G    | 5.9  |
| 50  | 2s    | 30   | LEU  | 5.8  |
| 45  | 2n    | 42   | ILE  | 5.8  |
| 54  | 2w    | 3    | C    | 5.8  |
| 45  | 2n    | 44   | LEU  | 5.8  |
| 54  | 2w    | 31   | A    | 5.8  |
| 1   | 2A    | 2154 | G    | 5.8  |
| 38  | 1g    | 84   | ASN  | 5.7  |
| 38  | 1g    | 85   | TYR  | 5.7  |
| 26  | 24    | 49   | PHE  | 5.7  |
| 54  | 2w    | 70   | G    | 5.7  |
| 35  | 2d    | 146  | ILE  | 5.7  |
| 45  | 2n    | 7    | ILE  | 5.7  |
| 38  | 2g    | 80   | VAL  | 5.7  |
| 44  | 2m    | 90   | LEU  | 5.6  |
| 21  | 2Z    | 170  | THR  | 5.6  |
| 36  | 2e    | 12   | LEU  | 5.6  |
| 34  | 2c    | 12   | LEU  | 5.5  |
| 45  | 2n    | 36   | PHE  | 5.5  |
| 45  | 2n    | 51   | GLY  | 5.5  |
| 34  | 2c    | 60   | ALA  | 5.5  |
| 44  | 2m    | 5    | ALA  | 5.4  |
| 34  | 2c    | 33   | LEU  | 5.4  |
| 44  | 2m    | 66   | LEU  | 5.4  |
| 45  | 2n    | 37   | PHE  | 5.4  |
| 1   | 1A    | 885  | C    | 5.4  |
| 41  | 2j    | 85   | LEU  | 5.4  |
| 1   | 1A    | 888  | C    | 5.4  |
| 34  | 2c    | 182  | ILE  | 5.3  |

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| Mol | Chain | Res     | Type | RSRZ |
|-----|-------|---------|------|------|
| 21  | 2Z    | 143     | GLY  | 5.3  |
| 35  | 2d    | 183     | GLY  | 5.3  |
| 45  | 2n    | 34      | TYR  | 5.3  |
| 21  | 2Z    | 155     | LEU  | 5.3  |
| 45  | 2n    | 61      | TRP  | 5.3  |
| 50  | 2s    | 49      | ILE  | 5.2  |
| 1   | 2A    | 883     | G    | 5.2  |
| 33  | 2b    | 201     | ILE  | 5.2  |
| 1   | 2A    | 888     | C    | 5.2  |
| 44  | 1m    | 123     | ALA  | 5.2  |
| 21  | 2Z    | 145     | GLU  | 5.2  |
| 21  | 2Z    | 141     | VAL  | 5.1  |
| 34  | 2c    | 6       | HIS  | 5.1  |
| 50  | 2s    | 40      | ILE  | 5.1  |
| 45  | 2n    | 29      | ARG  | 5.1  |
| 21  | 2Z    | 50      | GLN  | 5.1  |
| 38  | 2g    | 83      | ALA  | 5.1  |
| 1   | 1A    | 896     | A    | 5.0  |
| 33  | 2b    | 187     | LEU  | 5.0  |
| 9   | 2N    | 104     | LYS  | 5.0  |
| 26  | 24    | 50      | VAL  | 5.0  |
| 1   | 1A    | 1095    | A    | 4.9  |
| 45  | 2n    | 53      | LEU  | 4.9  |
| 53  | 2v    | 23      | A    | 4.9  |
| 34  | 2c    | 8       | ILE  | 4.9  |
| 50  | 2s    | 41      | VAL  | 4.9  |
| 32  | 2a    | 1036    | G    | 4.9  |
| 12  | 2Q    | 33      | GLY  | 4.9  |
| 38  | 2g    | 81      | GLY  | 4.9  |
| 54  | 2w    | 28      | G    | 4.8  |
| 54  | 2w    | 69      | G    | 4.8  |
| 21  | 2Z    | 154     | ASP  | 4.8  |
| 45  | 2n    | 10      | ALA  | 4.8  |
| 12  | 2Q    | 79      | LEU  | 4.8  |
| 32  | 2a    | 1030(B) | C    | 4.7  |
| 1   | 2A    | 884     | C    | 4.7  |
| 21  | 1Z    | 147     | GLY  | 4.7  |
| 34  | 2c    | 198     | VAL  | 4.7  |
| 36  | 2e    | 109     | ILE  | 4.7  |
| 1   | 2A    | 2146    | C    | 4.7  |
| 22  | 10    | 8       | GLY  | 4.7  |
| 12  | 2Q    | 5       | ARG  | 4.7  |

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| Mol | Chain | Res     | Type | RSRZ |
|-----|-------|---------|------|------|
| 27  | 15    | 60      | VAL  | 4.7  |
| 45  | 2n    | 55      | GLY  | 4.7  |
| 1   | 1A    | 2141    | G    | 4.6  |
| 40  | 2i    | 17      | VAL  | 4.6  |
| 45  | 2n    | 56      | VAL  | 4.6  |
| 41  | 2j    | 48      | THR  | 4.6  |
| 45  | 1n    | 2       | ALA  | 4.6  |
| 26  | 24    | 57      | GLU  | 4.6  |
| 54  | 2w    | 56      | C    | 4.6  |
| 35  | 2d    | 158     | ILE  | 4.6  |
| 34  | 2c    | 145     | GLY  | 4.6  |
| 42  | 1k    | 60      | ALA  | 4.6  |
| 44  | 2m    | 92      | HIS  | 4.6  |
| 45  | 2n    | 14      | PRO  | 4.6  |
| 54  | 1y    | 24      | G    | 4.5  |
| 6   | 2G    | 5       | VAL  | 4.5  |
| 12  | 2Q    | 6       | ARG  | 4.5  |
| 12  | 2Q    | 104     | PHE  | 4.5  |
| 20  | 2Y    | 44      | ILE  | 4.5  |
| 21  | 2Z    | 153     | SER  | 4.5  |
| 54  | 1y    | 36      | A    | 4.5  |
| 35  | 2d    | 166     | LYS  | 4.5  |
| 21  | 2Z    | 149     | SER  | 4.5  |
| 54  | 2w    | 29      | G    | 4.5  |
| 53  | 1v    | 12      | A    | 4.5  |
| 50  | 2s    | 35      | SER  | 4.5  |
| 21  | 1Z    | 168     | GLU  | 4.5  |
| 44  | 2m    | 84      | ILE  | 4.5  |
| 33  | 2b    | 188     | ALA  | 4.5  |
| 43  | 2l    | 28      | LYS  | 4.5  |
| 29  | 17    | 48      | LYS  | 4.4  |
| 25  | 23    | 60      | GLU  | 4.4  |
| 23  | 21    | 2       | SER  | 4.4  |
| 34  | 2c    | 157     | ILE  | 4.4  |
| 32  | 2a    | 1030(A) | G    | 4.4  |
| 50  | 2s    | 53      | ASN  | 4.4  |
| 54  | 1y    | 20      | U    | 4.4  |
| 41  | 2j    | 63      | PHE  | 4.4  |
| 41  | 2j    | 62      | HIS  | 4.3  |
| 36  | 2e    | 90      | VAL  | 4.3  |
| 34  | 2c    | 124     | ILE  | 4.3  |
| 45  | 2n    | 30      | ALA  | 4.3  |

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| Mol | Chain | Res     | Type | RSRZ |
|-----|-------|---------|------|------|
| 38  | 2g    | 79      | ARG  | 4.3  |
| 43  | 2l    | 64      | TYR  | 4.3  |
| 32  | 1a    | 1257    | U    | 4.3  |
| 49  | 2r    | 85      | LEU  | 4.3  |
| 44  | 1m    | 87      | TYR  | 4.3  |
| 54  | 2w    | 23      | A    | 4.3  |
| 50  | 2s    | 83      | HIS  | 4.3  |
| 32  | 1a    | 1028    | C    | 4.3  |
| 36  | 2e    | 133     | TYR  | 4.3  |
| 21  | 2Z    | 151     | HIS  | 4.2  |
| 23  | 1l    | 2       | SER  | 4.2  |
| 32  | 1a    | 1001(A) | G    | 4.2  |
| 54  | 2y    | 34      | G    | 4.2  |
| 6   | 2G    | 152     | LEU  | 4.2  |
| 7   | 2H    | 115     | VAL  | 4.2  |
| 9   | 2N    | 116     | LEU  | 4.2  |
| 41  | 2j    | 11      | PHE  | 4.2  |
| 1   | 1A    | 1509    | C    | 4.2  |
| 54  | 2w    | 2       | C    | 4.2  |
| 12  | 2Q    | 65      | PHE  | 4.2  |
| 34  | 2c    | 189     | ALA  | 4.2  |
| 34  | 1c    | 193     | TYR  | 4.2  |
| 1   | 2A    | 885     | C    | 4.2  |
| 34  | 2c    | 39      | ILE  | 4.2  |
| 41  | 2j    | 65      | LEU  | 4.2  |
| 35  | 2d    | 188     | LEU  | 4.1  |
| 41  | 2j    | 55      | LYS  | 4.1  |
| 1   | 2A    | 1026    | U    | 4.1  |
| 46  | 1o    | 88      | ARG  | 4.1  |
| 50  | 2s    | 82      | GLY  | 4.1  |
| 21  | 1Z    | 169     | GLU  | 4.1  |
| 32  | 2a    | 1035    | A    | 4.1  |
| 34  | 2c    | 53      | ALA  | 4.1  |
| 54  | 2w    | 5       | G    | 4.1  |
| 36  | 2e    | 99      | GLY  | 4.1  |
| 6   | 2G    | 140     | ILE  | 4.1  |
| 12  | 2Q    | 109     | VAL  | 4.1  |
| 54  | 1w    | 72      | C    | 4.1  |
| 34  | 1c    | 128     | PHE  | 4.1  |
| 50  | 2s    | 48      | THR  | 4.1  |
| 54  | 2w    | 24      | G    | 4.1  |
| 50  | 2s    | 62      | ILE  | 4.1  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 26         | 24           | 45         | GLY         | 4.1         |
| 43         | 2l           | 14         | GLY         | 4.1         |
| 38         | 2g           | 152        | ALA         | 4.1         |
| 21         | 2Z           | 121        | HIS         | 4.1         |
| 50         | 2s           | 80         | TYR         | 4.1         |
| 42         | 2k           | 89         | ALA         | 4.1         |
| 41         | 2j           | 46         | ARG         | 4.1         |
| 26         | 24           | 59         | PHE         | 4.1         |
| 45         | 2n           | 13         | THR         | 4.0         |
| 34         | 2c           | 180        | ALA         | 4.0         |
| 38         | 1g           | 78         | ARG         | 4.0         |
| 1          | 2A           | 2155       | G           | 4.0         |
| 19         | 2X           | 92         | LEU         | 4.0         |
| 6          | 2G           | 157        | ILE         | 4.0         |
| 33         | 2b           | 214        | ILE         | 4.0         |
| 21         | 2Z           | 122        | ARG         | 4.0         |
| 34         | 2c           | 184        | TYR         | 4.0         |
| 38         | 2g           | 154        | TYR         | 4.0         |
| 38         | 1g           | 153        | HIS         | 4.0         |
| 34         | 1c           | 39         | ILE         | 4.0         |
| 45         | 2n           | 12         | ARG         | 4.0         |
| 1          | 1A           | 884        | C           | 4.0         |
| 1          | 1A           | 1176       | G           | 4.0         |
| 54         | 2w           | 30         | G           | 4.0         |
| 38         | 1g           | 81         | GLY         | 4.0         |
| 35         | 2d           | 184        | LYS         | 4.0         |
| 33         | 2b           | 70         | PHE         | 4.0         |
| 25         | 23           | 26         | LEU         | 3.9         |
| 36         | 2e           | 10         | MET         | 3.9         |
| 1          | 1A           | 887        | A           | 3.9         |
| 1          | 1A           | 886        | C           | 3.9         |
| 20         | 2Y           | 1          | MET         | 3.9         |
| 34         | 1c           | 87         | LEU         | 3.9         |
| 42         | 2k           | 50         | TYR         | 3.9         |
| 12         | 2Q           | 59         | ARG         | 3.9         |
| 32         | 2a           | 1001(A)    | G           | 3.9         |
| 39         | 2h           | 135        | CYS         | 3.9         |
| 41         | 2j           | 96         | ILE         | 3.9         |
| 45         | 2n           | 31         | ARG         | 3.9         |
| 46         | 1o           | 82         | ILE         | 3.9         |
| 21         | 2Z           | 125        | LEU         | 3.9         |
| 45         | 2n           | 57         | ARG         | 3.9         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 42         | 2k           | 90         | GLY         | 3.9         |
| 44         | 2m           | 95         | GLY         | 3.9         |
| 54         | 2w           | 19         | G           | 3.9         |
| 54         | 2w           | 47         | U           | 3.9         |
| 45         | 2n           | 35         | ARG         | 3.9         |
| 6          | 2G           | 35         | GLU         | 3.9         |
| 54         | 2w           | 4          | C           | 3.9         |
| 25         | 23           | 35         | ARG         | 3.9         |
| 7          | 2H           | 106        | THR         | 3.9         |
| 33         | 2b           | 92         | TYR         | 3.9         |
| 36         | 2e           | 31         | LEU         | 3.8         |
| 32         | 2a           | 1033       | G           | 3.8         |
| 40         | 2i           | 114        | TYR         | 3.8         |
| 44         | 2m           | 103        | THR         | 3.8         |
| 21         | 2Z           | 46         | LYS         | 3.8         |
| 1          | 2A           | 2153       | G           | 3.8         |
| 36         | 2e           | 33         | VAL         | 3.8         |
| 43         | 2l           | 39         | VAL         | 3.8         |
| 2          | 2B           | 90         | A           | 3.8         |
| 12         | 2Q           | 15         | GLY         | 3.8         |
| 14         | 2S           | 5          | THR         | 3.8         |
| 7          | 2H           | 145        | ALA         | 3.8         |
| 45         | 2n           | 58         | LYS         | 3.8         |
| 1          | 1A           | 1096       | A           | 3.8         |
| 53         | 1v           | 24         | A           | 3.8         |
| 53         | 2v           | 14         | A           | 3.8         |
| 39         | 2h           | 128        | GLY         | 3.8         |
| 44         | 2m           | 78         | ILE         | 3.8         |
| 45         | 2n           | 2          | ALA         | 3.8         |
| 48         | 2q           | 30         | PRO         | 3.8         |
| 1          | 2A           | 2156       | G           | 3.8         |
| 35         | 2d           | 160        | GLN         | 3.8         |
| 52         | 2u           | 14         | TRP         | 3.8         |
| 36         | 2e           | 13         | ILE         | 3.8         |
| 54         | 2w           | 21         | A           | 3.8         |
| 50         | 2s           | 52         | TYR         | 3.7         |
| 1          | 1A           | 2159       | G           | 3.7         |
| 21         | 2Z           | 150        | LEU         | 3.7         |
| 1          | 1A           | 1097       | U           | 3.7         |
| 39         | 2h           | 83         | ILE         | 3.7         |
| 21         | 2Z           | 139        | VAL         | 3.7         |
| 1          | 2A           | 1509       | C           | 3.7         |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 54  | 2y    | 35   | A    | 3.7  |
| 34  | 2c    | 202  | ILE  | 3.7  |
| 39  | 2h    | 94   | TYR  | 3.7  |
| 21  | 1Z    | 165  | VAL  | 3.7  |
| 9   | 2N    | 23   | LEU  | 3.7  |
| 1   | 2A    | 887  | A    | 3.7  |
| 6   | 2G    | 39   | ILE  | 3.7  |
| 38  | 2g    | 85   | TYR  | 3.7  |
| 21  | 1Z    | 104  | PHE  | 3.7  |
| 38  | 2g    | 156  | TRP  | 3.7  |
| 22  | 20    | 11   | ARG  | 3.7  |
| 35  | 2d    | 176  | LEU  | 3.7  |
| 9   | 2N    | 47   | ALA  | 3.7  |
| 34  | 2c    | 58   | GLU  | 3.7  |
| 33  | 2b    | 37   | ASN  | 3.7  |
| 53  | 1v    | 13   | A    | 3.7  |
| 35  | 2d    | 64   | LEU  | 3.7  |
| 41  | 2j    | 98   | ILE  | 3.7  |
| 43  | 2l    | 94   | PRO  | 3.7  |
| 1   | 1A    | 883  | G    | 3.7  |
| 1   | 2A    | 2160 | G    | 3.7  |
| 54  | 2w    | 14   | A    | 3.6  |
| 35  | 1d    | 204  | ILE  | 3.6  |
| 12  | 2Q    | 10   | ARG  | 3.6  |
| 45  | 2n    | 11   | LYS  | 3.6  |
| 39  | 2h    | 93   | VAL  | 3.6  |
| 46  | 1o    | 87   | ILE  | 3.6  |
| 44  | 2m    | 67   | GLU  | 3.6  |
| 9   | 2N    | 26   | LEU  | 3.6  |
| 44  | 2m    | 119  | GLY  | 3.6  |
| 38  | 1g    | 156  | TRP  | 3.6  |
| 40  | 2i    | 109  | VAL  | 3.6  |
| 33  | 2b    | 216  | SER  | 3.6  |
| 41  | 2j    | 54   | PHE  | 3.6  |
| 42  | 1k    | 68   | ALA  | 3.6  |
| 6   | 2G    | 34   | LEU  | 3.6  |
| 12  | 2Q    | 103  | MET  | 3.6  |
| 53  | 2v    | 12   | A    | 3.6  |
| 12  | 2Q    | 108  | GLY  | 3.6  |
| 50  | 2s    | 50   | ALA  | 3.6  |
| 3   | 1D    | 276  | LYS  | 3.6  |
| 33  | 2b    | 51   | LEU  | 3.6  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 54         | 2w           | 6          | G           | 3.6         |
| 12         | 2Q           | 114        | ALA         | 3.6         |
| 44         | 2m           | 102        | ARG         | 3.6         |
| 40         | 2i           | 127        | LYS         | 3.6         |
| 21         | 2Z           | 172        | ALA         | 3.6         |
| 43         | 2l           | 8          | ASN         | 3.6         |
| 43         | 2l           | 56         | ALA         | 3.5         |
| 1          | 2A           | 896        | A           | 3.5         |
| 26         | 24           | 55         | ARG         | 3.5         |
| 43         | 2l           | 18         | VAL         | 3.5         |
| 35         | 1d           | 167        | GLY         | 3.5         |
| 38         | 2g           | 7          | ALA         | 3.5         |
| 6          | 2G           | 133        | LEU         | 3.5         |
| 49         | 1r           | 78         | LEU         | 3.5         |
| 34         | 2c           | 160        | ALA         | 3.5         |
| 35         | 2d           | 112        | VAL         | 3.5         |
| 1          | 2A           | 2897       | U           | 3.5         |
| 22         | 20           | 10         | THR         | 3.5         |
| 35         | 2d           | 179        | GLU         | 3.5         |
| 1          | 1A           | 2158       | A           | 3.5         |
| 21         | 2Z           | 148        | ASP         | 3.5         |
| 33         | 2b           | 44         | LEU         | 3.5         |
| 42         | 1k           | 98         | LEU         | 3.5         |
| 44         | 1m           | 96         | LEU         | 3.5         |
| 52         | 2u           | 16         | GLY         | 3.5         |
| 33         | 2b           | 200        | ILE         | 3.5         |
| 36         | 2e           | 11         | ILE         | 3.5         |
| 35         | 2d           | 19         | LEU         | 3.5         |
| 32         | 1a           | 1036       | G           | 3.5         |
| 54         | 2w           | 42         | C           | 3.5         |
| 21         | 2Z           | 105        | VAL         | 3.5         |
| 35         | 2d           | 148        | VAL         | 3.5         |
| 3          | 1D           | 275        | LYS         | 3.4         |
| 21         | 2Z           | 80         | ARG         | 3.5         |
| 46         | 1o           | 57         | LEU         | 3.5         |
| 50         | 2s           | 71         | LEU         | 3.5         |
| 42         | 1k           | 42         | TRP         | 3.4         |
| 1          | 2A           | 886        | C           | 3.4         |
| 9          | 2N           | 102        | ALA         | 3.4         |
| 38         | 1g           | 86         | GLN         | 3.4         |
| 6          | 2G           | 29         | TRP         | 3.4         |
| 32         | 1a           | 1030(B)    | C           | 3.4         |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 32  | 2a    | 1001 | A    | 3.4  |
| 41  | 2j    | 50   | ILE  | 3.4  |
| 51  | 2t    | 24   | LEU  | 3.4  |
| 1   | 1A    | 2131 | G    | 3.4  |
| 44  | 2m    | 121  | LYS  | 3.4  |
| 35  | 1d    | 168  | ARG  | 3.4  |
| 35  | 2d    | 20   | TYR  | 3.4  |
| 12  | 2Q    | 90   | VAL  | 3.4  |
| 36  | 2e    | 98   | THR  | 3.4  |
| 32  | 2a    | 1030 | C    | 3.4  |
| 50  | 2s    | 14   | HIS  | 3.4  |
| 1   | 2A    | 899  | A    | 3.4  |
| 20  | 2Y    | 5    | MET  | 3.4  |
| 54  | 2w    | 22   | G    | 3.4  |
| 12  | 2Q    | 32   | TYR  | 3.4  |
| 6   | 2G    | 2    | PRO  | 3.4  |
| 6   | 2G    | 142  | PRO  | 3.4  |
| 33  | 2b    | 115  | LEU  | 3.4  |
| 45  | 2n    | 8    | GLU  | 3.4  |
| 50  | 2s    | 66   | MET  | 3.4  |
| 7   | 2H    | 113  | VAL  | 3.4  |
| 20  | 2Y    | 45   | VAL  | 3.4  |
| 48  | 1q    | 27   | PHE  | 3.4  |
| 54  | 2w    | 41   | C    | 3.4  |
| 44  | 2m    | 87   | TYR  | 3.4  |
| 10  | 1O    | 91   | LEU  | 3.4  |
| 34  | 2c    | 21   | ARG  | 3.4  |
| 1   | 2A    | 2157 | G    | 3.3  |
| 7   | 2H    | 169  | VAL  | 3.3  |
| 45  | 2n    | 22   | THR  | 3.3  |
| 39  | 2h    | 104  | ARG  | 3.3  |
| 26  | 24    | 32   | TYR  | 3.3  |
| 6   | 2G    | 28   | VAL  | 3.3  |
| 42  | 1k    | 63   | LEU  | 3.3  |
| 41  | 2j    | 6    | ILE  | 3.3  |
| 44  | 2m    | 71   | ARG  | 3.3  |
| 1   | 2A    | 2159 | G    | 3.3  |
| 34  | 2c    | 190  | ARG  | 3.3  |
| 43  | 2l    | 95   | GLY  | 3.3  |
| 12  | 2Q    | 37   | LEU  | 3.3  |
| 12  | 2Q    | 93   | TYR  | 3.3  |
| 12  | 2Q    | 132  | VAL  | 3.3  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 21  | 1Z    | 100  | VAL  | 3.3  |
| 54  | 1w    | 70   | G    | 3.3  |
| 37  | 1f    | 21   | LEU  | 3.3  |
| 33  | 2b    | 203  | GLY  | 3.3  |
| 53  | 1v    | 14   | A    | 3.3  |
| 26  | 24    | 53   | GLU  | 3.3  |
| 26  | 24    | 40   | HIS  | 3.2  |
| 42  | 2k    | 25   | TYR  | 3.2  |
| 22  | 20    | 76   | GLY  | 3.2  |
| 7   | 2H    | 148  | ILE  | 3.2  |
| 54  | 2w    | 38   | A    | 3.2  |
| 39  | 2h    | 133  | LEU  | 3.2  |
| 1   | 1A    | 897  | C    | 3.2  |
| 40  | 2i    | 115  | GLY  | 3.2  |
| 7   | 2H    | 105  | LEU  | 3.2  |
| 1   | 2A    | 882  | G    | 3.2  |
| 14  | 2S    | 20   | ARG  | 3.2  |
| 21  | 1Z    | 164  | ALA  | 3.2  |
| 41  | 2j    | 44   | VAL  | 3.2  |
| 45  | 2n    | 23   | ARG  | 3.2  |
| 50  | 1s    | 81   | ARG  | 3.2  |
| 40  | 2i    | 79   | LEU  | 3.2  |
| 54  | 2w    | 12   | U    | 3.2  |
| 54  | 2w    | 13   | C    | 3.2  |
| 1   | 1A    | 2151 | G    | 3.2  |
| 54  | 1w    | 71   | G    | 3.2  |
| 40  | 2i    | 80   | GLY  | 3.2  |
| 50  | 1s    | 40   | ILE  | 3.2  |
| 36  | 2e    | 8    | GLU  | 3.2  |
| 14  | 2S    | 32   | LEU  | 3.2  |
| 25  | 23    | 28   | LEU  | 3.2  |
| 1   | 2A    | 897  | C    | 3.2  |
| 1   | 2A    | 2896 | C    | 3.2  |
| 33  | 2b    | 66   | GLY  | 3.2  |
| 44  | 2m    | 68   | GLY  | 3.2  |
| 34  | 2c    | 59   | ARG  | 3.2  |
| 33  | 2b    | 152  | PHE  | 3.2  |
| 14  | 2S    | 58   | LEU  | 3.2  |
| 36  | 2e    | 43   | LEU  | 3.2  |
| 1   | 2A    | 229  | A    | 3.2  |
| 12  | 2Q    | 86   | GLY  | 3.2  |
| 32  | 2a    | 1219 | U    | 3.2  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 35  | 2d    | 181  | MET  | 3.2  |
| 39  | 2h    | 91   | ARG  | 3.2  |
| 54  | 1y    | 12   | U    | 3.2  |
| 47  | 2p    | 9    | PHE  | 3.2  |
| 40  | 2i    | 36   | TYR  | 3.2  |
| 17  | 2V    | 71   | LEU  | 3.2  |
| 34  | 2c    | 206  | GLU  | 3.1  |
| 35  | 2d    | 121  | VAL  | 3.1  |
| 1   | 1A    | 889  | C    | 3.1  |
| 1   | 1A    | 1064 | C    | 3.1  |
| 1   | 1A    | 2129 | C    | 3.1  |
| 45  | 2n    | 26   | ARG  | 3.1  |
| 46  | 1o    | 89   | GLY  | 3.1  |
| 35  | 2d    | 33   | MET  | 3.1  |
| 54  | 2w    | 15   | G    | 3.1  |
| 34  | 2c    | 37   | GLN  | 3.1  |
| 12  | 2Q    | 28   | ALA  | 3.1  |
| 35  | 2d    | 108  | LEU  | 3.1  |
| 42  | 1k    | 25   | TYR  | 3.1  |
| 3   | 2D    | 275  | LYS  | 3.1  |
| 43  | 2l    | 32   | PHE  | 3.1  |
| 7   | 2H    | 166  | GLY  | 3.1  |
| 34  | 2c    | 13   | GLY  | 3.1  |
| 47  | 1p    | 7    | ALA  | 3.1  |
| 49  | 1r    | 79   | LEU  | 3.1  |
| 50  | 2s    | 67   | VAL  | 3.1  |
| 12  | 2Q    | 63   | LYS  | 3.1  |
| 45  | 2n    | 47   | LEU  | 3.1  |
| 29  | 17    | 47   | ARG  | 3.1  |
| 26  | 24    | 52   | THR  | 3.1  |
| 41  | 1j    | 10   | GLY  | 3.1  |
| 21  | 2Z    | 96   | VAL  | 3.1  |
| 33  | 2b    | 211  | ILE  | 3.1  |
| 32  | 2a    | 1257 | U    | 3.1  |
| 46  | 1o    | 78   | TYR  | 3.1  |
| 36  | 2e    | 81   | GLU  | 3.1  |
| 32  | 2a    | 1220 | G    | 3.1  |
| 36  | 2e    | 120  | THR  | 3.1  |
| 25  | 23    | 6    | VAL  | 3.1  |
| 25  | 23    | 23   | LEU  | 3.1  |
| 35  | 2d    | 150  | GLU  | 3.1  |
| 36  | 1e    | 6    | PHE  | 3.0  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | 1A    | 892  | G    | 3.0  |
| 42  | 1k    | 64   | ALA  | 3.0  |
| 44  | 2m    | 122  | LYS  | 3.0  |
| 1   | 2A    | 2140 | C    | 3.0  |
| 54  | 2w    | 58   | A    | 3.0  |
| 39  | 2h    | 65   | TYR  | 3.0  |
| 1   | 2A    | 2144 | U    | 3.0  |
| 33  | 2b    | 163  | PHE  | 3.0  |
| 35  | 2d    | 105  | VAL  | 3.0  |
| 39  | 2h    | 2    | LEU  | 3.0  |
| 41  | 2j    | 60   | ARG  | 3.0  |
| 50  | 2s    | 81   | ARG  | 3.0  |
| 40  | 2i    | 76   | ALA  | 3.0  |
| 1   | 2A    | 2802 | G    | 3.0  |
| 45  | 1n    | 7    | ILE  | 3.0  |
| 1   | 2A    | 2145 | C    | 3.0  |
| 1   | 1A    | 2132 | U    | 3.0  |
| 29  | 27    | 46   | VAL  | 3.0  |
| 29  | 27    | 47   | ARG  | 3.0  |
| 42  | 1k    | 57   | THR  | 3.0  |
| 45  | 2n    | 46   | GLU  | 3.0  |
| 12  | 2Q    | 40   | ALA  | 3.0  |
| 45  | 2n    | 49   | HIS  | 3.0  |
| 1   | 1A    | 2140 | C    | 3.0  |
| 1   | 1A    | 2146 | C    | 3.0  |
| 34  | 2c    | 15   | THR  | 3.0  |
| 45  | 2n    | 18   | VAL  | 3.0  |
| 34  | 2c    | 91   | LEU  | 3.0  |
| 35  | 1d    | 11   | LEU  | 3.0  |
| 35  | 1d    | 78   | LEU  | 3.0  |
| 50  | 2s    | 15   | LEU  | 3.0  |
| 21  | 2Z    | 152  | ALA  | 3.0  |
| 7   | 2H    | 89   | ILE  | 3.0  |
| 52  | 1u    | 11   | GLY  | 3.0  |
| 50  | 2s    | 57   | HIS  | 3.0  |
| 22  | 20    | 45   | PHE  | 3.0  |
| 41  | 2j    | 90   | LEU  | 3.0  |
| 36  | 2e    | 9    | LYS  | 3.0  |
| 48  | 1q    | 28   | PRO  | 3.0  |
| 40  | 2i    | 33   | PHE  | 3.0  |
| 9   | 2N    | 13   | TRP  | 3.0  |
| 49  | 1r    | 40   | LEU  | 3.0  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 21  | 2Z    | 51   | ALA  | 3.0  |
| 54  | 2w    | 68   | C    | 3.0  |
| 17  | 2V    | 73   | SER  | 3.0  |
| 9   | 2N    | 98   | VAL  | 3.0  |
| 10  | 2O    | 8    | LEU  | 3.0  |
| 22  | 20    | 13   | GLY  | 3.0  |
| 43  | 2l    | 15   | ARG  | 3.0  |
| 21  | 1Z    | 120  | ILE  | 2.9  |
| 35  | 2d    | 70   | ILE  | 2.9  |
| 54  | 1w    | 1    | G    | 2.9  |
| 54  | 2y    | 65   | G    | 2.9  |
| 32  | 1a    | 160  | A    | 2.9  |
| 32  | 1a    | 344  | A    | 2.9  |
| 50  | 2s    | 38   | SER  | 2.9  |
| 21  | 2Z    | 157  | LEU  | 2.9  |
| 28  | 26    | 28   | ARG  | 2.9  |
| 34  | 2c    | 85   | ARG  | 2.9  |
| 42  | 2k    | 35   | PRO  | 2.9  |
| 1   | 1A    | 1093 | G    | 2.9  |
| 35  | 2d    | 159  | ARG  | 2.9  |
| 36  | 2e    | 29   | GLY  | 2.9  |
| 20  | 2Y    | 42   | VAL  | 2.9  |
| 34  | 2c    | 200  | ALA  | 2.9  |
| 26  | 24    | 18   | CYS  | 2.9  |
| 39  | 2h    | 111  | ILE  | 2.9  |
| 44  | 2m    | 4    | ILE  | 2.9  |
| 45  | 2n    | 24   | CYS  | 2.9  |
| 35  | 2d    | 110  | PHE  | 2.9  |
| 1   | 1A    | 2142 | C    | 2.9  |
| 34  | 2c    | 80   | GLY  | 2.9  |
| 6   | 1G    | 152  | LEU  | 2.9  |
| 40  | 2i    | 7    | THR  | 2.9  |
| 7   | 2H    | 102  | ALA  | 2.9  |
| 10  | 2O    | 81   | ASP  | 2.9  |
| 53  | 1v    | 23   | A    | 2.9  |
| 21  | 2Z    | 53   | ILE  | 2.9  |
| 34  | 1c    | 124  | ILE  | 2.9  |
| 36  | 1e    | 89   | ILE  | 2.9  |
| 6   | 2G    | 115  | ARG  | 2.9  |
| 44  | 1m    | 91   | ARG  | 2.9  |
| 41  | 2j    | 67   | THR  | 2.9  |
| 34  | 2c    | 193  | TYR  | 2.9  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 12  | 2Q    | 91   | GLU  | 2.9  |
| 35  | 2d    | 98   | GLU  | 2.9  |
| 49  | 1r    | 73   | ALA  | 2.9  |
| 50  | 2s    | 33   | THR  | 2.9  |
| 38  | 1g    | 154  | TYR  | 2.9  |
| 3   | 1D    | 2    | ALA  | 2.9  |
| 45  | 2n    | 59   | ALA  | 2.9  |
| 32  | 1a    | 345  | C    | 2.9  |
| 35  | 2d    | 177  | ASP  | 2.9  |
| 54  | 1w    | 41   | C    | 2.9  |
| 35  | 2d    | 130  | GLY  | 2.9  |
| 48  | 2q    | 36   | ILE  | 2.9  |
| 1   | 2A    | 1042 | G    | 2.9  |
| 6   | 2G    | 19   | LEU  | 2.9  |
| 21  | 2Z    | 138  | GLU  | 2.9  |
| 32  | 1a    | 161  | A    | 2.9  |
| 34  | 1c    | 15   | THR  | 2.9  |
| 48  | 2q    | 100  | LYS  | 2.9  |
| 6   | 2G    | 159  | VAL  | 2.9  |
| 12  | 2Q    | 106  | VAL  | 2.9  |
| 43  | 2l    | 55   | VAL  | 2.9  |
| 1   | 1A    | 1026 | U    | 2.9  |
| 43  | 2l    | 7    | ILE  | 2.9  |
| 48  | 1q    | 98   | LEU  | 2.9  |
| 9   | 2N    | 50   | ASP  | 2.9  |
| 10  | 2O    | 58   | VAL  | 2.9  |
| 36  | 2e    | 105  | VAL  | 2.9  |
| 38  | 2g    | 78   | ARG  | 2.9  |
| 42  | 1k    | 47   | VAL  | 2.9  |
| 21  | 2Z    | 25   | PRO  | 2.9  |
| 7   | 2H    | 72   | ILE  | 2.8  |
| 44  | 2m    | 70   | LEU  | 2.8  |
| 49  | 1r    | 31   | LEU  | 2.8  |
| 39  | 2h    | 92   | ARG  | 2.8  |
| 12  | 2Q    | 81   | VAL  | 2.8  |
| 48  | 2q    | 32   | TYR  | 2.8  |
| 34  | 2c    | 18   | TRP  | 2.8  |
| 32  | 1a    | 1034 | G    | 2.8  |
| 1   | 2A    | 2602 | A    | 2.8  |
| 12  | 2Q    | 66   | ILE  | 2.8  |
| 12  | 2Q    | 56   | ARG  | 2.8  |
| 1   | 2A    | 1041 | C    | 2.8  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | 2A    | 2139 | C    | 2.8  |
| 6   | 2G    | 182  | LYS  | 2.8  |
| 12  | 1Q    | 81   | VAL  | 2.8  |
| 14  | 1S    | 37   | ALA  | 2.8  |
| 23  | 11    | 62   | VAL  | 2.8  |
| 50  | 2s    | 24   | ALA  | 2.8  |
| 41  | 2j    | 68   | HIS  | 2.8  |
| 52  | 1u    | 14   | TRP  | 2.8  |
| 10  | 2O    | 19   | ILE  | 2.8  |
| 5   | 2F    | 140  | LEU  | 2.8  |
| 44  | 1m    | 122  | LYS  | 2.8  |
| 1   | 2A    | 2803 | C    | 2.8  |
| 9   | 2N    | 9    | VAL  | 2.8  |
| 44  | 2m    | 15   | VAL  | 2.8  |
| 54  | 1w    | 2    | C    | 2.8  |
| 21  | 1Z    | 99   | TYR  | 2.8  |
| 25  | 23    | 11   | SER  | 2.8  |
| 35  | 2d    | 128  | VAL  | 2.8  |
| 50  | 2s    | 69   | HIS  | 2.8  |
| 3   | 2D    | 38   | LYS  | 2.8  |
| 35  | 2d    | 169  | LYS  | 2.8  |
| 12  | 2Q    | 64   | ILE  | 2.8  |
| 34  | 2c    | 17   | ASP  | 2.8  |
| 41  | 2j    | 12   | ASP  | 2.8  |
| 42  | 1k    | 81   | ASP  | 2.8  |
| 4   | 2E    | 71   | GLY  | 2.8  |
| 44  | 2m    | 72   | ALA  | 2.8  |
| 20  | 2Y    | 55   | TYR  | 2.8  |
| 40  | 1i    | 113  | LYS  | 2.8  |
| 12  | 2Q    | 3    | MET  | 2.8  |
| 25  | 23    | 54   | VAL  | 2.8  |
| 35  | 1d    | 170  | VAL  | 2.8  |
| 35  | 2d    | 122  | ARG  | 2.8  |
| 44  | 2m    | 94   | ARG  | 2.8  |
| 36  | 2e    | 89   | ILE  | 2.8  |
| 54  | 2w    | 18   | G    | 2.8  |
| 54  | 2w    | 43   | C    | 2.8  |
| 49  | 2r    | 87   | ARG  | 2.8  |
| 7   | 2H    | 114  | VAL  | 2.7  |
| 20  | 2Y    | 65   | ALA  | 2.7  |
| 23  | 11    | 26   | ARG  | 2.7  |
| 36  | 2e    | 107  | ARG  | 2.7  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 45  | 2n    | 41   | ARG  | 2.7  |
| 1   | 1A    | 2602 | A    | 2.7  |
| 32  | 1a    | 1531 | A    | 2.7  |
| 54  | 1w    | 29   | G    | 2.7  |
| 21  | 2Z    | 95   | PRO  | 2.7  |
| 26  | 14    | 50   | VAL  | 2.7  |
| 43  | 2l    | 96   | VAL  | 2.7  |
| 45  | 1n    | 56   | VAL  | 2.7  |
| 48  | 2q    | 28   | PRO  | 2.7  |
| 50  | 2s    | 42   | PRO  | 2.7  |
| 51  | 1t    | 76   | ALA  | 2.7  |
| 10  | 2O    | 7    | TYR  | 2.7  |
| 35  | 2d    | 120  | LEU  | 2.7  |
| 14  | 2S    | 35   | ILE  | 2.7  |
| 12  | 2Q    | 102  | VAL  | 2.7  |
| 34  | 2c    | 207  | VAL  | 2.7  |
| 35  | 2d    | 182  | LYS  | 2.7  |
| 42  | 1k    | 24   | SER  | 2.7  |
| 46  | 1o    | 60   | VAL  | 2.7  |
| 1   | 2A    | 2161 | C    | 2.7  |
| 54  | 1y    | 13   | C    | 2.7  |
| 32  | 2a    | 1202 | G    | 2.7  |
| 21  | 2Z    | 99   | TYR  | 2.7  |
| 36  | 2e    | 135  | THR  | 2.7  |
| 42  | 1k    | 87   | THR  | 2.7  |
| 9   | 2N    | 14   | VAL  | 2.7  |
| 17  | 2V    | 72   | VAL  | 2.7  |
| 36  | 2e    | 104  | ALA  | 2.7  |
| 42  | 1k    | 61   | ALA  | 2.7  |
| 46  | 2o    | 60   | VAL  | 2.7  |
| 36  | 1e    | 136  | MET  | 2.7  |
| 12  | 2Q    | 61   | GLY  | 2.7  |
| 28  | 26    | 4    | GLU  | 2.7  |
| 54  | 1y    | 23   | A    | 2.7  |
| 1   | 2A    | 1115 | G    | 2.7  |
| 32  | 1a    | 1002 | G    | 2.7  |
| 41  | 2j    | 8    | LEU  | 2.7  |
| 55  | 2x    | 70   | G    | 2.7  |
| 44  | 2m    | 120  | LYS  | 2.7  |
| 21  | 2Z    | 79   | ARG  | 2.7  |
| 41  | 2j    | 66   | ARG  | 2.7  |
| 6   | 1G    | 173  | LEU  | 2.7  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 20  | 2Y    | 43   | ASN  | 2.7  |
| 21  | 1Z    | 102  | LEU  | 2.7  |
| 36  | 2e    | 123  | LEU  | 2.7  |
| 34  | 2c    | 134  | ILE  | 2.7  |
| 9   | 2N    | 44   | PRO  | 2.7  |
| 21  | 1Z    | 51   | ALA  | 2.7  |
| 23  | 21    | 24   | ALA  | 2.7  |
| 34  | 2c    | 154  | SER  | 2.7  |
| 19  | 2X    | 68   | ARG  | 2.7  |
| 43  | 2l    | 31   | PRO  | 2.7  |
| 52  | 1u    | 15   | ARG  | 2.7  |
| 10  | 2O    | 57   | VAL  | 2.7  |
| 48  | 2q    | 33   | GLY  | 2.7  |
| 35  | 2d    | 196  | LEU  | 2.7  |
| 45  | 2n    | 16   | PHE  | 2.7  |
| 34  | 1c    | 134  | ILE  | 2.7  |
| 21  | 1Z    | 170  | THR  | 2.7  |
| 43  | 1l    | 16   | GLU  | 2.7  |
| 52  | 2u    | 15   | ARG  | 2.7  |
| 54  | 2w    | 11   | C    | 2.7  |
| 54  | 2w    | 7    | A    | 2.7  |
| 7   | 2H    | 25   | LYS  | 2.7  |
| 34  | 2c    | 4    | LYS  | 2.7  |
| 43  | 2l    | 13   | LYS  | 2.7  |
| 21  | 2Z    | 42   | VAL  | 2.7  |
| 39  | 2h    | 137  | VAL  | 2.7  |
| 42  | 1k    | 78   | GLN  | 2.7  |
| 38  | 2g    | 16   | LEU  | 2.7  |
| 10  | 2O    | 18   | LYS  | 2.7  |
| 21  | 2Z    | 137  | ILE  | 2.7  |
| 43  | 2l    | 85   | ILE  | 2.7  |
| 22  | 20    | 9    | SER  | 2.7  |
| 35  | 2d    | 127  | THR  | 2.7  |
| 1   | 1A    | 1078 | U    | 2.6  |
| 41  | 2j    | 52   | GLY  | 2.6  |
| 32  | 2a    | 973  | G    | 2.6  |
| 34  | 2c    | 19   | GLU  | 2.6  |
| 6   | 2G    | 136  | ARG  | 2.6  |
| 11  | 1P    | 15   | ARG  | 2.6  |
| 35  | 2d    | 175  | SER  | 2.6  |
| 37  | 2f    | 59   | TYR  | 2.6  |
| 9   | 2N    | 69   | GLN  | 2.6  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 42  | 1k    | 82   | VAL  | 2.6  |
| 1   | 2A    | 2131 | G    | 2.6  |
| 34  | 2c    | 159  | GLY  | 2.6  |
| 7   | 2H    | 111  | HIS  | 2.6  |
| 21  | 1Z    | 126  | VAL  | 2.6  |
| 42  | 1k    | 80   | VAL  | 2.6  |
| 48  | 2q    | 23   | VAL  | 2.6  |
| 6   | 1G    | 139  | LEU  | 2.6  |
| 43  | 2l    | 93   | LEU  | 2.6  |
| 44  | 1m    | 94   | ARG  | 2.6  |
| 34  | 2c    | 28   | GLN  | 2.6  |
| 35  | 2d    | 37   | PRO  | 2.6  |
| 36  | 2e    | 17   | ALA  | 2.6  |
| 40  | 2i    | 49   | PRO  | 2.6  |
| 44  | 1m    | 121  | LYS  | 2.6  |
| 48  | 1q    | 37   | LYS  | 2.6  |
| 35  | 2d    | 56   | VAL  | 2.6  |
| 44  | 1m    | 74   | VAL  | 2.6  |
| 10  | 2O    | 1    | MET  | 2.6  |
| 43  | 2l    | 60   | LEU  | 2.6  |
| 14  | 2S    | 12   | PHE  | 2.6  |
| 34  | 2c    | 57   | ILE  | 2.6  |
| 37  | 1f    | 81   | ILE  | 2.6  |
| 34  | 2c    | 174  | PRO  | 2.6  |
| 40  | 1i    | 125  | TYR  | 2.6  |
| 40  | 2i    | 123  | PRO  | 2.6  |
| 46  | 1o    | 69   | TYR  | 2.6  |
| 50  | 2s    | 77   | THR  | 2.6  |
| 9   | 2N    | 45   | ASN  | 2.6  |
| 35  | 2d    | 161  | ASN  | 2.6  |
| 7   | 2H    | 107  | VAL  | 2.6  |
| 42  | 2k    | 36   | ASP  | 2.6  |
| 34  | 1c    | 203  | PHE  | 2.6  |
| 54  | 2y    | 63   | G    | 2.6  |
| 10  | 2O    | 42   | SER  | 2.6  |
| 6   | 1G    | 136  | ARG  | 2.6  |
| 9   | 2N    | 85   | ILE  | 2.6  |
| 17  | 2V    | 50   | PRO  | 2.6  |
| 20  | 2Y    | 48   | ALA  | 2.6  |
| 9   | 2N    | 53   | VAL  | 2.6  |
| 31  | 29    | 25   | VAL  | 2.6  |
| 40  | 1i    | 19   | LEU  | 2.6  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 9   | 2N    | 125  | GLY  | 2.6  |
| 12  | 2Q    | 112  | GLU  | 2.6  |
| 32  | 2a    | 1021 | G    | 2.6  |
| 33  | 2b    | 226  | ARG  | 2.6  |
| 38  | 2g    | 155  | ARG  | 2.6  |
| 55  | 2x    | 4    | G    | 2.6  |
| 12  | 1Q    | 32   | TYR  | 2.6  |
| 43  | 1l    | 23   | LYS  | 2.6  |
| 54  | 2y    | 62   | C    | 2.6  |
| 55  | 2x    | 65   | C    | 2.6  |
| 36  | 2e    | 110  | LEU  | 2.6  |
| 45  | 2n    | 6    | LEU  | 2.6  |
| 6   | 2G    | 169  | ALA  | 2.5  |
| 43  | 2l    | 51   | ALA  | 2.5  |
| 44  | 2m    | 64   | TRP  | 2.5  |
| 1   | 2A    | 879  | G    | 2.5  |
| 48  | 2q    | 95   | TYR  | 2.5  |
| 13  | 1R    | 114  | VAL  | 2.5  |
| 33  | 2b    | 81   | VAL  | 2.5  |
| 34  | 2c    | 56   | ASP  | 2.5  |
| 49  | 1r    | 76   | LEU  | 2.5  |
| 32  | 1a    | 163  | C    | 2.5  |
| 50  | 2s    | 84   | GLY  | 2.5  |
| 3   | 2D    | 276  | LYS  | 2.5  |
| 7   | 2H    | 30   | LYS  | 2.5  |
| 28  | 26    | 2    | ALA  | 2.5  |
| 35  | 2d    | 164  | ALA  | 2.5  |
| 42  | 1k    | 97   | ALA  | 2.5  |
| 6   | 2G    | 116  | ASP  | 2.5  |
| 20  | 2Y    | 106  | LEU  | 2.5  |
| 36  | 2e    | 22   | GLY  | 2.5  |
| 50  | 2s    | 54   | GLY  | 2.5  |
| 38  | 2g    | 6    | ARG  | 2.5  |
| 1   | 1A    | 2161 | C    | 2.5  |
| 34  | 1c    | 8    | ILE  | 2.5  |
| 43  | 2l    | 48   | PRO  | 2.5  |
| 6   | 2G    | 3    | LEU  | 2.5  |
| 10  | 2O    | 10   | VAL  | 2.5  |
| 31  | 29    | 13   | LYS  | 2.5  |
| 31  | 29    | 33   | LYS  | 2.5  |
| 43  | 2l    | 47   | LYS  | 2.5  |
| 50  | 2s    | 11   | VAL  | 2.5  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 32  | 2a    | 1222 | G    | 2.5  |
| 1   | 1A    | 2138 | C    | 2.5  |
| 34  | 1c    | 65   | ALA  | 2.5  |
| 51  | 1t    | 55   | ILE  | 2.5  |
| 25  | 23    | 29   | ARG  | 2.5  |
| 38  | 2g    | 149  | ARG  | 2.5  |
| 39  | 2h    | 90   | GLY  | 2.5  |
| 42  | 1k    | 126  | ARG  | 2.5  |
| 21  | 2Z    | 3    | TYR  | 2.5  |
| 35  | 2d    | 106  | TYR  | 2.5  |
| 41  | 2j    | 49   | VAL  | 2.5  |
| 35  | 2d    | 89   | THR  | 2.5  |
| 39  | 2h    | 84   | ARG  | 2.5  |
| 40  | 2i    | 90   | PRO  | 2.5  |
| 40  | 2i    | 15   | ALA  | 2.5  |
| 44  | 2m    | 75   | ALA  | 2.5  |
| 48  | 2q    | 90   | ILE  | 2.5  |
| 12  | 2Q    | 80   | GLU  | 2.5  |
| 34  | 2c    | 89   | GLU  | 2.5  |
| 35  | 1d    | 62   | GLN  | 2.5  |
| 39  | 2h    | 112  | LEU  | 2.5  |
| 46  | 1o    | 62   | GLN  | 2.5  |
| 32  | 2a    | 1196 | U    | 2.5  |
| 54  | 1w    | 45   | U    | 2.5  |
| 3   | 1D    | 5    | LYS  | 2.5  |
| 12  | 2Q    | 77   | LYS  | 2.5  |
| 39  | 2h    | 124  | ALA  | 2.5  |
| 43  | 2l    | 29   | GLY  | 2.5  |
| 21  | 2Z    | 76   | LEU  | 2.5  |
| 35  | 1d    | 64   | LEU  | 2.5  |
| 3   | 1D    | 205  | VAL  | 2.5  |
| 35  | 2d    | 104  | VAL  | 2.5  |
| 9   | 2N    | 51   | PHE  | 2.5  |
| 20  | 2Y    | 63   | LYS  | 2.5  |
| 40  | 2i    | 125  | TYR  | 2.5  |
| 54  | 1w    | 24   | G    | 2.5  |
| 1   | 1A    | 1060 | U    | 2.5  |
| 9   | 2N    | 61   | ARG  | 2.5  |
| 6   | 2G    | 134  | GLY  | 2.5  |
| 12  | 2Q    | 19   | GLY  | 2.5  |
| 14  | 2S    | 34   | HIS  | 2.5  |
| 3   | 2D    | 271  | ILE  | 2.5  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 29  | 27    | 45   | ALA  | 2.5  |
| 39  | 1h    | 6    | ILE  | 2.5  |
| 47  | 1p    | 19   | ILE  | 2.5  |
| 34  | 2c    | 101  | LEU  | 2.5  |
| 47  | 2p    | 48   | TRP  | 2.5  |
| 7   | 2H    | 24   | VAL  | 2.5  |
| 35  | 1d    | 105  | VAL  | 2.5  |
| 39  | 2h    | 61   | VAL  | 2.5  |
| 19  | 2X    | 18   | TYR  | 2.5  |
| 36  | 2e    | 24   | ARG  | 2.5  |
| 32  | 2a    | 1017 | G    | 2.5  |
| 35  | 2d    | 69   | GLY  | 2.4  |
| 10  | 2O    | 53   | LYS  | 2.4  |
| 12  | 2Q    | 36   | ALA  | 2.4  |
| 31  | 29    | 15   | LYS  | 2.4  |
| 37  | 1f    | 48   | LEU  | 2.4  |
| 39  | 2h    | 134  | ILE  | 2.4  |
| 1   | 1A    | 1847 | A    | 2.4  |
| 26  | 24    | 56   | VAL  | 2.4  |
| 54  | 2w    | 9    | A    | 2.4  |
| 34  | 2c    | 36   | ASP  | 2.4  |
| 45  | 2n    | 40   | CYS  | 2.4  |
| 9   | 2N    | 43   | THR  | 2.4  |
| 21  | 2Z    | 164  | ALA  | 2.4  |
| 53  | 1v    | 25   | U    | 2.4  |
| 13  | 2R    | 65   | LEU  | 2.4  |
| 43  | 2l    | 100  | ILE  | 2.4  |
| 44  | 1m    | 90   | LEU  | 2.4  |
| 12  | 1Q    | 59   | ARG  | 2.4  |
| 21  | 1Z    | 128  | VAL  | 2.4  |
| 25  | 23    | 9    | VAL  | 2.4  |
| 31  | 29    | 16   | VAL  | 2.4  |
| 34  | 1c    | 127  | ARG  | 2.4  |
| 39  | 2h    | 122  | ARG  | 2.4  |
| 41  | 2j    | 61   | GLU  | 2.4  |
| 34  | 2c    | 23   | TYR  | 2.4  |
| 7   | 1H    | 166  | GLY  | 2.4  |
| 11  | 2P    | 20   | GLY  | 2.4  |
| 25  | 23    | 27   | GLY  | 2.4  |
| 54  | 1w    | 31   | A    | 2.4  |
| 38  | 2g    | 147  | ALA  | 2.4  |
| 36  | 2e    | 14   | ARG  | 2.4  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 42  | 2k    | 96   | ARG  | 2.4  |
| 46  | 1o    | 68   | ARG  | 2.4  |
| 6   | 2G    | 30   | GLU  | 2.4  |
| 12  | 2Q    | 18   | LYS  | 2.4  |
| 31  | 29    | 12   | ASP  | 2.4  |
| 33  | 2b    | 197  | VAL  | 2.4  |
| 34  | 1c    | 155  | GLY  | 2.4  |
| 21  | 1Z    | 167  | PRO  | 2.4  |
| 6   | 2G    | 181  | ARG  | 2.4  |
| 21  | 2Z    | 55   | HIS  | 2.4  |
| 12  | 2Q    | 2    | LEU  | 2.4  |
| 12  | 2Q    | 110  | THR  | 2.4  |
| 16  | 1U    | 4    | ALA  | 2.4  |
| 21  | 2Z    | 173  | ALA  | 2.4  |
| 50  | 2s    | 78   | ARG  | 2.4  |
| 34  | 2c    | 52   | LEU  | 2.4  |
| 42  | 1k    | 43   | SER  | 2.4  |
| 39  | 2h    | 131  | GLY  | 2.4  |
| 1   | 2A    | 1117 | G    | 2.4  |
| 38  | 2g    | 4    | ARG  | 2.4  |
| 41  | 2j    | 56   | HIS  | 2.4  |
| 35  | 1d    | 202  | LEU  | 2.4  |
| 35  | 2d    | 32   | ALA  | 2.4  |
| 45  | 1n    | 17   | LYS  | 2.4  |
| 6   | 2G    | 139  | LEU  | 2.4  |
| 34  | 2c    | 87   | LEU  | 2.4  |
| 45  | 1n    | 59   | ALA  | 2.4  |
| 50  | 2s    | 75   | ALA  | 2.4  |
| 36  | 1e    | 118  | ILE  | 2.4  |
| 36  | 2e    | 131  | ILE  | 2.4  |
| 34  | 2c    | 66   | VAL  | 2.4  |
| 40  | 2i    | 108  | VAL  | 2.4  |
| 53  | 2v    | 21   | C    | 2.4  |
| 55  | 2x    | 66   | C    | 2.4  |
| 43  | 2l    | 25   | PRO  | 2.4  |
| 1   | 2A    | 2793 | G    | 2.4  |
| 7   | 2H    | 103  | LEU  | 2.4  |
| 16  | 2U    | 20   | LEU  | 2.4  |
| 33  | 2b    | 34   | ALA  | 2.4  |
| 13  | 1R    | 34   | ILE  | 2.4  |
| 37  | 1f    | 55   | ASP  | 2.4  |
| 6   | 2G    | 109  | VAL  | 2.4  |

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| Mol | Chain | Res    | Type | RSRZ |
|-----|-------|--------|------|------|
| 39  | 1h    | 93     | VAL  | 2.4  |
| 1   | 1A    | 1077   | A    | 2.4  |
| 11  | 1P    | 102    | ARG  | 2.4  |
| 32  | 1a    | 162    | A    | 2.4  |
| 34  | 1c    | 126    | ARG  | 2.4  |
| 34  | 2c    | 179    | ARG  | 2.4  |
| 54  | 2y    | 33     | U    | 2.4  |
| 26  | 24    | 63     | TYR  | 2.4  |
| 31  | 29    | 24     | TYR  | 2.4  |
| 34  | 2c    | 201    | TYR  | 2.4  |
| 40  | 1i    | 117    | HIS  | 2.4  |
| 34  | 2c    | 204    | LEU  | 2.4  |
| 40  | 2i    | 19     | LEU  | 2.4  |
| 12  | 2Q    | 89     | ASN  | 2.4  |
| 14  | 2S    | 33     | LYS  | 2.4  |
| 16  | 1U    | 17     | ILE  | 2.4  |
| 32  | 2a    | 1221   | G    | 2.4  |
| 34  | 2c    | 9      | GLY  | 2.4  |
| 36  | 1e    | 129    | ILE  | 2.4  |
| 54  | 2w    | 57     | G    | 2.4  |
| 5   | 1F    | 72     | ARG  | 2.4  |
| 12  | 2Q    | 29     | PHE  | 2.4  |
| 16  | 2U    | 40     | PHE  | 2.4  |
| 21  | 2Z    | 126    | VAL  | 2.4  |
| 33  | 1b    | 165    | VAL  | 2.4  |
| 35  | 2d    | 187    | ARG  | 2.4  |
| 36  | 2e    | 6      | PHE  | 2.4  |
| 43  | 2l    | 16     | GLU  | 2.4  |
| 47  | 1p    | 59     | TRP  | 2.4  |
| 1   | 2A    | 614(A) | U    | 2.3  |
| 29  | 27    | 1      | MET  | 2.3  |
| 54  | 1y    | 38     | A    | 2.3  |
| 12  | 1Q    | 43     | THR  | 2.3  |
| 12  | 2Q    | 31     | ASP  | 2.3  |
| 27  | 25    | 29     | THR  | 2.3  |
| 34  | 2c    | 49     | SER  | 2.3  |
| 34  | 2c    | 94     | LEU  | 2.3  |
| 36  | 1e    | 95     | ALA  | 2.3  |
| 40  | 2i    | 78     | LYS  | 2.3  |
| 43  | 2l    | 62     | SER  | 2.3  |
| 3   | 1D    | 113    | VAL  | 2.3  |
| 42  | 1k    | 84     | VAL  | 2.3  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 43  | 1l    | 18   | VAL  | 2.3  |
| 1   | 2A    | 2112 | G    | 2.3  |
| 21  | 2Z    | 98   | MET  | 2.3  |
| 42  | 1k    | 20   | TYR  | 2.3  |
| 4   | 1E    | 195  | LEU  | 2.3  |
| 10  | 1O    | 122  | LEU  | 2.3  |
| 1   | 2A    | 2158 | A    | 2.3  |
| 12  | 2Q    | 44   | ALA  | 2.3  |
| 21  | 2Z    | 52   | SER  | 2.3  |
| 35  | 2d    | 157  | LEU  | 2.3  |
| 36  | 1e    | 134  | ALA  | 2.3  |
| 36  | 2e    | 132  | ALA  | 2.3  |
| 37  | 1f    | 53   | ALA  | 2.3  |
| 54  | 1w    | 23   | A    | 2.3  |
| 54  | 2y    | 64   | A    | 2.3  |
| 25  | 23    | 30   | ARG  | 2.3  |
| 42  | 2k    | 108  | ILE  | 2.3  |
| 52  | 2u    | 13   | ILE  | 2.3  |
| 9   | 2N    | 62   | VAL  | 2.3  |
| 34  | 1c    | 196  | LEU  | 2.3  |
| 35  | 1d    | 21   | LEU  | 2.3  |
| 35  | 2d    | 162  | LEU  | 2.3  |
| 40  | 2i    | 9    | ARG  | 2.3  |
| 41  | 1j    | 60   | ARG  | 2.3  |
| 43  | 2l    | 10   | LEU  | 2.3  |
| 54  | 1w    | 42   | C    | 2.3  |
| 54  | 2w    | 40   | C    | 2.3  |
| 54  | 2w    | 67   | C    | 2.3  |
| 36  | 2e    | 45   | PHE  | 2.3  |
| 54  | 2w    | 26   | A    | 2.3  |
| 16  | 2U    | 90   | VAL  | 2.3  |
| 31  | 29    | 11   | CYS  | 2.3  |
| 33  | 2b    | 220  | ASP  | 2.3  |
| 34  | 2c    | 7    | PRO  | 2.3  |
| 50  | 2s    | 13   | ASP  | 2.3  |
| 4   | 2E    | 182  | LEU  | 2.3  |
| 9   | 2N    | 57   | ALA  | 2.3  |
| 33  | 2b    | 33   | TYR  | 2.3  |
| 35  | 1d    | 101  | LEU  | 2.3  |
| 44  | 1m    | 75   | ALA  | 2.3  |
| 36  | 2e    | 80   | ILE  | 2.3  |
| 42  | 1k    | 21   | ILE  | 2.3  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 5   | 2F    | 37   | VAL  | 2.3  |
| 8   | 2I    | 19   | VAL  | 2.3  |
| 9   | 2N    | 46   | VAL  | 2.3  |
| 10  | 1O    | 115  | VAL  | 2.3  |
| 28  | 26    | 5    | VAL  | 2.3  |
| 21  | 2Z    | 93   | ASP  | 2.3  |
| 32  | 1a    | 1001 | A    | 2.3  |
| 28  | 26    | 50   | ARG  | 2.3  |
| 42  | 1k    | 18   | ARG  | 2.3  |
| 33  | 2b    | 215  | LEU  | 2.3  |
| 35  | 1d    | 97   | LEU  | 2.3  |
| 45  | 2n    | 32   | SER  | 2.3  |
| 48  | 2q    | 74   | LEU  | 2.3  |
| 21  | 1Z    | 69   | THR  | 2.3  |
| 33  | 2b    | 161  | ALA  | 2.3  |
| 34  | 1c    | 201  | TYR  | 2.3  |
| 35  | 2d    | 18   | LYS  | 2.3  |
| 50  | 2s    | 32   | LYS  | 2.3  |
| 38  | 1g    | 87   | VAL  | 2.3  |
| 6   | 2G    | 156  | ASP  | 2.3  |
| 54  | 2y    | 29   | G    | 2.3  |
| 11  | 1P    | 108  | LYS  | 2.3  |
| 9   | 2N    | 107  | LEU  | 2.3  |
| 41  | 2j    | 13   | HIS  | 2.3  |
| 42  | 2k    | 66   | LEU  | 2.3  |
| 40  | 2i    | 106  | ALA  | 2.3  |
| 42  | 1k    | 75   | TYR  | 2.3  |
| 42  | 1k    | 89   | ALA  | 2.3  |
| 14  | 2S    | 40   | ILE  | 2.3  |
| 21  | 2Z    | 124  | ILE  | 2.3  |
| 33  | 2b    | 58   | ILE  | 2.3  |
| 45  | 1n    | 29   | ARG  | 2.3  |
| 47  | 1p    | 21   | VAL  | 2.3  |
| 9   | 2N    | 20   | GLY  | 2.3  |
| 12  | 2Q    | 84   | GLY  | 2.3  |
| 34  | 1c    | 80   | GLY  | 2.3  |
| 43  | 2l    | 63   | GLY  | 2.3  |
| 11  | 1P    | 99   | LEU  | 2.3  |
| 54  | 1y    | 5    | G    | 2.3  |
| 1   | 2A    | 2174 | C    | 2.3  |
| 4   | 1E    | 28   | ALA  | 2.3  |
| 27  | 15    | 2    | ALA  | 2.3  |

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| Mol | Chain | Res     | Type | RSRZ |
|-----|-------|---------|------|------|
| 40  | 2i    | 82      | ALA  | 2.3  |
| 42  | 2k    | 23      | ALA  | 2.3  |
| 38  | 1g    | 151     | TYR  | 2.3  |
| 39  | 2h    | 99      | GLU  | 2.3  |
| 40  | 2i    | 62      | TYR  | 2.3  |
| 32  | 1a    | 1030(D) | A    | 2.3  |
| 12  | 2Q    | 87      | LYS  | 2.3  |
| 25  | 23    | 13      | ILE  | 2.3  |
| 40  | 1i    | 116     | LYS  | 2.3  |
| 43  | 2l    | 70      | ILE  | 2.3  |
| 6   | 2G    | 160     | VAL  | 2.3  |
| 21  | 1Z    | 161     | VAL  | 2.3  |
| 40  | 2i    | 26      | VAL  | 2.3  |
| 40  | 2i    | 28      | VAL  | 2.3  |
| 50  | 1s    | 58      | VAL  | 2.3  |
| 19  | 2X    | 94      | GLY  | 2.2  |
| 3   | 2D    | 37      | LEU  | 2.2  |
| 12  | 1Q    | 139     | GLU  | 2.2  |
| 38  | 1g    | 73      | MET  | 2.2  |
| 36  | 1e    | 132     | ALA  | 2.2  |
| 1   | 1A    | 2149    | G    | 2.2  |
| 1   | 2A    | 2794    | C    | 2.2  |
| 3   | 1D    | 38      | LYS  | 2.2  |
| 6   | 1G    | 51      | ARG  | 2.2  |
| 21  | 2Z    | 4       | ARG  | 2.2  |
| 35  | 1d    | 54      | TYR  | 2.2  |
| 54  | 1w    | 25      | C    | 2.2  |
| 21  | 1Z    | 154     | ASP  | 2.2  |
| 31  | 19    | 7       | VAL  | 2.2  |
| 31  | 19    | 17      | ILE  | 2.2  |
| 32  | 1a    | 1503    | A    | 2.2  |
| 36  | 2e    | 82      | VAL  | 2.2  |
| 42  | 1k    | 30      | VAL  | 2.2  |
| 50  | 2s    | 58      | VAL  | 2.2  |
| 46  | 1o    | 56      | LEU  | 2.2  |
| 40  | 1i    | 15      | ALA  | 2.2  |
| 48  | 2q    | 91      | ARG  | 2.2  |
| 33  | 2b    | 31      | TYR  | 2.2  |
| 31  | 29    | 37      | GLY  | 2.2  |
| 37  | 1f    | 58      | GLY  | 2.2  |
| 45  | 2n    | 52      | GLN  | 2.2  |
| 47  | 1p    | 2       | VAL  | 2.2  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 48  | 2q    | 59   | ILE  | 2.2  |
| 55  | 1x    | 67   | C    | 2.2  |
| 54  | 2w    | 27   | G    | 2.2  |
| 54  | 2y    | 5    | G    | 2.2  |
| 6   | 1G    | 182  | LYS  | 2.2  |
| 21  | 1Z    | 101  | PRO  | 2.2  |
| 33  | 2b    | 118  | LEU  | 2.2  |
| 39  | 2h    | 64   | LYS  | 2.2  |
| 40  | 1i    | 47   | LEU  | 2.2  |
| 48  | 2q    | 6    | LEU  | 2.2  |
| 1   | 1A    | 1081 | U    | 2.2  |
| 52  | 2u    | 22   | ARG  | 2.2  |
| 21  | 2Z    | 21   | ALA  | 2.2  |
| 42  | 2k    | 60   | ALA  | 2.2  |
| 5   | 1F    | 70   | THR  | 2.2  |
| 6   | 2G    | 161  | THR  | 2.2  |
| 28  | 16    | 47   | THR  | 2.2  |
| 22  | 20    | 8    | GLY  | 2.2  |
| 42  | 1k    | 59   | TYR  | 2.2  |
| 35  | 1d    | 110  | PHE  | 2.2  |
| 33  | 2b    | 222  | ILE  | 2.2  |
| 43  | 2l    | 65   | GLU  | 2.2  |
| 36  | 2e    | 130  | ASN  | 2.2  |
| 1   | 1A    | 2162 | G    | 2.2  |
| 50  | 1s    | 83   | HIS  | 2.2  |
| 7   | 2H    | 165  | ALA  | 2.2  |
| 42  | 1k    | 94   | ALA  | 2.2  |
| 54  | 1w    | 14   | A    | 2.2  |
| 35  | 2d    | 90   | GLY  | 2.2  |
| 7   | 2H    | 164  | TYR  | 2.2  |
| 35  | 2d    | 185  | PHE  | 2.2  |
| 5   | 2F    | 193  | VAL  | 2.2  |
| 34  | 2c    | 120  | VAL  | 2.2  |
| 7   | 1H    | 2    | SER  | 2.2  |
| 35  | 1d    | 73   | ARG  | 2.2  |
| 41  | 2j    | 59   | SER  | 2.2  |
| 6   | 1G    | 106  | LEU  | 2.2  |
| 23  | 1l    | 98   | LEU  | 2.2  |
| 45  | 2n    | 27   | CYS  | 2.2  |
| 49  | 1r    | 85   | LEU  | 2.2  |
| 6   | 2G    | 49   | ASP  | 2.2  |
| 31  | 19    | 1    | MET  | 2.2  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 26  | 24    | 19   | GLY  | 2.2  |
| 32  | 1a    | 117  | G    | 2.2  |
| 35  | 2d    | 23   | GLY  | 2.2  |
| 52  | 2u    | 17   | THR  | 2.2  |
| 54  | 2w    | 10   | G    | 2.2  |
| 19  | 2X    | 69   | TYR  | 2.2  |
| 21  | 2Z    | 48   | PHE  | 2.2  |
| 54  | 1w    | 21   | A    | 2.2  |
| 3   | 1D    | 145  | VAL  | 2.2  |
| 34  | 1c    | 14   | ILE  | 2.2  |
| 40  | 2i    | 63   | ILE  | 2.2  |
| 21  | 2Z    | 70   | LEU  | 2.2  |
| 40  | 2i    | 27   | THR  | 2.2  |
| 52  | 1u    | 17   | THR  | 2.2  |
| 35  | 2d    | 139  | ARG  | 2.2  |
| 35  | 2d    | 207  | TYR  | 2.2  |
| 3   | 2D    | 18   | VAL  | 2.2  |
| 40  | 1i    | 126  | SER  | 2.2  |
| 1   | 1A    | 2135 | A    | 2.2  |
| 1   | 2A    | 6    | A    | 2.2  |
| 12  | 2Q    | 85   | LYS  | 2.2  |
| 35  | 2d    | 94   | LEU  | 2.2  |
| 50  | 2s    | 28   | LYS  | 2.2  |
| 10  | 2O    | 11   | ALA  | 2.2  |
| 11  | 2P    | 1    | MET  | 2.2  |
| 9   | 2N    | 93   | THR  | 2.2  |
| 1   | 1A    | 1175 | U    | 2.1  |
| 42  | 2k    | 51   | LYS  | 2.1  |
| 21  | 1Z    | 124  | ILE  | 2.1  |
| 28  | 26    | 52   | VAL  | 2.1  |
| 35  | 1d    | 70   | ILE  | 2.1  |
| 46  | 2o    | 45   | VAL  | 2.1  |
| 25  | 23    | 53   | LEU  | 2.1  |
| 34  | 1c    | 34   | LEU  | 2.1  |
| 32  | 2a    | 1002 | G    | 2.1  |
| 1   | 1A    | 529  | A    | 2.1  |
| 54  | 1y    | 21   | A    | 2.1  |
| 31  | 29    | 9    | ARG  | 2.1  |
| 35  | 1d    | 50   | ARG  | 2.1  |
| 35  | 2d    | 47   | ARG  | 2.1  |
| 45  | 2n    | 19   | ARG  | 2.1  |
| 15  | 2T    | 46   | GLU  | 2.1  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 33  | 2b    | 55   | PHE  | 2.1  |
| 1   | 1A    | 2130 | U    | 2.1  |
| 4   | 2E    | 196  | VAL  | 2.1  |
| 7   | 2H    | 144  | VAL  | 2.1  |
| 41  | 1j    | 94   | VAL  | 2.1  |
| 41  | 2j    | 72   | VAL  | 2.1  |
| 42  | 2k    | 93   | GLN  | 2.1  |
| 46  | 1o    | 31   | LEU  | 2.1  |
| 49  | 2r    | 66   | LEU  | 2.1  |
| 5   | 2F    | 208  | GLY  | 2.1  |
| 23  | 2l    | 28   | GLY  | 2.1  |
| 50  | 2s    | 68   | GLY  | 2.1  |
| 35  | 1d    | 209  | ARG  | 2.1  |
| 40  | 2i    | 110  | GLU  | 2.1  |
| 12  | 2Q    | 113  | GLN  | 2.1  |
| 34  | 2c    | 10   | PHE  | 2.1  |
| 49  | 1r    | 29   | PHE  | 2.1  |
| 12  | 2Q    | 97   | VAL  | 2.1  |
| 15  | 1T    | 89   | VAL  | 2.1  |
| 35  | 1d    | 148  | VAL  | 2.1  |
| 36  | 2e    | 129  | ILE  | 2.1  |
| 42  | 1k    | 50   | TYR  | 2.1  |
| 43  | 2l    | 69   | TYR  | 2.1  |
| 11  | 2P    | 5    | ASP  | 2.1  |
| 21  | 2Z    | 163  | LEU  | 2.1  |
| 34  | 2c    | 155  | GLY  | 2.1  |
| 39  | 1h    | 4    | ASP  | 2.1  |
| 43  | 1l    | 60   | LEU  | 2.1  |
| 44  | 2m    | 88   | ARG  | 2.1  |
| 54  | 2w    | 25   | C    | 2.1  |
| 55  | 2x    | 3    | C    | 2.1  |
| 25  | 23    | 51   | ALA  | 2.1  |
| 35  | 2d    | 34   | GLU  | 2.1  |
| 42  | 1k    | 15   | ALA  | 2.1  |
| 5   | 2F    | 172  | TRP  | 2.1  |
| 38  | 2g    | 86   | GLN  | 2.1  |
| 42  | 1k    | 62   | GLN  | 2.1  |
| 42  | 2k    | 125  | PHE  | 2.1  |
| 1   | 2A    | 2133 | G    | 2.1  |
| 45  | 2n    | 60   | SER  | 2.1  |
| 54  | 1w    | 30   | G    | 2.1  |
| 54  | 1y    | 34   | G    | 2.1  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 3   | 2D    | 216  | GLY  | 2.1  |
| 5   | 2F    | 82   | ILE  | 2.1  |
| 10  | 1O    | 52   | VAL  | 2.1  |
| 12  | 1Q    | 66   | ILE  | 2.1  |
| 21  | 2Z    | 102  | LEU  | 2.1  |
| 31  | 29    | 19   | ARG  | 2.1  |
| 35  | 2d    | 198  | VAL  | 2.1  |
| 38  | 1g    | 141  | VAL  | 2.1  |
| 41  | 2j    | 89   | ASP  | 2.1  |
| 42  | 1k    | 29   | ILE  | 2.1  |
| 1   | 2A    | 2132 | U    | 2.1  |
| 35  | 2d    | 165  | MET  | 2.1  |
| 40  | 2i    | 126  | SER  | 2.1  |
| 6   | 1G    | 115  | ARG  | 2.1  |
| 12  | 1Q    | 5    | ARG  | 2.1  |
| 6   | 2G    | 43   | LEU  | 2.1  |
| 6   | 2G    | 85   | GLY  | 2.1  |
| 7   | 2H    | 35   | VAL  | 2.1  |
| 23  | 21    | 22   | GLY  | 2.1  |
| 50  | 2s    | 12   | ASP  | 2.1  |
| 50  | 1s    | 60   | VAL  | 2.1  |
| 1   | 1A    | 2152 | G    | 2.1  |
| 12  | 2Q    | 99   | PRO  | 2.1  |
| 16  | 2U    | 108  | GLU  | 2.1  |
| 21  | 2Z    | 167  | PRO  | 2.1  |
| 35  | 1d    | 4    | TYR  | 2.1  |
| 35  | 1d    | 138  | TYR  | 2.1  |
| 51  | 2t    | 13   | LEU  | 2.1  |
| 5   | 1F    | 42   | ALA  | 2.1  |
| 29  | 17    | 45   | ALA  | 2.1  |
| 31  | 19    | 34   | GLN  | 2.1  |
| 42  | 2k    | 65   | ALA  | 2.1  |
| 1   | 1A    | 2145 | C    | 2.1  |
| 36  | 2e    | 16   | THR  | 2.1  |
| 39  | 1h    | 3    | THR  | 2.1  |
| 48  | 2q    | 7    | THR  | 2.1  |
| 48  | 2q    | 27   | PHE  | 2.1  |
| 8   | 1I    | 38   | LEU  | 2.1  |
| 37  | 1f    | 98   | LEU  | 2.1  |
| 39  | 2h    | 132  | GLU  | 2.1  |
| 10  | 2O    | 47   | ILE  | 2.1  |
| 13  | 1R    | 97   | VAL  | 2.1  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 38  | 1g    | 105  | VAL  | 2.1  |
| 41  | 1j    | 65   | LEU  | 2.1  |
| 46  | 1o    | 34   | LEU  | 2.1  |
| 35  | 1d    | 207  | TYR  | 2.1  |
| 40  | 2i    | 88   | TYR  | 2.1  |
| 1   | 2A    | 2319 | G    | 2.1  |
| 32  | 2a    | 983  | A    | 2.1  |
| 54  | 2y    | 38   | A    | 2.1  |
| 34  | 2c    | 3    | ASN  | 2.1  |
| 12  | 1Q    | 65   | PHE  | 2.1  |
| 21  | 2Z    | 129  | SER  | 2.1  |
| 35  | 1d    | 137  | SER  | 2.1  |
| 35  | 2d    | 118  | ARG  | 2.1  |
| 35  | 2d    | 152  | SER  | 2.1  |
| 1   | 1A    | 1092 | C    | 2.1  |
| 7   | 2H    | 159  | GLU  | 2.1  |
| 16  | 1U    | 26   | GLY  | 2.1  |
| 34  | 2c    | 2    | GLY  | 2.1  |
| 54  | 1w    | 13   | C    | 2.1  |
| 21  | 1Z    | 70   | LEU  | 2.1  |
| 7   | 1H    | 21   | PRO  | 2.1  |
| 15  | 1T    | 48   | ILE  | 2.1  |
| 34  | 1c    | 64   | VAL  | 2.1  |
| 35  | 1d    | 120  | LEU  | 2.1  |
| 35  | 2d    | 135  | LEU  | 2.1  |
| 45  | 2n    | 17   | LYS  | 2.1  |
| 42  | 1k    | 65   | ALA  | 2.1  |
| 45  | 2n    | 45   | ARG  | 2.1  |
| 3   | 1D    | 50   | THR  | 2.1  |
| 21  | 1Z    | 166  | SER  | 2.1  |
| 42  | 1k    | 77   | MET  | 2.1  |
| 44  | 2m    | 73   | GLU  | 2.1  |
| 1   | 2A    | 2310 | A    | 2.1  |
| 16  | 1U    | 43   | GLY  | 2.1  |
| 32  | 1a    | 1532 | U    | 2.0  |
| 1   | 2A    | 2111 | C    | 2.0  |
| 12  | 2Q    | 17   | LEU  | 2.0  |
| 21  | 1Z    | 155  | LEU  | 2.0  |
| 39  | 1h    | 112  | LEU  | 2.0  |
| 43  | 2l    | 27   | LEU  | 2.0  |
| 47  | 2p    | 74   | LEU  | 2.0  |
| 49  | 2r    | 26   | LEU  | 2.0  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 34  | 2c    | 153  | VAL  | 2.0  |
| 35  | 1d    | 140  | VAL  | 2.0  |
| 47  | 2p    | 51   | VAL  | 2.0  |
| 50  | 2s    | 47   | HIS  | 2.0  |
| 3   | 1D    | 75   | ILE  | 2.0  |
| 21  | 1Z    | 133  | ILE  | 2.0  |
| 48  | 2q    | 60   | ILE  | 2.0  |
| 6   | 2G    | 146  | TYR  | 2.0  |
| 42  | 2k    | 59   | TYR  | 2.0  |
| 9   | 2N    | 92   | ALA  | 2.0  |
| 34  | 2c    | 100  | ALA  | 2.0  |
| 38  | 1g    | 147  | ALA  | 2.0  |
| 11  | 2P    | 28   | GLY  | 2.0  |
| 21  | 2Z    | 106  | GLY  | 2.0  |
| 23  | 2l    | 29   | GLY  | 2.0  |
| 33  | 2b    | 101  | MET  | 2.0  |
| 34  | 2c    | 194  | GLY  | 2.0  |
| 34  | 2c    | 197  | GLY  | 2.0  |
| 35  | 1d    | 208  | SER  | 2.0  |
| 43  | 1l    | 61   | THR  | 2.0  |
| 44  | 2m    | 112  | GLY  | 2.0  |
| 12  | 2Q    | 125  | LEU  | 2.0  |
| 35  | 1d    | 157  | LEU  | 2.0  |
| 41  | 1j    | 85   | LEU  | 2.0  |
| 47  | 1p    | 73   | LEU  | 2.0  |
| 55  | 1x    | 47   | U    | 2.0  |
| 1   | 2A    | 2148 | G    | 2.0  |
| 29  | 17    | 46   | VAL  | 2.0  |
| 44  | 2m    | 74   | VAL  | 2.0  |
| 50  | 2s    | 60   | VAL  | 2.0  |
| 53  | 1v    | 15   | A    | 2.0  |
| 9   | 2N    | 97   | ARG  | 2.0  |
| 10  | 2O    | 86   | ILE  | 2.0  |
| 12  | 2Q    | 16   | ARG  | 2.0  |
| 34  | 1c    | 164  | ARG  | 2.0  |
| 6   | 1G    | 48   | GLU  | 2.0  |
| 7   | 2H    | 124  | GLU  | 2.0  |
| 35  | 2d    | 163  | GLU  | 2.0  |
| 48  | 2q    | 42   | TYR  | 2.0  |
| 10  | 2O    | 41   | ALA  | 2.0  |
| 38  | 2g    | 145  | ALA  | 2.0  |
| 42  | 2k    | 117  | ASN  | 2.0  |

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| Mol | Chain | Res    | Type | RSRZ |
|-----|-------|--------|------|------|
| 21  | 2Z    | 45     | ASP  | 2.0  |
| 21  | 2Z    | 147    | GLY  | 2.0  |
| 35  | 1d    | 61     | LYS  | 2.0  |
| 44  | 1m    | 95     | GLY  | 2.0  |
| 3   | 2D    | 206    | LEU  | 2.0  |
| 18  | 2W    | 82     | LEU  | 2.0  |
| 9   | 2N    | 11     | PRO  | 2.0  |
| 12  | 1Q    | 78     | PRO  | 2.0  |
| 26  | 24    | 58     | ARG  | 2.0  |
| 39  | 2h    | 12     | ARG  | 2.0  |
| 42  | 2k    | 91     | ARG  | 2.0  |
| 44  | 2m    | 80     | ARG  | 2.0  |
| 6   | 2G    | 77     | ILE  | 2.0  |
| 36  | 2e    | 101    | ILE  | 2.0  |
| 47  | 2p    | 19     | ILE  | 2.0  |
| 1   | 2A    | 652(B) | A    | 2.0  |
| 1   | 1A    | 388    | G    | 2.0  |
| 2   | 2B    | 89     | G    | 2.0  |
| 7   | 2H    | 94     | TYR  | 2.0  |
| 9   | 2N    | 109    | LYS  | 2.0  |
| 12  | 2Q    | 22     | LYS  | 2.0  |
| 34  | 1c    | 72     | LYS  | 2.0  |
| 44  | 2m    | 42     | ALA  | 2.0  |
| 44  | 2m    | 65     | LYS  | 2.0  |
| 45  | 2n    | 4      | LYS  | 2.0  |
| 54  | 1w    | 10     | G    | 2.0  |
| 42  | 1k    | 33     | THR  | 2.0  |
| 4   | 2E    | 195    | LEU  | 2.0  |
| 6   | 2G    | 95     | ARG  | 2.0  |
| 20  | 2Y    | 31     | LEU  | 2.0  |
| 37  | 1f    | 79     | LEU  | 2.0  |
| 21  | 1Z    | 39     | VAL  | 2.0  |
| 21  | 1Z    | 141    | VAL  | 2.0  |
| 50  | 2s    | 51     | 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 54  | MIA  | 2y    | 37   | 22/30 | 0.84 | 0.34 | -    | 68,84,93,122                | 0     |
| 1   | 2MU  | 1A    | 2552 | 21/23 | 0.98 | 0.21 | -    | 24,30,37,41                 | 0     |
| 1   | 5MU  | 1A    | 1915 | 21/22 | 0.96 | 0.20 | -    | 54,67,70,77                 | 0     |
| 32  | M2G  | 1a    | 966  | 25/26 | 0.97 | 0.20 | -    | 39,49,58,74                 | 0     |
| 32  | 5MC  | 2a    | 1400 | 21/22 | 0.94 | 0.23 | -    | 61,73,83,87                 | 0     |
| 54  | 7MG  | 2w    | 46   | 24/25 | 0.82 | 0.41 | -    | 73,93,103,114               | 0     |
| 54  | 7MG  | 1y    | 46   | 24/25 | 0.84 | 0.22 | -    | 81,96,103,124               | 0     |
| 54  | 4SU  | 1y    | 8    | 20/21 | 0.87 | 0.18 | -    | 79,87,95,95                 | 0     |
| 32  | 5MC  | 1a    | 1404 | 21/22 | 0.98 | 0.20 | -    | 30,40,45,48                 | 0     |
| 54  | PSU  | 1y    | 32   | 20/21 | 0.85 | 0.36 | -    | 72,86,96,100                | 0     |
| 54  | 4SU  | 1w    | 8    | 20/21 | 0.93 | 0.18 | -    | 63,75,89,89                 | 0     |
| 1   | 2MA  | 2A    | 2503 | 23/24 | 0.98 | 0.20 | -    | 21,28,35,40                 | 0     |
| 1   | 5MU  | 1A    | 1939 | 21/22 | 0.98 | 0.21 | -    | 24,31,38,39                 | 0     |
| 54  | PSU  | 2y    | 32   | 20/21 | 0.81 | 0.32 | -    | 74,85,99,103                | 0     |
| 1   | PSU  | 1A    | 1917 | 20/21 | 0.95 | 0.18 | -    | 44,58,66,67                 | 0     |
| 1   | 5MC  | 1A    | 1962 | 21/22 | 0.97 | 0.22 | -    | 25,36,43,50                 | 0     |
| 1   | 5MU  | 2A    | 1915 | 21/22 | 0.94 | 0.14 | -    | 59,69,77,91                 | 0     |
| 54  | PSU  | 1y    | 55   | 20/21 | 0.79 | 0.29 | -    | 80,96,105,117               | 0     |
| 32  | 4OC  | 1a    | 1402 | 22/23 | 0.96 | 0.21 | -    | 35,45,57,62                 | 0     |
| 32  | 5MC  | 1a    | 967  | 21/22 | 0.96 | 0.21 | -    | 42,52,66,70                 | 0     |
| 54  | MIA  | 1w    | 37   | 29/30 | 0.95 | 0.26 | -    | 41,59,74,84                 | 0     |
| 54  | PSU  | 2w    | 39   | 20/21 | 0.92 | 0.39 | -    | 68,76,83,83                 | 0     |
| 54  | 7MG  | 1w    | 46   | 24/25 | 0.86 | 0.20 | -    | 66,84,103,123               | 0     |
| 1   | PSU  | 2A    | 1911 | 20/21 | 0.94 | 0.18 | -    | 40,58,64,67                 | 0     |
| 55  | 4SU  | 1x    | 8    | 20/21 | 0.95 | 0.19 | -    | 41,59,76,88                 | 0     |
| 32  | UR3  | 1a    | 1498 | 21/22 | 0.98 | 0.22 | -    | 35,43,51,52                 | 0     |
| 1   | PSU  | 2A    | 1917 | 20/21 | 0.95 | 0.16 | -    | 48,61,71,72                 | 0     |
| 32  | 7MG  | 2a    | 527  | 24/25 | 0.96 | 0.19 | -    | 54,66,75,89                 | 0     |
| 54  | PSU  | 2w    | 32   | 20/21 | 0.90 | 0.35 | -    | 69,80,91,97                 | 0     |
| 1   | OMG  | 1A    | 2251 | 24/25 | 0.98 | 0.22 | -    | 25,29,37,40                 | 0     |
| 32  | MA6  | 1a    | 1518 | 24/25 | 0.98 | 0.23 | -    | 28,42,50,51                 | 0     |
| 55  | 4SU  | 2x    | 8    | 20/21 | 0.89 | 0.15 | -    | 65,81,88,92                 | 0     |
| 32  | PSU  | 1a    | 516  | 20/21 | 0.94 | 0.15 | -    | 58,67,74,78                 | 0     |
| 1   | 4OC  | 1A    | 1920 | 21/23 | 0.97 | 0.24 | -    | 37,52,60,63                 | 0     |
| 55  | 5MU  | 1x    | 54   | 21/22 | 0.96 | 0.18 | -    | 40,62,68,69                 | 0     |
| 55  | 5MC  | 1x    | 32   | 21/22 | 0.97 | 0.23 | -    | 44,53,60,62                 | 0     |
| 54  | 5MU  | 2y    | 54   | 21/22 | 0.80 | 0.27 | -    | 81,94,101,117               | 0     |
| 54  | 4SU  | 2w    | 8    | 20/21 | 0.82 | 0.28 | -    | 68,89,101,117               | 0     |
| 54  | PSU  | 2y    | 39   | 20/21 | 0.84 | 0.30 | -    | 75,83,94,99                 | 0     |
| 54  | 5MU  | 1w    | 54   | 21/22 | 0.94 | 0.24 | -    | 48,66,72,87                 | 0     |
| 32  | MA6  | 2a    | 1519 | 24/25 | 0.96 | 0.25 | -    | 48,62,68,73                 | 0     |
| 43  | 0TD  | 2l    | 92   | 10/11 | 0.89 | 0.20 | -    | 62,70,72,90                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 1   | 2MA  | 1A    | 2503 | 23/24 | 0.98 | 0.24 | -    | 18,26,31,35                 | 0     |
| 54  | PSU  | 1w    | 39   | 20/21 | 0.94 | 0.24 | -    | 65,73,79,81                 | 0     |
| 54  | 5MU  | 2w    | 54   | 21/22 | 0.88 | 0.25 | -    | 55,78,91,98                 | 0     |
| 55  | PSU  | 1x    | 55   | 20/21 | 0.95 | 0.18 | -    | 48,55,72,72                 | 0     |
| 32  | 5MC  | 1a    | 1400 | 21/22 | 0.97 | 0.19 | -    | 36,52,62,67                 | 0     |
| 1   | PSU  | 2A    | 2605 | 20/21 | 0.97 | 0.19 | -    | 20,31,35,36                 | 0     |
| 32  | UR3  | 2a    | 1498 | 21/22 | 0.96 | 0.21 | -    | 36,56,67,69                 | 0     |
| 54  | 5MU  | 1y    | 54   | 21/22 | 0.84 | 0.21 | -    | 70,86,99,113                | 0     |
| 43  | 0TD  | 1l    | 92   | 10/11 | 0.93 | 0.21 | -    | 48,55,61,77                 | 0     |
| 54  | 7MG  | 2y    | 46   | 24/25 | 0.76 | 0.17 | -    | 84,98,104,130               | 0     |
| 32  | 5MC  | 2a    | 1404 | 21/22 | 0.94 | 0.19 | -    | 50,61,68,76                 | 0     |
| 32  | PSU  | 2a    | 516  | 20/21 | 0.92 | 0.16 | -    | 56,70,76,84                 | 0     |
| 54  | PSU  | 2w    | 55   | 20/21 | 0.82 | 0.35 | -    | 63,84,92,92                 | 0     |
| 1   | 5MU  | 2A    | 1939 | 21/22 | 0.97 | 0.18 | -    | 25,32,39,43                 | 0     |
| 54  | MIA  | 1y    | 37   | 22/30 | 0.91 | 0.27 | -    | 64,78,83,86                 | 0     |
| 32  | 2MG  | 2a    | 1207 | 24/25 | 0.92 | 0.17 | -    | 69,80,93,94                 | 0     |
| 32  | 5MC  | 2a    | 1407 | 21/22 | 0.96 | 0.18 | -    | 38,51,59,70                 | 0     |
| 54  | PSU  | 2y    | 55   | 20/21 | 0.68 | 0.23 | -    | 80,96,106,120               | 0     |
| 55  | M3O  | 1x    | 76   | 32/33 | 0.96 | 0.25 | -    | 21,39,51,79                 | 10    |
| 32  | M2G  | 2a    | 966  | 25/26 | 0.88 | 0.22 | -    | 52,72,85,96                 | 0     |
| 54  | MIA  | 2w    | 37   | 22/30 | 0.89 | 0.26 | -    | 60,78,83,89                 | 0     |
| 54  | PSU  | 1w    | 55   | 20/21 | 0.84 | 0.28 | -    | 61,81,88,95                 | 0     |
| 1   | PSU  | 1A    | 1911 | 20/21 | 0.97 | 0.21 | -    | 41,51,62,64                 | 0     |
| 1   | 5MC  | 2A    | 1942 | 21/22 | 0.97 | 0.18 | -    | 41,51,58,67                 | 0     |
| 55  | 5MU  | 2x    | 54   | 21/22 | 0.89 | 0.23 | -    | 68,79,84,102                | 0     |
| 55  | PSU  | 2x    | 55   | 20/21 | 0.91 | 0.20 | -    | 63,74,87,92                 | 0     |
| 54  | 4SU  | 2y    | 8    | 20/21 | 0.80 | 0.14 | -    | 80,97,107,114               | 0     |
| 54  | PSU  | 1y    | 39   | 20/21 | 0.90 | 0.27 | -    | 73,83,89,90                 | 0     |
| 32  | MA6  | 2a    | 1518 | 24/25 | 0.96 | 0.20 | -    | 44,63,70,76                 | 0     |
| 1   | 5MC  | 2A    | 1962 | 21/22 | 0.97 | 0.17 | -    | 27,40,49,52                 | 0     |
| 32  | 2MG  | 1a    | 1207 | 24/25 | 0.95 | 0.15 | -    | 49,69,77,81                 | 0     |
| 55  | M3O  | 2x    | 76   | 32/33 | 0.94 | 0.26 | -    | 35,55,69,90                 | 10    |
| 1   | OMG  | 2A    | 2251 | 24/25 | 0.98 | 0.21 | -    | 28,33,40,42                 | 0     |
| 1   | 2MU  | 2A    | 2552 | 21/23 | 0.97 | 0.20 | -    | 26,32,38,49                 | 0     |
| 1   | PSU  | 1A    | 2605 | 20/21 | 0.98 | 0.20 | -    | 19,24,34,35                 | 0     |
| 54  | PSU  | 1w    | 32   | 20/21 | 0.91 | 0.24 | -    | 67,79,90,93                 | 0     |
| 55  | 5MC  | 2x    | 32   | 21/22 | 0.96 | 0.19 | -    | 63,73,82,83                 | 0     |
| 1   | 4OC  | 2A    | 1920 | 21/23 | 0.95 | 0.20 | -    | 46,54,60,72                 | 0     |
| 1   | 5MC  | 1A    | 1942 | 21/22 | 0.97 | 0.19 | -    | 37,49,54,58                 | 0     |
| 32  | 4OC  | 2a    | 1402 | 22/23 | 0.91 | 0.19 | -    | 48,64,76,83                 | 0     |
| 32  | 5MC  | 2a    | 967  | 21/22 | 0.93 | 0.19 | -    | 61,67,75,87                 | 0     |
| 32  | 7MG  | 1a    | 527  | 24/25 | 0.96 | 0.17 | -    | 35,51,55,62                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 32  | MA6  | 1a    | 1519 | 24/25 | 0.97 | 0.24 | -    | 24,42,50,65                 | 0     |
| 32  | 5MC  | 1a    | 1407 | 21/22 | 0.98 | 0.22 | -    | 32,46,51,62                 | 0     |

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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  | LLDF  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 56  | MG   | 1A    | 3162 | 1/1   | 0.99 | 0.64 | 30.36 | 33,33,33,33                 | 0     |
| 56  | MG   | 1A    | 3958 | 1/1   | 0.93 | 0.73 | 25.82 | 49,49,49,49                 | 0     |
| 56  | MG   | 2A    | 3048 | 1/1   | 0.94 | 0.55 | 25.38 | 44,44,44,44                 | 0     |
| 56  | MG   | 1A    | 3917 | 1/1   | 0.95 | 0.56 | 23.47 | 40,40,40,40                 | 0     |
| 56  | MG   | 2A    | 3668 | 1/1   | 0.98 | 0.77 | 22.92 | 48,48,48,48                 | 0     |
| 56  | MG   | 1A    | 3235 | 1/1   | 0.91 | 0.47 | 22.16 | 32,32,32,32                 | 0     |
| 56  | MG   | 2a    | 1738 | 1/1   | 0.90 | 0.61 | 21.46 | 76,76,76,76                 | 0     |
| 56  | MG   | 1A    | 3769 | 1/1   | 0.94 | 0.43 | 18.58 | 39,39,39,39                 | 0     |
| 56  | MG   | 2A    | 3104 | 1/1   | 0.98 | 0.38 | 18.44 | 46,46,46,46                 | 0     |
| 56  | MG   | 1A    | 3030 | 1/1   | 0.98 | 0.46 | 17.65 | 33,33,33,33                 | 0     |
| 56  | MG   | 1A    | 3317 | 1/1   | 0.91 | 0.58 | 17.24 | 39,39,39,39                 | 0     |
| 56  | MG   | 1N    | 3006 | 1/1   | 0.84 | 0.63 | 17.23 | 50,50,50,50                 | 0     |
| 56  | MG   | 1A    | 3897 | 1/1   | 0.97 | 0.49 | 15.77 | 38,38,38,38                 | 0     |
| 56  | MG   | 2A    | 3482 | 1/1   | 0.90 | 0.29 | 14.74 | 46,46,46,46                 | 0     |
| 56  | MG   | 1A    | 3362 | 1/1   | 0.93 | 0.33 | 14.29 | 36,36,36,36                 | 0     |
| 56  | MG   | 2A    | 3090 | 1/1   | 0.92 | 0.47 | 13.75 | 53,53,53,53                 | 0     |
| 56  | MG   | 1A    | 3930 | 1/1   | 0.95 | 0.52 | 13.64 | 36,36,36,36                 | 0     |
| 56  | MG   | 1A    | 3770 | 1/1   | 0.65 | 0.52 | 13.61 | 63,63,63,63                 | 0     |
| 56  | MG   | 2a    | 1633 | 1/1   | 0.81 | 0.55 | 13.58 | 61,61,61,61                 | 0     |
| 56  | MG   | 1A    | 3202 | 1/1   | 0.98 | 0.33 | 13.45 | 31,31,31,31                 | 0     |
| 56  | MG   | 2D    | 303  | 1/1   | 0.91 | 0.63 | 13.21 | 45,45,45,45                 | 0     |
| 56  | MG   | 1A    | 3940 | 1/1   | 0.97 | 0.51 | 12.50 | 33,33,33,33                 | 0     |
| 56  | MG   | 2A    | 3659 | 1/1   | 0.96 | 0.58 | 12.46 | 43,43,43,43                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 56  | MG   | 2A    | 3071 | 1/1   | 0.93 | 0.42 | 12.18 | 34,34,34,34                 | 0     |
| 56  | MG   | 1A    | 3680 | 1/1   | 0.96 | 0.33 | 12.04 | 36,36,36,36                 | 0     |
| 56  | MG   | 1A    | 3908 | 1/1   | 0.96 | 0.42 | 10.82 | 38,38,38,38                 | 0     |
| 56  | MG   | 2A    | 3022 | 1/1   | 0.97 | 0.34 | 10.79 | 43,43,43,43                 | 0     |
| 56  | MG   | 1A    | 3234 | 1/1   | 0.96 | 0.31 | 10.42 | 34,34,34,34                 | 0     |
| 56  | MG   | 1a    | 1761 | 1/1   | 0.78 | 0.30 | 10.25 | 72,72,72,72                 | 0     |
| 56  | MG   | 1N    | 3004 | 1/1   | 0.96 | 0.48 | 9.77  | 56,56,56,56                 | 0     |
| 56  | MG   | 1A    | 3738 | 1/1   | 0.84 | 0.39 | 9.62  | 44,44,44,44                 | 0     |
| 56  | MG   | 1A    | 3159 | 1/1   | 0.93 | 0.31 | 9.61  | 34,34,34,34                 | 0     |
| 56  | MG   | 2A    | 3497 | 1/1   | 0.71 | 0.25 | 9.11  | 56,56,56,56                 | 0     |
| 56  | MG   | 2A    | 3656 | 1/1   | 0.96 | 0.46 | 8.96  | 44,44,44,44                 | 0     |
| 56  | MG   | 1A    | 3934 | 1/1   | 0.92 | 0.32 | 8.94  | 30,30,30,30                 | 0     |
| 56  | MG   | 1A    | 3314 | 1/1   | 0.93 | 0.36 | 8.71  | 42,42,42,42                 | 0     |
| 56  | MG   | 2A    | 3421 | 1/1   | 0.92 | 0.23 | 8.68  | 52,52,52,52                 | 0     |
| 56  | MG   | 2D    | 301  | 1/1   | 0.85 | 0.49 | 8.43  | 39,39,39,39                 | 0     |
| 56  | MG   | 1A    | 3319 | 1/1   | 0.97 | 0.42 | 7.99  | 28,28,28,28                 | 0     |
| 56  | MG   | 2U    | 204  | 1/1   | 0.90 | 0.45 | 7.92  | 45,45,45,45                 | 0     |
| 56  | MG   | 1B    | 3011 | 1/1   | 0.89 | 0.33 | 7.90  | 54,54,54,54                 | 0     |
| 56  | MG   | 1a    | 1656 | 1/1   | 0.80 | 0.28 | 7.83  | 46,46,46,46                 | 0     |
| 56  | MG   | 2A    | 3167 | 1/1   | 0.96 | 0.24 | 7.66  | 39,39,39,39                 | 0     |
| 56  | MG   | 1N    | 3001 | 1/1   | 0.97 | 0.42 | 7.63  | 38,38,38,38                 | 0     |
| 56  | MG   | 1A    | 3249 | 1/1   | 0.98 | 0.40 | 7.49  | 29,29,29,29                 | 0     |
| 56  | MG   | 2A    | 3304 | 1/1   | 0.95 | 0.23 | 7.43  | 53,53,53,53                 | 0     |
| 56  | MG   | 1a    | 1608 | 1/1   | 0.88 | 0.33 | 7.40  | 57,57,57,57                 | 0     |
| 56  | MG   | 2a    | 1715 | 1/1   | 0.93 | 0.29 | 7.12  | 53,53,53,53                 | 0     |
| 56  | MG   | 1S    | 3001 | 1/1   | 0.92 | 0.47 | 7.04  | 52,52,52,52                 | 0     |
| 56  | MG   | 2Q    | 201  | 1/1   | 0.91 | 1.00 | 7.02  | 61,61,61,61                 | 0     |
| 56  | MG   | 1A    | 3929 | 1/1   | 0.98 | 0.43 | 6.98  | 45,45,45,45                 | 0     |
| 56  | MG   | 2A    | 3159 | 1/1   | 0.95 | 0.23 | 6.97  | 41,41,41,41                 | 0     |
| 56  | MG   | 1A    | 3296 | 1/1   | 0.90 | 0.26 | 6.58  | 40,40,40,40                 | 0     |
| 56  | MG   | 1A    | 3919 | 1/1   | 0.92 | 0.34 | 6.53  | 33,33,33,33                 | 0     |
| 56  | MG   | 2A    | 3123 | 1/1   | 0.93 | 0.26 | 6.52  | 47,47,47,47                 | 0     |
| 56  | MG   | 1A    | 3315 | 1/1   | 0.97 | 0.36 | 6.42  | 37,37,37,37                 | 0     |
| 56  | MG   | 2A    | 3405 | 1/1   | 0.94 | 0.21 | 6.23  | 49,49,49,49                 | 0     |
| 56  | MG   | 1F    | 304  | 1/1   | 0.98 | 0.32 | 5.97  | 37,37,37,37                 | 0     |
| 56  | MG   | 1A    | 3957 | 1/1   | 0.97 | 0.32 | 5.79  | 37,37,37,37                 | 0     |
| 56  | MG   | 2A    | 3015 | 1/1   | 0.97 | 0.24 | 5.70  | 36,36,36,36                 | 0     |
| 56  | MG   | 1a    | 1837 | 1/1   | 0.88 | 0.41 | 5.69  | 60,60,60,60                 | 0     |
| 56  | MG   | 1B    | 3003 | 1/1   | 0.92 | 0.28 | 5.58  | 62,62,62,62                 | 0     |
| 56  | MG   | 1a    | 1653 | 1/1   | 0.92 | 0.19 | 5.57  | 59,59,59,59                 | 0     |
| 56  | MG   | 1a    | 1669 | 1/1   | 0.87 | 0.26 | 5.43  | 58,58,58,58                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56  | MG   | 2A    | 3664 | 1/1   | 0.97 | 0.51 | 5.38 | 46,46,46,46                 | 0     |
| 56  | MG   | 1A    | 3199 | 1/1   | 0.90 | 0.30 | 5.38 | 35,35,35,35                 | 0     |
| 56  | MG   | 1A    | 3121 | 1/1   | 0.84 | 0.31 | 5.26 | 55,55,55,55                 | 0     |
| 56  | MG   | 2A    | 3264 | 1/1   | 0.96 | 0.25 | 5.16 | 40,40,40,40                 | 0     |
| 56  | MG   | 2A    | 3201 | 1/1   | 0.78 | 0.23 | 5.09 | 61,61,61,61                 | 0     |
| 56  | MG   | 2a    | 1679 | 1/1   | 0.92 | 0.19 | 5.02 | 64,64,64,64                 | 0     |
| 56  | MG   | 1A    | 3126 | 1/1   | 0.99 | 0.36 | 5.01 | 39,39,39,39                 | 0     |
| 56  | MG   | 2a    | 1659 | 1/1   | 0.87 | 0.33 | 4.82 | 66,66,66,66                 | 0     |
| 56  | MG   | 1A    | 3935 | 1/1   | 0.94 | 0.32 | 4.77 | 48,48,48,48                 | 0     |
| 56  | MG   | 1A    | 3125 | 1/1   | 0.95 | 0.32 | 4.50 | 36,36,36,36                 | 0     |
| 56  | MG   | 2A    | 3481 | 1/1   | 0.94 | 0.24 | 4.45 | 58,58,58,58                 | 0     |
| 56  | MG   | 1A    | 3094 | 1/1   | 0.95 | 0.26 | 4.34 | 58,58,58,58                 | 0     |
| 56  | MG   | 1F    | 307  | 1/1   | 0.91 | 0.38 | 4.12 | 57,57,57,57                 | 0     |
| 56  | MG   | 1B    | 3024 | 1/1   | 0.89 | 0.27 | 4.05 | 63,63,63,63                 | 0     |
| 56  | MG   | 1a    | 1713 | 1/1   | 0.98 | 0.25 | 3.91 | 53,53,53,53                 | 0     |
| 56  | MG   | 1A    | 3652 | 1/1   | 0.98 | 0.25 | 3.90 | 25,25,25,25                 | 0     |
| 56  | MG   | 1A    | 3192 | 1/1   | 0.90 | 0.29 | 3.85 | 39,39,39,39                 | 0     |
| 56  | MG   | 1A    | 3910 | 1/1   | 0.90 | 0.30 | 3.79 | 40,40,40,40                 | 0     |
| 56  | MG   | 1A    | 3198 | 1/1   | 0.94 | 0.29 | 3.74 | 34,34,34,34                 | 0     |
| 56  | MG   | 2A    | 3662 | 1/1   | 0.96 | 0.27 | 3.65 | 29,29,29,29                 | 0     |
| 56  | MG   | 2a    | 1747 | 1/1   | 0.92 | 0.22 | 3.59 | 72,72,72,72                 | 0     |
| 56  | MG   | 1A    | 3178 | 1/1   | 0.90 | 0.27 | 3.55 | 36,36,36,36                 | 0     |
| 56  | MG   | 2A    | 3622 | 1/1   | 0.88 | 0.26 | 3.46 | 41,41,41,41                 | 0     |
| 56  | MG   | 1A    | 3658 | 1/1   | 0.98 | 0.33 | 3.45 | 35,35,35,35                 | 0     |
| 56  | MG   | 1A    | 3123 | 1/1   | 0.95 | 0.24 | 3.39 | 43,43,43,43                 | 0     |
| 56  | MG   | 1A    | 3827 | 1/1   | 0.88 | 0.25 | 3.37 | 51,51,51,51                 | 0     |
| 56  | MG   | 1A    | 3268 | 1/1   | 0.97 | 0.23 | 3.36 | 33,33,33,33                 | 0     |
| 56  | MG   | 2A    | 3215 | 1/1   | 0.91 | 0.24 | 3.34 | 50,50,50,50                 | 0     |
| 56  | MG   | 1a    | 1644 | 1/1   | 0.79 | 0.23 | 3.23 | 56,56,56,56                 | 0     |
| 56  | MG   | 1A    | 3251 | 1/1   | 0.94 | 0.29 | 3.22 | 25,25,25,25                 | 0     |
| 56  | MG   | 2A    | 3303 | 1/1   | 0.94 | 0.21 | 3.21 | 60,60,60,60                 | 0     |
| 56  | MG   | 1A    | 3604 | 1/1   | 0.95 | 0.25 | 3.20 | 29,29,29,29                 | 0     |
| 56  | MG   | 1a    | 1625 | 1/1   | 0.97 | 0.22 | 3.11 | 53,53,53,53                 | 0     |
| 56  | MG   | 2A    | 3451 | 1/1   | 0.96 | 0.32 | 3.05 | 36,36,36,36                 | 0     |
| 56  | MG   | 1A    | 3944 | 1/1   | 0.97 | 0.30 | 3.02 | 33,33,33,33                 | 0     |
| 56  | MG   | 2A    | 3598 | 1/1   | 0.91 | 0.20 | 2.89 | 45,45,45,45                 | 0     |
| 56  | MG   | 1a    | 1649 | 1/1   | 0.89 | 0.19 | 2.74 | 56,56,56,56                 | 0     |
| 56  | MG   | 1A    | 3965 | 1/1   | 0.98 | 0.28 | 2.69 | 38,38,38,38                 | 0     |
| 56  | MG   | 1A    | 3313 | 1/1   | 0.92 | 0.32 | 2.69 | 41,41,41,41                 | 0     |
| 56  | MG   | 2A    | 3495 | 1/1   | 0.91 | 0.23 | 2.69 | 61,61,61,61                 | 0     |
| 56  | MG   | 1A    | 3926 | 1/1   | 0.97 | 0.27 | 2.59 | 29,29,29,29                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56  | MG   | 18    | 101  | 1/1   | 0.96 | 0.31 | 2.59 | 45,45,45,45                 | 0     |
| 56  | MG   | 1A    | 3736 | 1/1   | 0.96 | 0.23 | 2.53 | 38,38,38,38                 | 0     |
| 56  | MG   | 2A    | 3559 | 1/1   | 0.74 | 0.23 | 2.50 | 59,59,59,59                 | 0     |
| 56  | MG   | 1A    | 3762 | 1/1   | 0.90 | 0.27 | 2.44 | 31,31,31,31                 | 0     |
| 56  | MG   | 1A    | 3670 | 1/1   | 0.83 | 0.23 | 2.39 | 58,58,58,58                 | 0     |
| 56  | MG   | 2F    | 302  | 1/1   | 0.96 | 0.24 | 2.29 | 50,50,50,50                 | 0     |
| 56  | MG   | 2A    | 3205 | 1/1   | 0.96 | 0.29 | 2.27 | 53,53,53,53                 | 0     |
| 56  | MG   | 1A    | 3039 | 1/1   | 0.93 | 0.26 | 2.24 | 50,50,50,50                 | 0     |
| 56  | MG   | 2A    | 3669 | 1/1   | 0.95 | 0.33 | 2.21 | 44,44,44,44                 | 0     |
| 56  | MG   | 1A    | 3947 | 1/1   | 0.93 | 0.28 | 2.16 | 49,49,49,49                 | 0     |
| 56  | MG   | 17    | 101  | 1/1   | 0.94 | 0.27 | 2.16 | 48,48,48,48                 | 0     |
| 56  | MG   | 2A    | 3202 | 1/1   | 0.97 | 0.19 | 2.06 | 44,44,44,44                 | 0     |
| 56  | MG   | 1X    | 3004 | 1/1   | 0.94 | 0.27 | 2.05 | 64,64,64,64                 | 0     |
| 56  | MG   | 1a    | 1730 | 1/1   | 0.94 | 0.22 | 2.03 | 71,71,71,71                 | 0     |
| 56  | MG   | 2a    | 1787 | 1/1   | 0.96 | 0.23 | 2.02 | 51,51,51,51                 | 0     |
| 56  | MG   | 2A    | 3057 | 1/1   | 0.94 | 0.22 | 1.99 | 57,57,57,57                 | 0     |
| 56  | MG   | 2A    | 3189 | 1/1   | 0.99 | 0.20 | 1.98 | 31,31,31,31                 | 0     |
| 56  | MG   | 1A    | 3013 | 1/1   | 0.96 | 0.26 | 1.97 | 24,24,24,24                 | 0     |
| 56  | MG   | 2a    | 1616 | 1/1   | 0.90 | 0.20 | 1.95 | 52,52,52,52                 | 0     |
| 56  | MG   | 1N    | 3005 | 1/1   | 0.95 | 0.20 | 1.93 | 51,51,51,51                 | 0     |
| 56  | MG   | 2A    | 3567 | 1/1   | 0.89 | 0.23 | 1.92 | 58,58,58,58                 | 0     |
| 56  | MG   | 1b    | 3002 | 1/1   | 0.80 | 0.22 | 1.87 | 74,74,74,74                 | 0     |
| 56  | MG   | 1A    | 3939 | 1/1   | 0.94 | 0.31 | 1.86 | 42,42,42,42                 | 0     |
| 56  | MG   | 2A    | 3310 | 1/1   | 0.96 | 0.21 | 1.79 | 34,34,34,34                 | 0     |
| 56  | MG   | 2A    | 3088 | 1/1   | 0.92 | 0.17 | 1.78 | 53,53,53,53                 | 0     |
| 56  | MG   | 1A    | 3601 | 1/1   | 0.91 | 0.24 | 1.75 | 45,45,45,45                 | 0     |
| 56  | MG   | 1A    | 3914 | 1/1   | 0.88 | 0.23 | 1.74 | 38,38,38,38                 | 0     |
| 56  | MG   | 1P    | 203  | 1/1   | 0.96 | 0.29 | 1.59 | 27,27,27,27                 | 0     |
| 56  | MG   | 1N    | 3002 | 1/1   | 0.94 | 0.25 | 1.56 | 49,49,49,49                 | 0     |
| 56  | MG   | 1A    | 3936 | 1/1   | 0.97 | 0.28 | 1.54 | 29,29,29,29                 | 0     |
| 56  | MG   | 1A    | 3945 | 1/1   | 0.91 | 0.24 | 1.47 | 39,39,39,39                 | 0     |
| 56  | MG   | 2A    | 3389 | 1/1   | 0.94 | 0.24 | 1.40 | 52,52,52,52                 | 0     |
| 56  | MG   | 1A    | 3924 | 1/1   | 0.98 | 0.26 | 1.38 | 28,28,28,28                 | 0     |
| 56  | MG   | 2A    | 3381 | 1/1   | 0.92 | 0.19 | 1.35 | 46,46,46,46                 | 0     |
| 56  | MG   | 1A    | 3564 | 1/1   | 0.87 | 0.26 | 1.31 | 24,24,24,24                 | 0     |
| 56  | MG   | 2A    | 3150 | 1/1   | 0.88 | 0.22 | 1.31 | 35,35,35,35                 | 0     |
| 56  | MG   | 1A    | 3129 | 1/1   | 0.86 | 0.22 | 1.30 | 38,38,38,38                 | 0     |
| 56  | MG   | 2A    | 3663 | 1/1   | 0.98 | 0.28 | 1.28 | 42,42,42,42                 | 0     |
| 56  | MG   | 1a    | 1708 | 1/1   | 0.97 | 0.21 | 1.27 | 34,34,34,34                 | 0     |
| 56  | MG   | 1A    | 3900 | 1/1   | 0.88 | 0.24 | 1.20 | 28,28,28,28                 | 0     |
| 56  | MG   | 1X    | 3001 | 1/1   | 0.96 | 0.27 | 1.14 | 33,33,33,33                 | 0     |
| 56  | MG   | 2A    | 3039 | 1/1   | 0.89 | 0.17 | 1.09 | 46,46,46,46                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56  | MG   | 2A    | 3461 | 1/1   | 0.95 | 0.17 | 1.09 | 39,39,39,39                 | 0     |
| 56  | MG   | 1A    | 3265 | 1/1   | 0.92 | 0.21 | 1.08 | 40,40,40,40                 | 0     |
| 56  | MG   | 1A    | 3073 | 1/1   | 0.95 | 0.22 | 1.04 | 29,29,29,29                 | 0     |
| 56  | MG   | 2A    | 3342 | 1/1   | 0.98 | 0.22 | 1.02 | 31,31,31,31                 | 0     |
| 56  | MG   | 1A    | 3485 | 1/1   | 0.97 | 0.23 | 0.94 | 38,38,38,38                 | 0     |
| 56  | MG   | 2A    | 3223 | 1/1   | 0.90 | 0.18 | 0.92 | 51,51,51,51                 | 0     |
| 56  | MG   | 1a    | 1717 | 1/1   | 0.78 | 0.31 | 0.89 | 80,80,80,80                 | 0     |
| 56  | MG   | 1A    | 3432 | 1/1   | 0.99 | 0.21 | 0.89 | 22,22,22,22                 | 0     |
| 56  | MG   | 1a    | 1680 | 1/1   | 0.95 | 0.22 | 0.84 | 56,56,56,56                 | 0     |
| 56  | MG   | 1P    | 202  | 1/1   | 0.92 | 0.26 | 0.79 | 33,33,33,33                 | 0     |
| 56  | MG   | 1A    | 3765 | 1/1   | 0.91 | 0.30 | 0.77 | 46,46,46,46                 | 0     |
| 56  | MG   | 1A    | 3920 | 1/1   | 0.92 | 0.24 | 0.75 | 33,33,33,33                 | 0     |
| 56  | MG   | 1a    | 1833 | 1/1   | 0.94 | 0.27 | 0.73 | 52,52,52,52                 | 0     |
| 56  | MG   | 1A    | 3772 | 1/1   | 0.95 | 0.27 | 0.72 | 29,29,29,29                 | 0     |
| 56  | MG   | 2A    | 3165 | 1/1   | 0.95 | 0.21 | 0.71 | 36,36,36,36                 | 0     |
| 56  | MG   | 2D    | 304  | 1/1   | 0.99 | 0.23 | 0.70 | 42,42,42,42                 | 0     |
| 56  | MG   | 1A    | 3952 | 1/1   | 0.94 | 0.23 | 0.64 | 33,33,33,33                 | 0     |
| 56  | MG   | 2A    | 3549 | 1/1   | 0.92 | 0.21 | 0.59 | 45,45,45,45                 | 0     |
| 56  | MG   | 1A    | 3949 | 1/1   | 0.99 | 0.27 | 0.58 | 28,28,28,28                 | 0     |
| 56  | MG   | 1U    | 203  | 1/1   | 0.98 | 0.27 | 0.55 | 27,27,27,27                 | 0     |
| 56  | MG   | 2A    | 3347 | 1/1   | 0.82 | 0.16 | 0.52 | 45,45,45,45                 | 0     |
| 56  | MG   | 1A    | 3955 | 1/1   | 0.93 | 0.24 | 0.52 | 29,29,29,29                 | 0     |
| 56  | MG   | 2a    | 1745 | 1/1   | 0.93 | 0.20 | 0.50 | 78,78,78,78                 | 0     |
| 56  | MG   | 2A    | 3542 | 1/1   | 0.91 | 0.21 | 0.48 | 37,37,37,37                 | 0     |
| 59  | ZN   | 26    | 501  | 1/1   | 0.99 | 0.19 | 0.47 | 54,54,54,54                 | 0     |
| 56  | MG   | 2A    | 3585 | 1/1   | 0.85 | 0.27 | 0.44 | 44,44,44,44                 | 0     |
| 56  | MG   | 1Y    | 502  | 1/1   | 0.96 | 0.28 | 0.42 | 50,50,50,50                 | 0     |
| 59  | ZN   | 19    | 103  | 1/1   | 0.98 | 0.26 | 0.39 | 61,61,61,61                 | 0     |
| 56  | MG   | 1A    | 3801 | 1/1   | 0.95 | 0.24 | 0.35 | 45,45,45,45                 | 0     |
| 56  | MG   | 2A    | 3151 | 1/1   | 0.95 | 0.19 | 0.35 | 31,31,31,31                 | 0     |
| 56  | MG   | 2a    | 1774 | 1/1   | 0.83 | 0.17 | 0.35 | 72,72,72,72                 | 0     |
| 56  | MG   | 1A    | 3903 | 1/1   | 0.84 | 0.23 | 0.35 | 51,51,51,51                 | 0     |
| 56  | MG   | 2a    | 1696 | 1/1   | 0.86 | 0.20 | 0.32 | 50,50,50,50                 | 0     |
| 56  | MG   | 1A    | 3060 | 1/1   | 0.92 | 0.18 | 0.32 | 31,31,31,31                 | 0     |
| 56  | MG   | 1A    | 3398 | 1/1   | 0.99 | 0.19 | 0.29 | 27,27,27,27                 | 0     |
| 59  | ZN   | 25    | 101  | 1/1   | 0.99 | 0.18 | 0.28 | 64,64,64,64                 | 0     |
| 56  | MG   | 1A    | 3222 | 1/1   | 0.87 | 0.26 | 0.28 | 37,37,37,37                 | 0     |
| 56  | MG   | 1A    | 3956 | 1/1   | 0.98 | 0.26 | 0.25 | 35,35,35,35                 | 0     |
| 56  | MG   | 2a    | 1662 | 1/1   | 0.96 | 0.21 | 0.22 | 42,42,42,42                 | 0     |
| 56  | MG   | 2A    | 3505 | 1/1   | 0.98 | 0.20 | 0.22 | 48,48,48,48                 | 0     |
| 56  | MG   | 2A    | 3309 | 1/1   | 0.91 | 0.19 | 0.21 | 31,31,31,31                 | 0     |
| 56  | MG   | 2B    | 3004 | 1/1   | 0.95 | 0.23 | 0.20 | 62,62,62,62                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 56  | MG   | 2A    | 3423 | 1/1   | 0.96 | 0.19 | 0.19  | 47,47,47,47                 | 0     |
| 59  | ZN   | 1Y    | 501  | 1/1   | 0.98 | 0.18 | 0.18  | 67,67,67,67                 | 0     |
| 56  | MG   | 2A    | 3311 | 1/1   | 0.94 | 0.18 | 0.18  | 45,45,45,45                 | 0     |
| 56  | MG   | 1A    | 3061 | 1/1   | 0.94 | 0.20 | 0.15  | 36,36,36,36                 | 0     |
| 56  | MG   | 1X    | 3003 | 1/1   | 0.97 | 0.23 | 0.13  | 32,32,32,32                 | 0     |
| 56  | MG   | 2A    | 3168 | 1/1   | 0.93 | 0.20 | 0.11  | 46,46,46,46                 | 0     |
| 56  | MG   | 1A    | 3921 | 1/1   | 0.98 | 0.26 | 0.10  | 40,40,40,40                 | 0     |
| 56  | MG   | 1D    | 305  | 1/1   | 0.97 | 0.23 | 0.06  | 31,31,31,31                 | 0     |
| 56  | MG   | 2A    | 3108 | 1/1   | 0.95 | 0.15 | 0.04  | 30,30,30,30                 | 0     |
| 56  | MG   | 2A    | 3653 | 1/1   | 0.89 | 0.20 | 0.04  | 36,36,36,36                 | 0     |
| 56  | MG   | 1B    | 3009 | 1/1   | 0.95 | 0.19 | 0.04  | 42,42,42,42                 | 0     |
| 56  | MG   | 1A    | 3931 | 1/1   | 0.86 | 0.19 | 0.01  | 57,57,57,57                 | 0     |
| 56  | MG   | 1A    | 3084 | 1/1   | 0.81 | 0.23 | 0.00  | 42,42,42,42                 | 0     |
| 58  | HGR  | 2A    | 3652 | 36/36 | 0.96 | 0.24 | -0.01 | 21,36,48,50                 | 0     |
| 56  | MG   | 1Z    | 3001 | 1/1   | 0.83 | 0.24 | -0.05 | 50,50,50,50                 | 0     |
| 56  | MG   | 2a    | 1631 | 1/1   | 0.72 | 0.18 | -0.07 | 58,58,58,58                 | 0     |
| 56  | MG   | 2a    | 1776 | 1/1   | 0.95 | 0.18 | -0.10 | 66,66,66,66                 | 0     |
| 58  | HGR  | 1A    | 3915 | 36/36 | 0.97 | 0.23 | -0.17 | 15,30,37,44                 | 0     |
| 56  | MG   | 2A    | 3550 | 1/1   | 0.88 | 0.18 | -0.21 | 52,52,52,52                 | 0     |
| 56  | MG   | 2q    | 3002 | 1/1   | 0.97 | 0.18 | -0.21 | 63,63,63,63                 | 0     |
| 56  | MG   | 1a    | 1603 | 1/1   | 0.90 | 0.21 | -0.21 | 66,66,66,66                 | 0     |
| 56  | MG   | 1A    | 3064 | 1/1   | 0.98 | 0.20 | -0.25 | 35,35,35,35                 | 0     |
| 56  | MG   | 1A    | 3342 | 1/1   | 0.98 | 0.27 | -0.26 | 33,33,33,33                 | 0     |
| 56  | MG   | 1a    | 1794 | 1/1   | 0.90 | 0.17 | -0.27 | 45,45,45,45                 | 0     |
| 56  | MG   | 2t    | 3001 | 1/1   | 0.80 | 0.19 | -0.28 | 48,48,48,48                 | 0     |
| 56  | MG   | 2A    | 3302 | 1/1   | 0.92 | 0.20 | -0.30 | 38,38,38,38                 | 0     |
| 56  | MG   | 2A    | 3092 | 1/1   | 0.93 | 0.15 | -0.30 | 38,38,38,38                 | 0     |
| 56  | MG   | 1a    | 1806 | 1/1   | 0.65 | 0.18 | -0.31 | 68,68,68,68                 | 0     |
| 56  | MG   | 2A    | 3504 | 1/1   | 0.88 | 0.17 | -0.33 | 45,45,45,45                 | 0     |
| 56  | MG   | 1a    | 1639 | 1/1   | 0.92 | 0.18 | -0.34 | 45,45,45,45                 | 0     |
| 56  | MG   | 2A    | 3570 | 1/1   | 0.81 | 0.15 | -0.36 | 57,57,57,57                 | 0     |
| 56  | MG   | 1A    | 3173 | 1/1   | 0.95 | 0.22 | -0.37 | 36,36,36,36                 | 0     |
| 56  | MG   | 1Q    | 201  | 1/1   | 0.91 | 0.23 | -0.39 | 30,30,30,30                 | 0     |
| 56  | MG   | 2a    | 1650 | 1/1   | 0.92 | 0.17 | -0.40 | 47,47,47,47                 | 0     |
| 56  | MG   | 2A    | 3066 | 1/1   | 0.87 | 0.14 | -0.43 | 46,46,46,46                 | 0     |
| 56  | MG   | 1A    | 3458 | 1/1   | 0.94 | 0.19 | -0.44 | 42,42,42,42                 | 0     |
| 59  | ZN   | 16    | 501  | 1/1   | 0.99 | 0.20 | -0.44 | 35,35,35,35                 | 0     |
| 56  | MG   | 2X    | 101  | 1/1   | 0.92 | 0.16 | -0.45 | 37,37,37,37                 | 0     |
| 56  | MG   | 1A    | 3174 | 1/1   | 0.96 | 0.22 | -0.49 | 34,34,34,34                 | 0     |
| 59  | ZN   | 2Y    | 501  | 1/1   | 0.97 | 0.14 | -0.53 | 83,83,83,83                 | 0     |
| 56  | MG   | 1A    | 3493 | 1/1   | 0.95 | 0.21 | -0.53 | 21,21,21,21                 | 0     |
| 56  | MG   | 1A    | 3522 | 1/1   | 0.76 | 0.21 | -0.54 | 38,38,38,38                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 56  | MG   | 2A    | 3144 | 1/1   | 0.94 | 0.13 | -0.57 | 43,43,43,43                 | 0     |
| 56  | MG   | 1U    | 205  | 1/1   | 0.96 | 0.21 | -0.60 | 29,29,29,29                 | 0     |
| 56  | MG   | 1A    | 3457 | 1/1   | 0.93 | 0.19 | -0.60 | 30,30,30,30                 | 0     |
| 56  | MG   | 1a    | 1765 | 1/1   | 0.97 | 0.18 | -0.63 | 69,69,69,69                 | 0     |
| 56  | MG   | 2A    | 3354 | 1/1   | 0.96 | 0.18 | -0.63 | 43,43,43,43                 | 0     |
| 56  | MG   | 2A    | 3254 | 1/1   | 0.99 | 0.16 | -0.65 | 38,38,38,38                 | 0     |
| 56  | MG   | 2a    | 1758 | 1/1   | 0.96 | 0.16 | -0.67 | 46,46,46,46                 | 0     |
| 56  | MG   | 2a    | 1779 | 1/1   | 0.82 | 0.16 | -0.67 | 74,74,74,74                 | 0     |
| 56  | MG   | 1A    | 3467 | 1/1   | 0.98 | 0.17 | -0.68 | 43,43,43,43                 | 0     |
| 56  | MG   | 1a    | 1818 | 1/1   | 0.95 | 0.21 | -0.68 | 55,55,55,55                 | 0     |
| 56  | MG   | 1O    | 202  | 1/1   | 0.93 | 0.21 | -0.69 | 63,63,63,63                 | 0     |
| 56  | MG   | 1A    | 3029 | 1/1   | 0.94 | 0.23 | -0.69 | 28,28,28,28                 | 0     |
| 56  | MG   | 2A    | 3267 | 1/1   | 0.98 | 0.17 | -0.70 | 53,53,53,53                 | 0     |
| 56  | MG   | 1A    | 3300 | 1/1   | 0.97 | 0.21 | -0.72 | 31,31,31,31                 | 0     |
| 56  | MG   | 1a    | 1666 | 1/1   | 0.98 | 0.17 | -0.78 | 36,36,36,36                 | 0     |
| 56  | MG   | 1a    | 1752 | 1/1   | 0.89 | 0.18 | -0.79 | 59,59,59,59                 | 0     |
| 56  | MG   | 1A    | 3113 | 1/1   | 0.90 | 0.20 | -0.79 | 40,40,40,40                 | 0     |
| 56  | MG   | 2a    | 1643 | 1/1   | 0.90 | 0.18 | -0.83 | 58,58,58,58                 | 0     |
| 56  | MG   | 1a    | 1642 | 1/1   | 0.91 | 0.18 | -0.84 | 42,42,42,42                 | 0     |
| 56  | MG   | 1a    | 1712 | 1/1   | 0.97 | 0.20 | -0.85 | 49,49,49,49                 | 0     |
| 56  | MG   | 2A    | 3021 | 1/1   | 0.99 | 0.19 | -0.86 | 38,38,38,38                 | 0     |
| 56  | MG   | 2A    | 3190 | 1/1   | 0.76 | 0.18 | -0.89 | 44,44,44,44                 | 0     |
| 56  | MG   | 1A    | 3946 | 1/1   | 0.93 | 0.21 | -0.90 | 38,38,38,38                 | 0     |
| 56  | MG   | 1A    | 3911 | 1/1   | 0.98 | 0.20 | -0.90 | 53,53,53,53                 | 0     |
| 56  | MG   | 2U    | 201  | 1/1   | 0.95 | 0.17 | -0.91 | 39,39,39,39                 | 0     |
| 56  | MG   | 2d    | 302  | 1/1   | 0.93 | 0.21 | -0.95 | 67,67,67,67                 | 0     |
| 56  | MG   | 1E    | 305  | 1/1   | 0.96 | 0.20 | -0.96 | 37,37,37,37                 | 0     |
| 56  | MG   | 2U    | 203  | 1/1   | 0.96 | 0.24 | -0.97 | 42,42,42,42                 | 0     |
| 59  | ZN   | 1n    | 501  | 1/1   | 0.98 | 0.16 | -0.98 | 58,58,58,58                 | 0     |
| 56  | MG   | 2A    | 3406 | 1/1   | 0.95 | 0.17 | -0.99 | 47,47,47,47                 | 0     |
| 56  | MG   | 2A    | 3396 | 1/1   | 0.78 | 0.16 | -1.00 | 36,36,36,36                 | 0     |
| 56  | MG   | 1a    | 1836 | 1/1   | 0.89 | 0.17 | -1.00 | 60,60,60,60                 | 0     |
| 56  | MG   | 1A    | 3595 | 1/1   | 0.94 | 0.20 | -1.01 | 26,26,26,26                 | 0     |
| 56  | MG   | 1A    | 3183 | 1/1   | 0.69 | 0.21 | -1.04 | 50,50,50,50                 | 0     |
| 56  | MG   | 1a    | 1722 | 1/1   | 0.97 | 0.13 | -1.04 | 50,50,50,50                 | 0     |
| 56  | MG   | 1A    | 3089 | 1/1   | 0.97 | 0.15 | -1.07 | 40,40,40,40                 | 0     |
| 56  | MG   | 20    | 101  | 1/1   | 0.84 | 0.12 | -1.08 | 57,57,57,57                 | 0     |
| 56  | MG   | 2A    | 3443 | 1/1   | 0.96 | 0.14 | -1.09 | 36,36,36,36                 | 0     |
| 56  | MG   | 1A    | 3171 | 1/1   | 0.93 | 0.20 | -1.09 | 43,43,43,43                 | 0     |
| 56  | MG   | 2a    | 1705 | 1/1   | 0.94 | 0.12 | -1.09 | 60,60,60,60                 | 0     |
| 56  | MG   | 2A    | 3431 | 1/1   | 0.98 | 0.16 | -1.10 | 52,52,52,52                 | 0     |
| 56  | MG   | 1G    | 203  | 1/1   | 0.92 | 0.18 | -1.10 | 71,71,71,71                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 56  | MG   | 2A    | 3094 | 1/1   | 0.91 | 0.15 | -1.10 | 43,43,43,43                 | 0     |
| 56  | MG   | 1a    | 1747 | 1/1   | 0.94 | 0.17 | -1.14 | 55,55,55,55                 | 0     |
| 56  | MG   | 1A    | 3566 | 1/1   | 0.91 | 0.16 | -1.15 | 55,55,55,55                 | 0     |
| 56  | MG   | 2A    | 3391 | 1/1   | 0.89 | 0.16 | -1.16 | 53,53,53,53                 | 0     |
| 56  | MG   | 2a    | 1639 | 1/1   | 0.94 | 0.17 | -1.17 | 52,52,52,52                 | 0     |
| 56  | MG   | 2A    | 3091 | 1/1   | 0.95 | 0.17 | -1.17 | 29,29,29,29                 | 0     |
| 56  | MG   | 1A    | 3898 | 1/1   | 0.86 | 0.20 | -1.21 | 25,25,25,25                 | 0     |
| 56  | MG   | 1a    | 1834 | 1/1   | 0.97 | 0.21 | -1.21 | 44,44,44,44                 | 0     |
| 56  | MG   | 2A    | 3647 | 1/1   | 0.97 | 0.19 | -1.22 | 41,41,41,41                 | 0     |
| 56  | MG   | 1a    | 1611 | 1/1   | 0.87 | 0.16 | -1.23 | 57,57,57,57                 | 0     |
| 60  | SF4  | 1d    | 501  | 8/8   | 0.98 | 0.16 | -1.24 | 55,66,73,80                 | 0     |
| 56  | MG   | 2a    | 1671 | 1/1   | 0.81 | 0.15 | -1.24 | 54,54,54,54                 | 0     |
| 56  | MG   | 1A    | 3488 | 1/1   | 0.94 | 0.19 | -1.25 | 28,28,28,28                 | 0     |
| 56  | MG   | 1A    | 3038 | 1/1   | 0.96 | 0.21 | -1.25 | 36,36,36,36                 | 0     |
| 56  | MG   | 1N    | 3003 | 1/1   | 0.99 | 0.17 | -1.26 | 36,36,36,36                 | 0     |
| 56  | MG   | 19    | 101  | 1/1   | 0.83 | 0.20 | -1.27 | 41,41,41,41                 | 0     |
| 56  | MG   | 1A    | 3729 | 1/1   | 0.89 | 0.20 | -1.27 | 39,39,39,39                 | 0     |
| 56  | MG   | 1A    | 3735 | 1/1   | 0.96 | 0.19 | -1.28 | 25,25,25,25                 | 0     |
| 56  | MG   | 1A    | 3637 | 1/1   | 0.89 | 0.20 | -1.28 | 39,39,39,39                 | 0     |
| 56  | MG   | 1D    | 302  | 1/1   | 0.94 | 0.18 | -1.30 | 21,21,21,21                 | 0     |
| 56  | MG   | 1A    | 3456 | 1/1   | 0.97 | 0.18 | -1.31 | 28,28,28,28                 | 0     |
| 56  | MG   | 2A    | 3666 | 1/1   | 0.97 | 0.18 | -1.32 | 48,48,48,48                 | 0     |
| 56  | MG   | 1A    | 3193 | 1/1   | 0.93 | 0.19 | -1.33 | 33,33,33,33                 | 0     |
| 56  | MG   | 2a    | 1688 | 1/1   | 0.94 | 0.17 | -1.33 | 56,56,56,56                 | 0     |
| 56  | MG   | 2a    | 1697 | 1/1   | 0.96 | 0.14 | -1.33 | 37,37,37,37                 | 0     |
| 56  | MG   | 2A    | 3016 | 1/1   | 0.97 | 0.15 | -1.33 | 41,41,41,41                 | 0     |
| 56  | MG   | 2A    | 3146 | 1/1   | 0.98 | 0.16 | -1.34 | 33,33,33,33                 | 0     |
| 56  | MG   | 1B    | 3027 | 1/1   | 0.95 | 0.16 | -1.36 | 48,48,48,48                 | 0     |
| 56  | MG   | 1A    | 3591 | 1/1   | 0.95 | 0.20 | -1.37 | 49,49,49,49                 | 0     |
| 56  | MG   | 2A    | 3169 | 1/1   | 0.85 | 0.14 | -1.37 | 41,41,41,41                 | 0     |
| 56  | MG   | 2A    | 3081 | 1/1   | 0.93 | 0.15 | -1.38 | 39,39,39,39                 | 0     |
| 56  | MG   | 1A    | 3245 | 1/1   | 0.96 | 0.20 | -1.38 | 29,29,29,29                 | 0     |
| 56  | MG   | 2a    | 1792 | 1/1   | 0.94 | 0.15 | -1.38 | 50,50,50,50                 | 0     |
| 56  | MG   | 2A    | 3024 | 1/1   | 0.83 | 0.16 | -1.39 | 33,33,33,33                 | 0     |
| 56  | MG   | 2A    | 3436 | 1/1   | 0.96 | 0.17 | -1.40 | 39,39,39,39                 | 0     |
| 56  | MG   | 1A    | 3443 | 1/1   | 0.98 | 0.19 | -1.40 | 26,26,26,26                 | 0     |
| 56  | MG   | 2A    | 3291 | 1/1   | 0.92 | 0.17 | -1.41 | 49,49,49,49                 | 0     |
| 56  | MG   | 1A    | 3796 | 1/1   | 0.88 | 0.16 | -1.44 | 47,47,47,47                 | 0     |
| 56  | MG   | 2A    | 3140 | 1/1   | 0.90 | 0.14 | -1.45 | 50,50,50,50                 | 0     |
| 56  | MG   | 2A    | 3064 | 1/1   | 0.85 | 0.15 | -1.46 | 58,58,58,58                 | 0     |
| 56  | MG   | 1U    | 201  | 1/1   | 0.95 | 0.19 | -1.47 | 33,33,33,33                 | 0     |
| 56  | MG   | 2a    | 1739 | 1/1   | 0.89 | 0.15 | -1.49 | 74,74,74,74                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 56  | MG   | 2A    | 3556 | 1/1   | 0.88 | 0.07 | -1.49 | 49,49,49,49                 | 0     |
| 56  | MG   | 2A    | 3042 | 1/1   | 0.98 | 0.15 | -1.49 | 37,37,37,37                 | 0     |
| 56  | MG   | 2A    | 3569 | 1/1   | 0.95 | 0.14 | -1.49 | 51,51,51,51                 | 0     |
| 56  | MG   | 2R    | 201  | 1/1   | 0.96 | 0.15 | -1.54 | 48,48,48,48                 | 0     |
| 56  | MG   | 1A    | 3912 | 1/1   | 0.87 | 0.15 | -1.57 | 35,35,35,35                 | 0     |
| 56  | MG   | 2a    | 1648 | 1/1   | 0.85 | 0.12 | -1.57 | 61,61,61,61                 | 0     |
| 56  | MG   | 2A    | 3587 | 1/1   | 0.94 | 0.17 | -1.59 | 48,48,48,48                 | 0     |
| 56  | MG   | 2j    | 8002 | 1/1   | 0.88 | 0.10 | -1.60 | 66,66,66,66                 | 0     |
| 56  | MG   | 1A    | 3837 | 1/1   | 0.93 | 0.18 | -1.60 | 21,21,21,21                 | 0     |
| 56  | MG   | 2A    | 3621 | 1/1   | 0.92 | 0.15 | -1.61 | 57,57,57,57                 | 0     |
| 56  | MG   | 2A    | 3531 | 1/1   | 0.94 | 0.18 | -1.66 | 45,45,45,45                 | 0     |
| 56  | MG   | 2a    | 1757 | 1/1   | 0.94 | 0.10 | -1.72 | 70,70,70,70                 | 0     |
| 56  | MG   | 1A    | 3668 | 1/1   | 0.95 | 0.20 | -1.72 | 35,35,35,35                 | 0     |
| 56  | MG   | 1A    | 3848 | 1/1   | 0.87 | 0.19 | -1.72 | 29,29,29,29                 | 0     |
| 60  | SF4  | 2d    | 301  | 8/8   | 0.98 | 0.12 | -1.73 | 51,72,83,98                 | 0     |
| 56  | MG   | 1A    | 3045 | 1/1   | 0.97 | 0.19 | -1.74 | 19,19,19,19                 | 0     |
| 59  | ZN   | 29    | 501  | 1/1   | 0.92 | 0.12 | -1.77 | 62,62,62,62                 | 0     |
| 56  | MG   | 1D    | 304  | 1/1   | 0.93 | 0.19 | -1.77 | 44,44,44,44                 | 0     |
| 56  | MG   | 2A    | 3345 | 1/1   | 0.85 | 0.15 | -1.81 | 40,40,40,40                 | 0     |
| 56  | MG   | 1a    | 1805 | 1/1   | 0.95 | 0.16 | -1.82 | 49,49,49,49                 | 0     |
| 56  | MG   | 1a    | 1760 | 1/1   | 0.95 | 0.17 | -1.83 | 36,36,36,36                 | 0     |
| 56  | MG   | 2A    | 3095 | 1/1   | 0.98 | 0.16 | -1.85 | 47,47,47,47                 | 0     |
| 56  | MG   | 2A    | 3163 | 1/1   | 0.97 | 0.17 | -1.86 | 32,32,32,32                 | 0     |
| 56  | MG   | 1A    | 3592 | 1/1   | 0.80 | 0.18 | -1.88 | 32,32,32,32                 | 0     |
| 56  | MG   | 1A    | 3954 | 1/1   | 0.97 | 0.19 | -1.89 | 28,28,28,28                 | 0     |
| 56  | MG   | 2G    | 3001 | 1/1   | 0.88 | 0.14 | -1.90 | 54,54,54,54                 | 0     |
| 56  | MG   | 2A    | 3337 | 1/1   | 0.96 | 0.16 | -1.90 | 42,42,42,42                 | 0     |
| 56  | MG   | 2A    | 3281 | 1/1   | 0.86 | 0.14 | -1.90 | 40,40,40,40                 | 0     |
| 56  | MG   | 1A    | 3933 | 1/1   | 0.97 | 0.17 | -1.91 | 28,28,28,28                 | 0     |
| 56  | MG   | 2a    | 1773 | 1/1   | 0.91 | 0.13 | -1.91 | 66,66,66,66                 | 0     |
| 56  | MG   | 1A    | 3899 | 1/1   | 0.95 | 0.18 | -1.95 | 14,14,14,14                 | 0     |
| 56  | MG   | 1A    | 3010 | 1/1   | 0.98 | 0.15 | -1.95 | 29,29,29,29                 | 0     |
| 56  | MG   | 1a    | 1808 | 1/1   | 0.77 | 0.16 | -1.96 | 67,67,67,67                 | 0     |
| 56  | MG   | 2A    | 3642 | 1/1   | 0.96 | 0.17 | -1.98 | 32,32,32,32                 | 0     |
| 56  | MG   | 1l    | 201  | 1/1   | 0.96 | 0.14 | -1.98 | 34,34,34,34                 | 0     |
| 56  | MG   | 2A    | 3428 | 1/1   | 0.97 | 0.14 | -1.99 | 27,27,27,27                 | 0     |
| 56  | MG   | 1x    | 3001 | 1/1   | 0.84 | 0.13 | -1.99 | 44,44,44,44                 | 0     |
| 56  | MG   | 1A    | 3477 | 1/1   | 0.93 | 0.17 | -2.02 | 23,23,23,23                 | 0     |
| 56  | MG   | 1A    | 3953 | 1/1   | 0.95 | 0.19 | -2.03 | 48,48,48,48                 | 0     |
| 56  | MG   | 2A    | 3533 | 1/1   | 0.87 | 0.16 | -2.03 | 26,26,26,26                 | 0     |
| 56  | MG   | 2A    | 3173 | 1/1   | 0.80 | 0.14 | -2.03 | 45,45,45,45                 | 0     |
| 56  | MG   | 1A    | 3269 | 1/1   | 0.91 | 0.16 | -2.04 | 30,30,30,30                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 56  | MG   | 2A    | 3401 | 1/1   | 0.93 | 0.12 | -2.08 | 45,45,45,45                 | 0     |
| 56  | MG   | 2A    | 3478 | 1/1   | 0.91 | 0.15 | -2.08 | 56,56,56,56                 | 0     |
| 59  | ZN   | 2n    | 501  | 1/1   | 0.93 | 0.08 | -2.10 | 108,108,108,108             | 0     |
| 56  | MG   | 1A    | 3875 | 1/1   | 0.90 | 0.16 | -2.11 | 32,32,32,32                 | 0     |
| 56  | MG   | 2A    | 3459 | 1/1   | 0.96 | 0.15 | -2.13 | 49,49,49,49                 | 0     |
| 56  | MG   | 1A    | 3913 | 1/1   | 0.95 | 0.15 | -2.14 | 39,39,39,39                 | 0     |
| 56  | MG   | 1A    | 3942 | 1/1   | 0.98 | 0.19 | -2.16 | 32,32,32,32                 | 0     |
| 56  | MG   | 2f    | 3001 | 1/1   | 0.96 | 0.13 | -2.17 | 39,39,39,39                 | 0     |
| 56  | MG   | 2A    | 3395 | 1/1   | 0.92 | 0.14 | -2.17 | 46,46,46,46                 | 0     |
| 56  | MG   | 2A    | 3285 | 1/1   | 0.78 | 0.12 | -2.18 | 64,64,64,64                 | 0     |
| 56  | MG   | 1A    | 3290 | 1/1   | 0.87 | 0.19 | -2.18 | 33,33,33,33                 | 0     |
| 56  | MG   | 1A    | 3106 | 1/1   | 0.96 | 0.18 | -2.19 | 37,37,37,37                 | 0     |
| 56  | MG   | 2A    | 3298 | 1/1   | 0.82 | 0.12 | -2.19 | 39,39,39,39                 | 0     |
| 56  | MG   | 1A    | 3687 | 1/1   | 0.95 | 0.20 | -2.21 | 39,39,39,39                 | 0     |
| 56  | MG   | 2a    | 1702 | 1/1   | 0.93 | 0.12 | -2.21 | 60,60,60,60                 | 0     |
| 56  | MG   | 2B    | 3008 | 1/1   | 0.89 | 0.12 | -2.22 | 55,55,55,55                 | 0     |
| 56  | MG   | 26    | 502  | 1/1   | 0.92 | 0.14 | -2.23 | 45,45,45,45                 | 0     |
| 56  | MG   | 1A    | 3948 | 1/1   | 0.90 | 0.18 | -2.23 | 34,34,34,34                 | 0     |
| 56  | MG   | 2A    | 3400 | 1/1   | 0.96 | 0.12 | -2.24 | 49,49,49,49                 | 0     |
| 56  | MG   | 2A    | 3434 | 1/1   | 0.88 | 0.15 | -2.24 | 39,39,39,39                 | 0     |
| 56  | MG   | 1x    | 3003 | 1/1   | 0.90 | 0.13 | -2.25 | 53,53,53,53                 | 0     |
| 56  | MG   | 2a    | 1667 | 1/1   | 0.61 | 0.14 | -2.26 | 73,73,73,73                 | 0     |
| 56  | MG   | 2A    | 3402 | 1/1   | 0.82 | 0.14 | -2.26 | 53,53,53,53                 | 0     |
| 56  | MG   | 1t    | 3001 | 1/1   | 0.97 | 0.15 | -2.26 | 47,47,47,47                 | 0     |
| 56  | MG   | 2A    | 3643 | 1/1   | 0.81 | 0.15 | -2.27 | 38,38,38,38                 | 0     |
| 56  | MG   | 2A    | 3413 | 1/1   | 0.91 | 0.10 | -2.28 | 50,50,50,50                 | 0     |
| 56  | MG   | 2Q    | 202  | 1/1   | 0.98 | 0.14 | -2.29 | 46,46,46,46                 | 0     |
| 56  | MG   | 1a    | 1601 | 1/1   | 0.94 | 0.14 | -2.29 | 53,53,53,53                 | 0     |
| 56  | MG   | 1A    | 3502 | 1/1   | 0.91 | 0.18 | -2.30 | 23,23,23,23                 | 0     |
| 56  | MG   | 1A    | 3535 | 1/1   | 0.95 | 0.18 | -2.32 | 45,45,45,45                 | 0     |
| 56  | MG   | 2A    | 3349 | 1/1   | 0.96 | 0.18 | -2.33 | 18,18,18,18                 | 0     |
| 56  | MG   | 1a    | 1602 | 1/1   | 0.93 | 0.17 | -2.33 | 68,68,68,68                 | 0     |
| 56  | MG   | 1A    | 3103 | 1/1   | 0.94 | 0.18 | -2.35 | 36,36,36,36                 | 0     |
| 56  | MG   | 1A    | 3110 | 1/1   | 0.97 | 0.19 | -2.37 | 29,29,29,29                 | 0     |
| 56  | MG   | 2a    | 1794 | 1/1   | 0.92 | 0.13 | -2.37 | 51,51,51,51                 | 0     |
| 56  | MG   | 1A    | 3468 | 1/1   | 0.92 | 0.18 | -2.38 | 44,44,44,44                 | 0     |
| 56  | MG   | 2A    | 3294 | 1/1   | 0.97 | 0.13 | -2.38 | 38,38,38,38                 | 0     |
| 56  | MG   | 2A    | 3033 | 1/1   | 0.96 | 0.14 | -2.38 | 29,29,29,29                 | 0     |
| 56  | MG   | 1b    | 3001 | 1/1   | 0.95 | 0.10 | -2.40 | 75,75,75,75                 | 0     |
| 56  | MG   | 1a    | 1689 | 1/1   | 0.78 | 0.13 | -2.40 | 63,63,63,63                 | 0     |
| 56  | MG   | 1A    | 3487 | 1/1   | 0.98 | 0.18 | -2.42 | 24,24,24,24                 | 0     |
| 56  | MG   | 19    | 102  | 1/1   | 0.94 | 0.12 | -2.42 | 50,50,50,50                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 56  | MG   | 2A    | 3599 | 1/1   | 0.94 | 0.14 | -2.44 | 54,54,54,54                 | 0     |
| 56  | MG   | 2a    | 1632 | 1/1   | 0.96 | 0.13 | -2.45 | 59,59,59,59                 | 0     |
| 56  | MG   | 1A    | 3474 | 1/1   | 0.88 | 0.20 | -2.49 | 29,29,29,29                 | 0     |
| 56  | MG   | 2A    | 3317 | 1/1   | 0.98 | 0.15 | -2.51 | 38,38,38,38                 | 0     |
| 56  | MG   | 1A    | 3402 | 1/1   | 0.95 | 0.15 | -2.52 | 38,38,38,38                 | 0     |
| 56  | MG   | 2A    | 3609 | 1/1   | 0.97 | 0.16 | -2.53 | 36,36,36,36                 | 0     |
| 56  | MG   | 1A    | 3841 | 1/1   | 0.98 | 0.18 | -2.54 | 22,22,22,22                 | 0     |
| 56  | MG   | 2A    | 3142 | 1/1   | 0.92 | 0.18 | -2.54 | 37,37,37,37                 | 0     |
| 56  | MG   | 1a    | 1628 | 1/1   | 0.94 | 0.14 | -2.55 | 43,43,43,43                 | 0     |
| 56  | MG   | 1A    | 3885 | 1/1   | 0.93 | 0.19 | -2.58 | 44,44,44,44                 | 0     |
| 56  | MG   | 2l    | 201  | 1/1   | 0.96 | 0.09 | -2.59 | 61,61,61,61                 | 0     |
| 56  | MG   | 1A    | 3190 | 1/1   | 0.93 | 0.19 | -2.59 | 43,43,43,43                 | 0     |
| 56  | MG   | 1A    | 3918 | 1/1   | 0.93 | 0.18 | -2.59 | 35,35,35,35                 | 0     |
| 56  | MG   | 2A    | 3620 | 1/1   | 0.96 | 0.14 | -2.60 | 39,39,39,39                 | 0     |
| 56  | MG   | 1A    | 3469 | 1/1   | 0.97 | 0.16 | -2.62 | 33,33,33,33                 | 0     |
| 56  | MG   | 1A    | 3577 | 1/1   | 0.95 | 0.18 | -2.62 | 47,47,47,47                 | 0     |
| 56  | MG   | 1A    | 3384 | 1/1   | 0.90 | 0.19 | -2.63 | 52,52,52,52                 | 0     |
| 56  | MG   | 1B    | 3025 | 1/1   | 0.86 | 0.14 | -2.63 | 49,49,49,49                 | 0     |
| 56  | MG   | 1a    | 1621 | 1/1   | 0.91 | 0.15 | -2.64 | 49,49,49,49                 | 0     |
| 56  | MG   | 1A    | 3472 | 1/1   | 0.98 | 0.17 | -2.65 | 32,32,32,32                 | 0     |
| 56  | MG   | 2A    | 3006 | 1/1   | 0.93 | 0.13 | -2.67 | 53,53,53,53                 | 0     |
| 56  | MG   | 2A    | 3658 | 1/1   | 0.95 | 0.11 | -2.68 | 39,39,39,39                 | 0     |
| 56  | MG   | 1a    | 1727 | 1/1   | 0.91 | 0.07 | -2.68 | 65,65,65,65                 | 0     |
| 59  | ZN   | 24    | 501  | 1/1   | 0.69 | 0.07 | -2.68 | 143,143,143,143             | 0     |
| 56  | MG   | 2a    | 1672 | 1/1   | 0.76 | 0.16 | -2.68 | 72,72,72,72                 | 0     |
| 56  | MG   | 1A    | 3950 | 1/1   | 0.95 | 0.16 | -2.68 | 35,35,35,35                 | 0     |
| 56  | MG   | 1a    | 1753 | 1/1   | 0.91 | 0.13 | -2.69 | 58,58,58,58                 | 0     |
| 56  | MG   | 1A    | 3700 | 1/1   | 0.93 | 0.17 | -2.70 | 40,40,40,40                 | 0     |
| 56  | MG   | 1R    | 201  | 1/1   | 0.88 | 0.14 | -2.71 | 34,34,34,34                 | 0     |
| 56  | MG   | 1A    | 3688 | 1/1   | 0.97 | 0.15 | -2.73 | 41,41,41,41                 | 0     |
| 56  | MG   | 1A    | 3012 | 1/1   | 0.98 | 0.16 | -2.74 | 28,28,28,28                 | 0     |
| 59  | ZN   | 14    | 501  | 1/1   | 0.94 | 0.07 | -2.75 | 97,97,97,97                 | 0     |
| 56  | MG   | 2E    | 302  | 1/1   | 0.88 | 0.12 | -2.75 | 39,39,39,39                 | 0     |
| 56  | MG   | 2A    | 3099 | 1/1   | 0.95 | 0.15 | -2.79 | 24,24,24,24                 | 0     |
| 56  | MG   | 1A    | 3630 | 1/1   | 0.90 | 0.19 | -2.80 | 35,35,35,35                 | 0     |
| 56  | MG   | 1A    | 3008 | 1/1   | 0.96 | 0.17 | -2.84 | 26,26,26,26                 | 0     |
| 56  | MG   | 1A    | 3814 | 1/1   | 0.96 | 0.19 | -2.87 | 16,16,16,16                 | 0     |
| 56  | MG   | 1A    | 3583 | 1/1   | 0.97 | 0.18 | -2.88 | 57,57,57,57                 | 0     |
| 56  | MG   | 2A    | 3307 | 1/1   | 0.94 | 0.14 | -2.92 | 31,31,31,31                 | 0     |
| 56  | MG   | 1A    | 3071 | 1/1   | 0.96 | 0.16 | -2.93 | 47,47,47,47                 | 0     |
| 56  | MG   | 2A    | 3373 | 1/1   | 0.86 | 0.15 | -2.93 | 27,27,27,27                 | 0     |
| 56  | MG   | 1A    | 3377 | 1/1   | 0.96 | 0.17 | -2.94 | 36,36,36,36                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 56  | MG   | 1A    | 3127 | 1/1   | 0.98 | 0.18 | -2.96 | 47,47,47,47                 | 0     |
| 56  | MG   | 2A    | 3001 | 1/1   | 0.94 | 0.16 | -2.98 | 28,28,28,28                 | 0     |
| 56  | MG   | 2A    | 3418 | 1/1   | 0.95 | 0.17 | -2.98 | 44,44,44,44                 | 0     |
| 56  | MG   | 1A    | 3464 | 1/1   | 0.95 | 0.16 | -2.98 | 35,35,35,35                 | 0     |
| 56  | MG   | 2A    | 3035 | 1/1   | 0.95 | 0.12 | -2.99 | 41,41,41,41                 | 0     |
| 56  | MG   | 1A    | 3403 | 1/1   | 0.95 | 0.16 | -3.00 | 52,52,52,52                 | 0     |
| 56  | MG   | 1F    | 303  | 1/1   | 0.84 | 0.18 | -3.02 | 34,34,34,34                 | 0     |
| 56  | MG   | 2A    | 3327 | 1/1   | 0.96 | 0.14 | -3.03 | 33,33,33,33                 | 0     |
| 56  | MG   | 1a    | 1629 | 1/1   | 0.88 | 0.13 | -3.03 | 58,58,58,58                 | 0     |
| 56  | MG   | 2A    | 3465 | 1/1   | 0.94 | 0.12 | -3.04 | 39,39,39,39                 | 0     |
| 56  | MG   | 2A    | 3380 | 1/1   | 0.94 | 0.09 | -3.04 | 35,35,35,35                 | 0     |
| 56  | MG   | 1A    | 3229 | 1/1   | 0.94 | 0.15 | -3.05 | 40,40,40,40                 | 0     |
| 56  | MG   | 1A    | 3750 | 1/1   | 0.76 | 0.14 | -3.05 | 53,53,53,53                 | 0     |
| 56  | MG   | 2A    | 3576 | 1/1   | 0.89 | 0.09 | -3.06 | 59,59,59,59                 | 0     |
| 56  | MG   | 1A    | 3767 | 1/1   | 0.96 | 0.14 | -3.06 | 39,39,39,39                 | 0     |
| 56  | MG   | 1a    | 1757 | 1/1   | 0.96 | 0.14 | -3.08 | 39,39,39,39                 | 0     |
| 56  | MG   | 2A    | 3419 | 1/1   | 0.95 | 0.14 | -3.08 | 37,37,37,37                 | 0     |
| 56  | MG   | 1d    | 503  | 1/1   | 0.85 | 0.08 | -3.11 | 66,66,66,66                 | 0     |
| 56  | MG   | 2a    | 1606 | 1/1   | 0.92 | 0.12 | -3.12 | 61,61,61,61                 | 0     |
| 56  | MG   | 2A    | 3319 | 1/1   | 0.95 | 0.16 | -3.12 | 29,29,29,29                 | 0     |
| 56  | MG   | 1A    | 3397 | 1/1   | 0.95 | 0.18 | -3.13 | 56,56,56,56                 | 0     |
| 56  | MG   | 1A    | 3508 | 1/1   | 0.95 | 0.17 | -3.18 | 38,38,38,38                 | 0     |
| 56  | MG   | 2A    | 3009 | 1/1   | 0.94 | 0.13 | -3.21 | 41,41,41,41                 | 0     |
| 56  | MG   | 1U    | 202  | 1/1   | 0.94 | 0.13 | -3.22 | 31,31,31,31                 | 0     |
| 56  | MG   | 1A    | 3187 | 1/1   | 0.92 | 0.12 | -3.23 | 60,60,60,60                 | 0     |
| 56  | MG   | 1a    | 1674 | 1/1   | 0.94 | 0.13 | -3.26 | 42,42,42,42                 | 0     |
| 56  | MG   | 1a    | 1838 | 1/1   | 0.94 | 0.10 | -3.26 | 51,51,51,51                 | 0     |
| 56  | MG   | 1A    | 3922 | 1/1   | 0.98 | 0.15 | -3.28 | 41,41,41,41                 | 0     |
| 56  | MG   | 1a    | 1830 | 1/1   | 0.98 | 0.15 | -3.28 | 44,44,44,44                 | 0     |
| 56  | MG   | 2A    | 3522 | 1/1   | 0.86 | 0.13 | -3.32 | 53,53,53,53                 | 0     |
| 56  | MG   | 2A    | 3568 | 1/1   | 0.97 | 0.11 | -3.33 | 54,54,54,54                 | 0     |
| 56  | MG   | 1A    | 3963 | 1/1   | 0.95 | 0.18 | -3.38 | 34,34,34,34                 | 0     |
| 56  | MG   | 1A    | 3858 | 1/1   | 0.97 | 0.13 | -3.42 | 36,36,36,36                 | 0     |
| 56  | MG   | 1A    | 3584 | 1/1   | 0.89 | 0.17 | -3.42 | 19,19,19,19                 | 0     |
| 56  | MG   | 1A    | 3715 | 1/1   | 0.79 | 0.12 | -3.44 | 50,50,50,50                 | 0     |
| 56  | MG   | 2A    | 3117 | 1/1   | 0.91 | 0.14 | -3.46 | 43,43,43,43                 | 0     |
| 56  | MG   | 1A    | 3462 | 1/1   | 0.86 | 0.14 | -3.47 | 53,53,53,53                 | 0     |
| 56  | MG   | 1A    | 3200 | 1/1   | 0.90 | 0.14 | -3.47 | 49,49,49,49                 | 0     |
| 56  | MG   | 2A    | 3058 | 1/1   | 0.86 | 0.12 | -3.48 | 47,47,47,47                 | 0     |
| 56  | MG   | 2A    | 3253 | 1/1   | 0.97 | 0.11 | -3.49 | 47,47,47,47                 | 0     |
| 56  | MG   | 1A    | 3452 | 1/1   | 0.91 | 0.15 | -3.52 | 43,43,43,43                 | 0     |
| 56  | MG   | 1A    | 3046 | 1/1   | 0.98 | 0.17 | -3.52 | 29,29,29,29                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 56  | MG   | 1A    | 3962 | 1/1   | 0.93 | 0.15 | -3.58 | 35,35,35,35                 | 0     |
| 56  | MG   | 2e    | 3001 | 1/1   | 0.97 | 0.10 | -3.59 | 53,53,53,53                 | 0     |
| 56  | MG   | 1A    | 3775 | 1/1   | 0.90 | 0.12 | -3.59 | 47,47,47,47                 | 0     |
| 56  | MG   | 1A    | 3691 | 1/1   | 0.92 | 0.17 | -3.62 | 41,41,41,41                 | 0     |
| 56  | MG   | 1A    | 3901 | 1/1   | 0.98 | 0.16 | -3.63 | 46,46,46,46                 | 0     |
| 56  | MG   | 2A    | 3282 | 1/1   | 0.92 | 0.13 | -3.65 | 33,33,33,33                 | 0     |
| 56  | MG   | 1A    | 3842 | 1/1   | 0.92 | 0.15 | -3.65 | 39,39,39,39                 | 0     |
| 56  | MG   | 2A    | 3118 | 1/1   | 0.98 | 0.11 | -3.65 | 37,37,37,37                 | 0     |
| 56  | MG   | 1A    | 3461 | 1/1   | 0.89 | 0.16 | -3.67 | 27,27,27,27                 | 0     |
| 56  | MG   | 1A    | 3479 | 1/1   | 0.94 | 0.19 | -3.67 | 48,48,48,48                 | 0     |
| 56  | MG   | 2A    | 3061 | 1/1   | 0.84 | 0.15 | -3.67 | 43,43,43,43                 | 0     |
| 56  | MG   | 2A    | 3010 | 1/1   | 0.97 | 0.13 | -3.68 | 30,30,30,30                 | 0     |
| 56  | MG   | 2A    | 3017 | 1/1   | 0.96 | 0.14 | -3.73 | 26,26,26,26                 | 0     |
| 56  | MG   | 1A    | 3434 | 1/1   | 0.86 | 0.10 | -3.73 | 39,39,39,39                 | 0     |
| 56  | MG   | 2A    | 3650 | 1/1   | 0.97 | 0.12 | -3.73 | 37,37,37,37                 | 0     |
| 56  | MG   | 1a    | 1832 | 1/1   | 0.94 | 0.10 | -3.75 | 47,47,47,47                 | 0     |
| 59  | ZN   | 15    | 101  | 1/1   | 0.99 | 0.12 | -3.77 | 25,25,25,25                 | 0     |
| 56  | MG   | 1A    | 3854 | 1/1   | 0.96 | 0.15 | -3.77 | 33,33,33,33                 | 0     |
| 56  | MG   | 2O    | 8001 | 1/1   | 0.91 | 0.12 | -3.79 | 52,52,52,52                 | 0     |
| 56  | MG   | 1a    | 1646 | 1/1   | 0.94 | 0.19 | -3.80 | 25,25,25,25                 | 0     |
| 56  | MG   | 1a    | 1745 | 1/1   | 0.96 | 0.13 | -3.81 | 43,43,43,43                 | 0     |
| 56  | MG   | 1A    | 3896 | 1/1   | 0.99 | 0.20 | -3.82 | 13,13,13,13                 | 0     |
| 56  | MG   | 1A    | 3401 | 1/1   | 0.86 | 0.16 | -3.82 | 38,38,38,38                 | 0     |
| 56  | MG   | 1l    | 202  | 1/1   | 0.96 | 0.14 | -3.82 | 52,52,52,52                 | 0     |
| 56  | MG   | 2a    | 1732 | 1/1   | 0.98 | 0.10 | -3.83 | 45,45,45,45                 | 0     |
| 56  | MG   | 1G    | 201  | 1/1   | 0.94 | 0.10 | -3.84 | 37,37,37,37                 | 0     |
| 56  | MG   | 1A    | 3553 | 1/1   | 0.95 | 0.14 | -3.85 | 28,28,28,28                 | 0     |
| 56  | MG   | 1A    | 3600 | 1/1   | 0.76 | 0.16 | -3.85 | 41,41,41,41                 | 0     |
| 56  | MG   | 1A    | 3838 | 1/1   | 0.91 | 0.17 | -3.88 | 38,38,38,38                 | 0     |
| 56  | MG   | 1A    | 3097 | 1/1   | 0.95 | 0.18 | -3.89 | 16,16,16,16                 | 0     |
| 56  | MG   | 2A    | 3489 | 1/1   | 0.94 | 0.12 | -3.92 | 57,57,57,57                 | 0     |
| 56  | MG   | 2A    | 3541 | 1/1   | 0.98 | 0.11 | -3.93 | 51,51,51,51                 | 0     |
| 56  | MG   | 1A    | 3394 | 1/1   | 0.98 | 0.18 | -3.94 | 12,12,12,12                 | 0     |
| 56  | MG   | 2A    | 3256 | 1/1   | 0.93 | 0.11 | -3.97 | 33,33,33,33                 | 0     |
| 56  | MG   | 2D    | 302  | 1/1   | 0.99 | 0.10 | -3.98 | 27,27,27,27                 | 0     |
| 56  | MG   | 1W    | 3005 | 1/1   | 0.96 | 0.09 | -3.98 | 30,30,30,30                 | 0     |
| 56  | MG   | 1A    | 3316 | 1/1   | 0.89 | 0.11 | -3.99 | 44,44,44,44                 | 0     |
| 56  | MG   | 2A    | 3012 | 1/1   | 0.89 | 0.12 | -4.04 | 40,40,40,40                 | 0     |
| 56  | MG   | 2a    | 1611 | 1/1   | 0.77 | 0.11 | -4.05 | 62,62,62,62                 | 0     |
| 56  | MG   | 2a    | 1692 | 1/1   | 0.98 | 0.14 | -4.08 | 54,54,54,54                 | 0     |
| 56  | MG   | 1A    | 3614 | 1/1   | 0.97 | 0.16 | -4.08 | 42,42,42,42                 | 0     |
| 56  | MG   | 1A    | 3794 | 1/1   | 0.90 | 0.10 | -4.08 | 21,21,21,21                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 56  | MG   | 2A    | 3472 | 1/1   | 0.97 | 0.15 | -4.10 | 55,55,55,55                 | 0     |
| 56  | MG   | 2A    | 3275 | 1/1   | 0.97 | 0.13 | -4.10 | 46,46,46,46                 | 0     |
| 56  | MG   | 1A    | 3613 | 1/1   | 0.89 | 0.15 | -4.11 | 36,36,36,36                 | 0     |
| 56  | MG   | 2a    | 1622 | 1/1   | 0.86 | 0.13 | -4.11 | 44,44,44,44                 | 0     |
| 56  | MG   | 2A    | 3654 | 1/1   | 0.96 | 0.13 | -4.11 | 34,34,34,34                 | 0     |
| 56  | MG   | 1A    | 3593 | 1/1   | 0.91 | 0.14 | -4.12 | 29,29,29,29                 | 0     |
| 56  | MG   | 1A    | 3033 | 1/1   | 0.98 | 0.16 | -4.12 | 22,22,22,22                 | 0     |
| 56  | MG   | 1a    | 1679 | 1/1   | 0.92 | 0.16 | -4.14 | 48,48,48,48                 | 0     |
| 56  | MG   | 2A    | 3660 | 1/1   | 0.93 | 0.08 | -4.15 | 42,42,42,42                 | 0     |
| 56  | MG   | 2A    | 3132 | 1/1   | 0.97 | 0.13 | -4.15 | 44,44,44,44                 | 0     |
| 56  | MG   | 2a    | 1714 | 1/1   | 0.94 | 0.13 | -4.17 | 55,55,55,55                 | 0     |
| 56  | MG   | 2a    | 1733 | 1/1   | 0.95 | 0.16 | -4.18 | 61,61,61,61                 | 0     |
| 56  | MG   | 2a    | 1687 | 1/1   | 0.93 | 0.12 | -4.18 | 52,52,52,52                 | 0     |
| 56  | MG   | 1a    | 1813 | 1/1   | 0.94 | 0.14 | -4.18 | 72,72,72,72                 | 0     |
| 56  | MG   | 2a    | 1795 | 1/1   | 0.94 | 0.07 | -4.19 | 55,55,55,55                 | 0     |
| 56  | MG   | 2A    | 3526 | 1/1   | 0.97 | 0.13 | -4.20 | 49,49,49,49                 | 0     |
| 56  | MG   | 1A    | 3902 | 1/1   | 0.94 | 0.17 | -4.21 | 28,28,28,28                 | 0     |
| 56  | MG   | 1A    | 3804 | 1/1   | 0.98 | 0.16 | -4.21 | 26,26,26,26                 | 0     |
| 56  | MG   | 1A    | 3632 | 1/1   | 0.97 | 0.17 | -4.23 | 57,57,57,57                 | 0     |
| 56  | MG   | 1A    | 3447 | 1/1   | 0.93 | 0.17 | -4.24 | 36,36,36,36                 | 0     |
| 56  | MG   | 1A    | 3572 | 1/1   | 0.96 | 0.12 | -4.24 | 33,33,33,33                 | 0     |
| 56  | MG   | 1A    | 3960 | 1/1   | 0.83 | 0.16 | -4.29 | 38,38,38,38                 | 0     |
| 56  | MG   | 1W    | 3003 | 1/1   | 0.98 | 0.14 | -4.30 | 25,25,25,25                 | 0     |
| 56  | MG   | 1A    | 3620 | 1/1   | 0.96 | 0.15 | -4.34 | 32,32,32,32                 | 0     |
| 56  | MG   | 1A    | 3927 | 1/1   | 0.92 | 0.15 | -4.35 | 40,40,40,40                 | 0     |
| 56  | MG   | 1A    | 3473 | 1/1   | 0.85 | 0.18 | -4.39 | 26,26,26,26                 | 0     |
| 56  | MG   | 2A    | 3301 | 1/1   | 0.97 | 0.09 | -4.39 | 35,35,35,35                 | 0     |
| 56  | MG   | 1A    | 3664 | 1/1   | 0.96 | 0.15 | -4.40 | 39,39,39,39                 | 0     |
| 56  | MG   | 1a    | 1734 | 1/1   | 0.90 | 0.16 | -4.40 | 30,30,30,30                 | 0     |
| 56  | MG   | 1A    | 3792 | 1/1   | 0.98 | 0.11 | -4.41 | 17,17,17,17                 | 0     |
| 56  | MG   | 2A    | 3655 | 1/1   | 0.87 | 0.10 | -4.45 | 31,31,31,31                 | 0     |
| 56  | MG   | 2A    | 3119 | 1/1   | 0.92 | 0.12 | -4.48 | 37,37,37,37                 | 0     |
| 56  | MG   | 1A    | 3389 | 1/1   | 0.94 | 0.14 | -4.50 | 50,50,50,50                 | 0     |
| 56  | MG   | 2A    | 3470 | 1/1   | 0.93 | 0.13 | -4.55 | 30,30,30,30                 | 0     |
| 56  | MG   | 1A    | 3165 | 1/1   | 0.85 | 0.15 | -4.58 | 38,38,38,38                 | 0     |
| 56  | MG   | 1A    | 3892 | 1/1   | 0.84 | 0.15 | -4.61 | 41,41,41,41                 | 0     |
| 56  | MG   | 1w    | 3001 | 1/1   | 0.94 | 0.10 | -4.61 | 44,44,44,44                 | 0     |
| 56  | MG   | 1A    | 3217 | 1/1   | 0.89 | 0.10 | -4.62 | 42,42,42,42                 | 0     |
| 56  | MG   | 1A    | 3043 | 1/1   | 0.96 | 0.12 | -4.64 | 27,27,27,27                 | 0     |
| 56  | MG   | 1A    | 3417 | 1/1   | 0.87 | 0.17 | -4.67 | 32,32,32,32                 | 0     |
| 56  | MG   | 11    | 102  | 1/1   | 0.97 | 0.14 | -4.70 | 38,38,38,38                 | 0     |
| 56  | MG   | 1A    | 3396 | 1/1   | 0.95 | 0.15 | -4.71 | 45,45,45,45                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 56  | MG   | 1A    | 3774 | 1/1   | 0.91 | 0.17 | -4.71 | 42,42,42,42                 | 0     |
| 56  | MG   | 1I    | 101  | 1/1   | 0.95 | 0.07 | -4.72 | 41,41,41,41                 | 0     |
| 56  | MG   | 1A    | 3905 | 1/1   | 0.97 | 0.12 | -4.73 | 35,35,35,35                 | 0     |
| 56  | MG   | 1A    | 3212 | 1/1   | 0.90 | 0.10 | -4.73 | 67,67,67,67                 | 0     |
| 56  | MG   | 2A    | 3385 | 1/1   | 0.81 | 0.13 | -4.74 | 43,43,43,43                 | 0     |
| 56  | MG   | 2A    | 3543 | 1/1   | 0.98 | 0.11 | -4.74 | 28,28,28,28                 | 0     |
| 56  | MG   | 2A    | 3240 | 1/1   | 0.94 | 0.12 | -4.79 | 46,46,46,46                 | 0     |
| 56  | MG   | 1E    | 303  | 1/1   | 0.98 | 0.12 | -4.84 | 26,26,26,26                 | 0     |
| 56  | MG   | 1a    | 1741 | 1/1   | 0.94 | 0.11 | -4.84 | 47,47,47,47                 | 0     |
| 56  | MG   | 2A    | 3028 | 1/1   | 0.91 | 0.10 | -4.87 | 43,43,43,43                 | 0     |
| 56  | MG   | 1A    | 3781 | 1/1   | 0.99 | 0.13 | -4.91 | 23,23,23,23                 | 0     |
| 56  | MG   | 1a    | 1672 | 1/1   | 0.85 | 0.11 | -4.94 | 55,55,55,55                 | 0     |
| 56  | MG   | 1A    | 3585 | 1/1   | 0.98 | 0.13 | -4.94 | 49,49,49,49                 | 0     |
| 56  | MG   | 1a    | 1619 | 1/1   | 0.98 | 0.09 | -4.99 | 56,56,56,56                 | 0     |
| 56  | MG   | 1a    | 1771 | 1/1   | 0.95 | 0.10 | -5.00 | 54,54,54,54                 | 0     |
| 56  | MG   | 2a    | 1647 | 1/1   | 0.83 | 0.13 | -5.01 | 64,64,64,64                 | 0     |
| 56  | MG   | 2A    | 3571 | 1/1   | 0.96 | 0.14 | -5.01 | 47,47,47,47                 | 0     |
| 56  | MG   | 1A    | 3780 | 1/1   | 0.94 | 0.16 | -5.01 | 26,26,26,26                 | 0     |
| 56  | MG   | 1A    | 3819 | 1/1   | 0.87 | 0.10 | -5.03 | 51,51,51,51                 | 0     |
| 56  | MG   | 1A    | 3209 | 1/1   | 0.93 | 0.16 | -5.04 | 35,35,35,35                 | 0     |
| 56  | MG   | 2a    | 1700 | 1/1   | 0.92 | 0.09 | -5.07 | 60,60,60,60                 | 0     |
| 56  | MG   | 1A    | 3093 | 1/1   | 0.90 | 0.14 | -5.08 | 43,43,43,43                 | 0     |
| 56  | MG   | 1a    | 1677 | 1/1   | 0.91 | 0.12 | -5.11 | 56,56,56,56                 | 0     |
| 56  | MG   | 2A    | 3561 | 1/1   | 0.88 | 0.05 | -5.12 | 71,71,71,71                 | 0     |
| 56  | MG   | 1A    | 3590 | 1/1   | 0.95 | 0.16 | -5.13 | 24,24,24,24                 | 0     |
| 56  | MG   | 1A    | 3684 | 1/1   | 0.96 | 0.16 | -5.16 | 29,29,29,29                 | 0     |
| 56  | MG   | 1A    | 3051 | 1/1   | 0.91 | 0.15 | -5.18 | 38,38,38,38                 | 0     |
| 56  | MG   | 2A    | 3640 | 1/1   | 0.91 | 0.12 | -5.25 | 45,45,45,45                 | 0     |
| 56  | MG   | 1A    | 3040 | 1/1   | 0.96 | 0.12 | -5.26 | 32,32,32,32                 | 0     |
| 56  | MG   | 1B    | 3017 | 1/1   | 0.96 | 0.12 | -5.27 | 44,44,44,44                 | 0     |
| 56  | MG   | 1A    | 3203 | 1/1   | 0.92 | 0.14 | -5.27 | 44,44,44,44                 | 0     |
| 56  | MG   | 1A    | 3612 | 1/1   | 0.91 | 0.14 | -5.32 | 30,30,30,30                 | 0     |
| 56  | MG   | 2a    | 1704 | 1/1   | 0.88 | 0.13 | -5.34 | 40,40,40,40                 | 0     |
| 56  | MG   | 1A    | 3714 | 1/1   | 0.93 | 0.13 | -5.42 | 48,48,48,48                 | 0     |
| 56  | MG   | 1A    | 3530 | 1/1   | 0.97 | 0.13 | -5.42 | 14,14,14,14                 | 0     |
| 56  | MG   | 1A    | 3134 | 1/1   | 0.96 | 0.12 | -5.43 | 35,35,35,35                 | 0     |
| 56  | MG   | 2a    | 1619 | 1/1   | 0.93 | 0.08 | -5.46 | 46,46,46,46                 | 0     |
| 56  | MG   | 1a    | 1831 | 1/1   | 0.79 | 0.11 | -5.48 | 58,58,58,58                 | 0     |
| 56  | MG   | 1A    | 3515 | 1/1   | 0.79 | 0.17 | -5.49 | 37,37,37,37                 | 0     |
| 56  | MG   | 2A    | 3646 | 1/1   | 0.93 | 0.11 | -5.49 | 39,39,39,39                 | 0     |
| 56  | MG   | 1a    | 1839 | 1/1   | 0.92 | 0.10 | -5.50 | 37,37,37,37                 | 0     |
| 56  | MG   | 2A    | 3560 | 1/1   | 0.98 | 0.11 | -5.50 | 51,51,51,51                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 56  | MG   | 1B    | 3029 | 1/1   | 0.96 | 0.12 | -5.51 | 28,28,28,28                 | 0     |
| 56  | MG   | 2A    | 3548 | 1/1   | 0.91 | 0.10 | -5.52 | 35,35,35,35                 | 0     |
| 56  | MG   | 2A    | 3390 | 1/1   | 0.93 | 0.11 | -5.55 | 30,30,30,30                 | 0     |
| 56  | MG   | 2A    | 3325 | 1/1   | 0.96 | 0.09 | -5.56 | 25,25,25,25                 | 0     |
| 56  | MG   | 1A    | 3496 | 1/1   | 0.96 | 0.16 | -5.56 | 28,28,28,28                 | 0     |
| 56  | MG   | 1A    | 3873 | 1/1   | 0.95 | 0.15 | -5.59 | 39,39,39,39                 | 0     |
| 56  | MG   | 1A    | 3856 | 1/1   | 0.95 | 0.14 | -5.63 | 29,29,29,29                 | 0     |
| 56  | MG   | 2A    | 3469 | 1/1   | 0.92 | 0.09 | -5.63 | 46,46,46,46                 | 0     |
| 56  | MG   | 1A    | 3019 | 1/1   | 0.97 | 0.13 | -5.64 | 27,27,27,27                 | 0     |
| 56  | MG   | 1A    | 3602 | 1/1   | 0.84 | 0.18 | -5.72 | 22,22,22,22                 | 0     |
| 56  | MG   | 1A    | 3188 | 1/1   | 0.95 | 0.13 | -5.72 | 39,39,39,39                 | 0     |
| 56  | MG   | 1a    | 1661 | 1/1   | 0.87 | 0.13 | -5.72 | 56,56,56,56                 | 0     |
| 56  | MG   | 1A    | 3358 | 1/1   | 0.97 | 0.14 | -5.74 | 33,33,33,33                 | 0     |
| 56  | MG   | 2A    | 3479 | 1/1   | 0.98 | 0.11 | -5.80 | 39,39,39,39                 | 0     |
| 56  | MG   | 1F    | 302  | 1/1   | 0.91 | 0.10 | -5.80 | 54,54,54,54                 | 0     |
| 56  | MG   | 1A    | 3442 | 1/1   | 0.97 | 0.16 | -5.81 | 36,36,36,36                 | 0     |
| 56  | MG   | 2A    | 3457 | 1/1   | 0.97 | 0.09 | -5.81 | 48,48,48,48                 | 0     |
| 56  | MG   | 2a    | 1641 | 1/1   | 0.95 | 0.11 | -5.81 | 65,65,65,65                 | 0     |
| 56  | MG   | 1A    | 3748 | 1/1   | 0.94 | 0.13 | -5.82 | 29,29,29,29                 | 0     |
| 56  | MG   | 2A    | 3523 | 1/1   | 0.91 | 0.14 | -5.83 | 54,54,54,54                 | 0     |
| 56  | MG   | 1a    | 1673 | 1/1   | 0.89 | 0.09 | -5.89 | 65,65,65,65                 | 0     |
| 56  | MG   | 2A    | 3358 | 1/1   | 0.96 | 0.10 | -5.89 | 52,52,52,52                 | 0     |
| 56  | MG   | 1A    | 3471 | 1/1   | 0.97 | 0.13 | -5.92 | 26,26,26,26                 | 0     |
| 56  | MG   | 1a    | 1763 | 1/1   | 0.95 | 0.07 | -5.98 | 56,56,56,56                 | 0     |
| 56  | MG   | 1A    | 3928 | 1/1   | 0.98 | 0.13 | -5.99 | 24,24,24,24                 | 0     |
| 56  | MG   | 1A    | 3629 | 1/1   | 0.92 | 0.13 | -6.02 | 42,42,42,42                 | 0     |
| 56  | MG   | 2A    | 3398 | 1/1   | 0.90 | 0.04 | -6.03 | 47,47,47,47                 | 0     |
| 56  | MG   | 2a    | 1717 | 1/1   | 0.92 | 0.15 | -6.07 | 59,59,59,59                 | 0     |
| 56  | MG   | 1A    | 3594 | 1/1   | 0.89 | 0.13 | -6.09 | 35,35,35,35                 | 0     |
| 56  | MG   | 2A    | 3356 | 1/1   | 0.98 | 0.07 | -6.10 | 29,29,29,29                 | 0     |
| 56  | MG   | 1A    | 3172 | 1/1   | 0.99 | 0.12 | -6.12 | 32,32,32,32                 | 0     |
| 56  | MG   | 1A    | 3478 | 1/1   | 0.96 | 0.16 | -6.15 | 20,20,20,20                 | 0     |
| 56  | MG   | 1A    | 3500 | 1/1   | 0.98 | 0.13 | -6.20 | 26,26,26,26                 | 0     |
| 56  | MG   | 2A    | 3157 | 1/1   | 0.98 | 0.10 | -6.22 | 29,29,29,29                 | 0     |
| 56  | MG   | 1A    | 3540 | 1/1   | 0.93 | 0.14 | -6.31 | 33,33,33,33                 | 0     |
| 56  | MG   | 1A    | 3682 | 1/1   | 0.97 | 0.14 | -6.31 | 50,50,50,50                 | 0     |
| 56  | MG   | 2A    | 3502 | 1/1   | 0.97 | 0.05 | -6.32 | 35,35,35,35                 | 0     |
| 56  | MG   | 1A    | 3431 | 1/1   | 0.92 | 0.12 | -6.40 | 45,45,45,45                 | 0     |
| 56  | MG   | 1A    | 3175 | 1/1   | 0.94 | 0.15 | -6.41 | 31,31,31,31                 | 0     |
| 56  | MG   | 1A    | 3445 | 1/1   | 0.96 | 0.11 | -6.42 | 53,53,53,53                 | 0     |
| 56  | MG   | 1A    | 3104 | 1/1   | 0.95 | 0.15 | -6.42 | 33,33,33,33                 | 0     |
| 56  | MG   | 2A    | 3124 | 1/1   | 0.94 | 0.10 | -6.46 | 50,50,50,50                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 56  | MG   | 2a    | 1707 | 1/1   | 0.92 | 0.07 | -6.51 | 60,60,60,60                 | 0     |
| 56  | MG   | 1A    | 3400 | 1/1   | 0.98 | 0.14 | -6.53 | 28,28,28,28                 | 0     |
| 56  | MG   | 1A    | 3480 | 1/1   | 0.94 | 0.16 | -6.53 | 26,26,26,26                 | 0     |
| 56  | MG   | 1A    | 3941 | 1/1   | 0.96 | 0.10 | -6.54 | 43,43,43,43                 | 0     |
| 56  | MG   | 1B    | 3019 | 1/1   | 0.97 | 0.14 | -6.54 | 22,22,22,22                 | 0     |
| 56  | MG   | 1a    | 1631 | 1/1   | 0.95 | 0.14 | -6.63 | 59,59,59,59                 | 0     |
| 56  | MG   | 2A    | 3299 | 1/1   | 0.95 | 0.09 | -6.65 | 36,36,36,36                 | 0     |
| 56  | MG   | 2A    | 3579 | 1/1   | 0.92 | 0.13 | -6.69 | 65,65,65,65                 | 0     |
| 56  | MG   | 2A    | 3552 | 1/1   | 0.97 | 0.10 | -6.70 | 57,57,57,57                 | 0     |
| 56  | MG   | 1T    | 203  | 1/1   | 0.93 | 0.09 | -6.76 | 42,42,42,42                 | 0     |
| 56  | MG   | 1A    | 3031 | 1/1   | 0.94 | 0.14 | -6.76 | 31,31,31,31                 | 0     |
| 56  | MG   | 1A    | 3751 | 1/1   | 0.74 | 0.11 | -6.77 | 63,63,63,63                 | 0     |
| 56  | MG   | 2A    | 3078 | 1/1   | 0.92 | 0.14 | -6.77 | 47,47,47,47                 | 0     |
| 56  | MG   | 2A    | 3297 | 1/1   | 0.86 | 0.15 | -6.79 | 32,32,32,32                 | 0     |
| 56  | MG   | 2A    | 3238 | 1/1   | 0.91 | 0.10 | -6.83 | 42,42,42,42                 | 0     |
| 56  | MG   | 1a    | 1670 | 1/1   | 0.92 | 0.15 | -6.84 | 40,40,40,40                 | 0     |
| 56  | MG   | 2A    | 3030 | 1/1   | 0.97 | 0.11 | -6.88 | 28,28,28,28                 | 0     |
| 56  | MG   | 1A    | 3862 | 1/1   | 0.99 | 0.11 | -6.88 | 19,19,19,19                 | 0     |
| 56  | MG   | 1A    | 3386 | 1/1   | 0.96 | 0.16 | -6.92 | 42,42,42,42                 | 0     |
| 56  | MG   | 2A    | 3508 | 1/1   | 0.97 | 0.09 | -6.92 | 38,38,38,38                 | 0     |
| 56  | MG   | 1A    | 3421 | 1/1   | 0.88 | 0.08 | -7.01 | 60,60,60,60                 | 0     |
| 56  | MG   | 2A    | 3393 | 1/1   | 0.90 | 0.09 | -7.03 | 21,21,21,21                 | 0     |
| 56  | MG   | 2A    | 3258 | 1/1   | 0.98 | 0.06 | -7.04 | 35,35,35,35                 | 0     |
| 56  | MG   | 1A    | 3871 | 1/1   | 0.96 | 0.16 | -7.23 | 18,18,18,18                 | 0     |
| 56  | MG   | 2A    | 3572 | 1/1   | 0.98 | 0.09 | -7.27 | 43,43,43,43                 | 0     |
| 56  | MG   | 2A    | 3228 | 1/1   | 0.93 | 0.11 | -7.29 | 43,43,43,43                 | 0     |
| 56  | MG   | 2A    | 3031 | 1/1   | 0.97 | 0.07 | -7.31 | 24,24,24,24                 | 0     |
| 56  | MG   | 2A    | 3273 | 1/1   | 0.96 | 0.12 | -7.38 | 35,35,35,35                 | 0     |
| 56  | MG   | 1A    | 3793 | 1/1   | 0.89 | 0.17 | -7.47 | 28,28,28,28                 | 0     |
| 56  | MG   | 2A    | 3447 | 1/1   | 0.95 | 0.07 | -7.62 | 46,46,46,46                 | 0     |
| 56  | MG   | 1A    | 3565 | 1/1   | 0.97 | 0.14 | -7.76 | 28,28,28,28                 | 0     |
| 56  | MG   | 1A    | 3204 | 1/1   | 0.96 | 0.15 | -7.87 | 24,24,24,24                 | 0     |
| 56  | MG   | 1A    | 3482 | 1/1   | 0.93 | 0.14 | -7.90 | 27,27,27,27                 | 0     |
| 56  | MG   | 2A    | 3265 | 1/1   | 0.98 | 0.11 | -7.92 | 51,51,51,51                 | 0     |
| 56  | MG   | 1A    | 3070 | 1/1   | 0.90 | 0.11 | -7.95 | 33,33,33,33                 | 0     |
| 56  | MG   | 1A    | 3517 | 1/1   | 0.98 | 0.12 | -8.00 | 9,9,9,9                     | 0     |
| 56  | MG   | 1A    | 3369 | 1/1   | 0.91 | 0.14 | -8.10 | 40,40,40,40                 | 0     |
| 56  | MG   | 1A    | 3651 | 1/1   | 0.94 | 0.13 | -8.33 | 41,41,41,41                 | 0     |
| 56  | MG   | 1A    | 3567 | 1/1   | 0.98 | 0.13 | -8.35 | 15,15,15,15                 | 0     |
| 56  | MG   | 1A    | 3690 | 1/1   | 0.96 | 0.11 | -8.36 | 48,48,48,48                 | 0     |
| 56  | MG   | 1A    | 3587 | 1/1   | 0.95 | 0.15 | -8.39 | 25,25,25,25                 | 0     |
| 56  | MG   | 1a    | 1615 | 1/1   | 0.95 | 0.11 | -8.41 | 65,65,65,65                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF   | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|--------|-----------------------------|-------|
| 56  | MG   | 1A    | 3436 | 1/1   | 0.95 | 0.15 | -8.48  | 31,31,31,31                 | 0     |
| 56  | MG   | 1A    | 3363 | 1/1   | 0.85 | 0.15 | -8.63  | 58,58,58,58                 | 0     |
| 56  | MG   | 2A    | 3673 | 1/1   | 0.96 | 0.12 | -8.65  | 33,33,33,33                 | 0     |
| 56  | MG   | 1A    | 3861 | 1/1   | 0.91 | 0.11 | -8.80  | 26,26,26,26                 | 0     |
| 56  | MG   | 2A    | 3432 | 1/1   | 0.98 | 0.12 | -8.88  | 36,36,36,36                 | 0     |
| 56  | MG   | 1a    | 1652 | 1/1   | 0.92 | 0.12 | -9.05  | 51,51,51,51                 | 0     |
| 56  | MG   | 2A    | 3323 | 1/1   | 0.88 | 0.09 | -9.08  | 47,47,47,47                 | 0     |
| 56  | MG   | 1A    | 3430 | 1/1   | 0.96 | 0.10 | -9.11  | 21,21,21,21                 | 0     |
| 56  | MG   | 1A    | 3248 | 1/1   | 0.88 | 0.10 | -9.11  | 32,32,32,32                 | 0     |
| 56  | MG   | 2a    | 1727 | 1/1   | 0.95 | 0.09 | -9.22  | 62,62,62,62                 | 0     |
| 56  | MG   | 2A    | 3365 | 1/1   | 0.94 | 0.09 | -9.30  | 29,29,29,29                 | 0     |
| 56  | MG   | 2A    | 3007 | 1/1   | 0.95 | 0.12 | -9.32  | 38,38,38,38                 | 0     |
| 56  | MG   | 1A    | 3419 | 1/1   | 0.90 | 0.15 | -9.49  | 43,43,43,43                 | 0     |
| 56  | MG   | 1A    | 3160 | 1/1   | 0.98 | 0.13 | -9.83  | 26,26,26,26                 | 0     |
| 56  | MG   | 2A    | 3196 | 1/1   | 0.96 | 0.10 | -9.84  | 35,35,35,35                 | 0     |
| 56  | MG   | 1A    | 3865 | 1/1   | 0.92 | 0.13 | -9.91  | 41,41,41,41                 | 0     |
| 56  | MG   | 1A    | 3020 | 1/1   | 0.91 | 0.11 | -10.06 | 23,23,23,23                 | 0     |
| 56  | MG   | 2A    | 3314 | 1/1   | 0.96 | 0.15 | -10.10 | 40,40,40,40                 | 0     |
| 56  | MG   | 1A    | 3615 | 1/1   | 0.97 | 0.12 | -10.11 | 45,45,45,45                 | 0     |
| 56  | MG   | 1a    | 1815 | 1/1   | 0.82 | 0.08 | -10.26 | 76,76,76,76                 | 0     |
| 56  | MG   | 1A    | 3206 | 1/1   | 0.93 | 0.15 | -10.34 | 36,36,36,36                 | 0     |
| 56  | MG   | 2A    | 3152 | 1/1   | 0.96 | 0.12 | -10.41 | 32,32,32,32                 | 0     |
| 56  | MG   | 1a    | 1690 | 1/1   | 0.92 | 0.14 | -10.46 | 47,47,47,47                 | 0     |
| 56  | MG   | 1A    | 3642 | 1/1   | 0.86 | 0.12 | -10.85 | 39,39,39,39                 | 0     |
| 56  | MG   | 2A    | 3510 | 1/1   | 0.95 | 0.11 | -10.94 | 31,31,31,31                 | 0     |
| 56  | MG   | 1a    | 1715 | 1/1   | 0.94 | 0.13 | -10.98 | 51,51,51,51                 | 0     |
| 56  | MG   | 1A    | 3580 | 1/1   | 0.97 | 0.11 | -11.00 | 32,32,32,32                 | 0     |
| 56  | MG   | 1A    | 3044 | 1/1   | 0.91 | 0.13 | -11.02 | 23,23,23,23                 | 0     |
| 56  | MG   | 2A    | 3442 | 1/1   | 0.94 | 0.08 | -11.23 | 46,46,46,46                 | 0     |
| 56  | MG   | 2A    | 3224 | 1/1   | 0.89 | 0.10 | -11.33 | 46,46,46,46                 | 0     |
| 56  | MG   | 1a    | 1610 | 1/1   | 0.97 | 0.10 | -11.42 | 22,22,22,22                 | 0     |
| 56  | MG   | 1a    | 1660 | 1/1   | 0.94 | 0.13 | -11.55 | 47,47,47,47                 | 0     |
| 56  | MG   | 2A    | 3332 | 1/1   | 0.92 | 0.06 | -12.42 | 37,37,37,37                 | 0     |
| 56  | MG   | 1A    | 3207 | 1/1   | 0.84 | 0.12 | -12.45 | 52,52,52,52                 | 0     |
| 56  | MG   | 1a    | 1738 | 1/1   | 0.94 | 0.05 | -12.51 | 43,43,43,43                 | 0     |
| 56  | MG   | 1A    | 3685 | 1/1   | 0.95 | 0.14 | -12.54 | 26,26,26,26                 | 0     |
| 56  | MG   | 1A    | 3654 | 1/1   | 0.97 | 0.10 | -12.64 | 40,40,40,40                 | 0     |
| 56  | MG   | 2A    | 3366 | 1/1   | 0.89 | 0.11 | -12.78 | 41,41,41,41                 | 0     |
| 56  | MG   | 1A    | 3001 | 1/1   | 0.97 | 0.10 | -12.87 | 33,33,33,33                 | 0     |
| 56  | MG   | 1A    | 3650 | 1/1   | 0.98 | 0.14 | -12.98 | 31,31,31,31                 | 0     |
| 56  | MG   | 1A    | 3644 | 1/1   | 0.86 | 0.07 | -13.18 | 57,57,57,57                 | 0     |
| 56  | MG   | 2A    | 3089 | 1/1   | 0.97 | 0.10 | -14.52 | 27,27,27,27                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF   | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|--------|-----------------------------|-------|
| 56  | MG   | 2A    | 3306 | 1/1   | 0.94 | 0.11 | -14.76 | 33,33,33,33                 | 0     |
| 56  | MG   | 1A    | 3111 | 1/1   | 0.95 | 0.15 | -15.59 | 40,40,40,40                 | 0     |
| 56  | MG   | 1A    | 3576 | 1/1   | 0.97 | 0.10 | -16.60 | 41,41,41,41                 | 0     |
| 56  | MG   | 1A    | 3518 | 1/1   | 0.95 | 0.17 | -16.66 | 40,40,40,40                 | 0     |
| 56  | MG   | 1A    | 3388 | 1/1   | 0.94 | 0.12 | -17.48 | 49,49,49,49                 | 0     |
| 56  | MG   | 2A    | 3511 | 1/1   | 0.95 | 0.11 | -17.95 | 68,68,68,68                 | 0     |
| 56  | MG   | 1a    | 1804 | 1/1   | 0.94 | 0.09 | -19.03 | 65,65,65,65                 | 0     |
| 56  | MG   | 1A    | 3561 | 1/1   | 0.96 | 0.16 | -      | 54,54,54,54                 | 0     |
| 56  | MG   | 1a    | 1612 | 1/1   | 0.74 | 0.17 | -      | 63,63,63,63                 | 0     |
| 56  | MG   | 2A    | 3627 | 1/1   | 0.94 | 0.11 | -      | 56,56,56,56                 | 0     |
| 56  | MG   | 1A    | 3586 | 1/1   | 0.99 | 0.17 | -      | 41,41,41,41                 | 0     |
| 56  | MG   | 2A    | 3453 | 1/1   | 0.96 | 0.10 | -      | 37,37,37,37                 | 0     |
| 56  | MG   | 2A    | 3415 | 1/1   | 0.99 | 0.16 | -      | 30,30,30,30                 | 0     |
| 56  | MG   | 2A    | 3295 | 1/1   | 0.95 | 0.11 | -      | 39,39,39,39                 | 0     |
| 56  | MG   | 2A    | 3412 | 1/1   | 0.92 | 0.17 | -      | 40,40,40,40                 | 0     |
| 56  | MG   | 1a    | 1793 | 1/1   | 0.93 | 0.09 | -      | 45,45,45,45                 | 0     |
| 56  | MG   | 1A    | 3374 | 1/1   | 0.89 | 0.13 | -      | 47,47,47,47                 | 0     |
| 56  | MG   | 2a    | 1793 | 1/1   | 0.94 | 0.13 | -      | 41,41,41,41                 | 0     |
| 56  | MG   | 2A    | 3293 | 1/1   | 0.94 | 0.09 | -      | 33,33,33,33                 | 0     |
| 56  | MG   | 1A    | 3425 | 1/1   | 0.98 | 0.17 | -      | 36,36,36,36                 | 0     |
| 56  | MG   | 1A    | 3139 | 1/1   | 0.95 | 0.17 | -      | 33,33,33,33                 | 0     |
| 56  | MG   | 1A    | 3698 | 1/1   | 0.92 | 0.21 | -      | 43,43,43,43                 | 0     |
| 56  | MG   | 1A    | 3554 | 1/1   | 0.94 | 0.27 | -      | 32,32,32,32                 | 0     |
| 56  | MG   | 2A    | 3341 | 1/1   | 0.91 | 0.19 | -      | 45,45,45,45                 | 0     |
| 56  | MG   | 1A    | 3641 | 1/1   | 0.90 | 0.26 | -      | 35,35,35,35                 | 0     |
| 56  | MG   | 1A    | 3608 | 1/1   | 0.81 | 0.15 | -      | 40,40,40,40                 | 0     |
| 56  | MG   | 1a    | 1696 | 1/1   | 0.89 | 0.15 | -      | 66,66,66,66                 | 0     |
| 56  | MG   | 1A    | 3305 | 1/1   | 0.93 | 0.17 | -      | 42,42,42,42                 | 0     |
| 56  | MG   | 1A    | 3525 | 1/1   | 0.90 | 0.09 | -      | 53,53,53,53                 | 0     |
| 56  | MG   | 2A    | 3578 | 1/1   | 0.74 | 0.30 | -      | 65,65,65,65                 | 0     |
| 56  | MG   | 1A    | 3291 | 1/1   | 0.95 | 0.27 | -      | 28,28,28,28                 | 0     |
| 56  | MG   | 2A    | 3222 | 1/1   | 0.78 | 0.17 | -      | 47,47,47,47                 | 0     |
| 56  | MG   | 2A    | 3631 | 1/1   | 0.95 | 0.14 | -      | 51,51,51,51                 | 0     |
| 56  | MG   | 2a    | 1725 | 1/1   | 0.88 | 0.07 | -      | 69,69,69,69                 | 0     |
| 56  | MG   | 1a    | 1651 | 1/1   | 0.75 | 0.21 | -      | 62,62,62,62                 | 0     |
| 56  | MG   | 1A    | 3244 | 1/1   | 0.85 | 0.34 | -      | 39,39,39,39                 | 0     |
| 56  | MG   | 2A    | 3308 | 1/1   | 0.92 | 0.08 | -      | 45,45,45,45                 | 0     |
| 56  | MG   | 2A    | 3586 | 1/1   | 0.98 | 0.11 | -      | 44,44,44,44                 | 0     |
| 56  | MG   | 1A    | 3782 | 1/1   | 0.93 | 0.16 | -      | 34,34,34,34                 | 0     |
| 56  | MG   | 2A    | 3133 | 1/1   | 0.93 | 0.17 | -      | 49,49,49,49                 | 0     |
| 56  | MG   | 1A    | 3145 | 1/1   | 0.93 | 0.28 | -      | 36,36,36,36                 | 0     |
| 56  | MG   | 2A    | 3339 | 1/1   | 0.93 | 0.16 | -      | 38,38,38,38                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56  | MG   | 1A    | 3707 | 1/1   | 0.95 | 0.16 | -    | 54,54,54,54                 | 0     |
| 56  | MG   | 2A    | 3375 | 1/1   | 0.92 | 0.10 | -    | 53,53,53,53                 | 0     |
| 56  | MG   | 1B    | 3002 | 1/1   | 0.89 | 0.19 | -    | 48,48,48,48                 | 0     |
| 56  | MG   | 2a    | 1723 | 1/1   | 0.95 | 0.07 | -    | 54,54,54,54                 | 0     |
| 56  | MG   | 1A    | 3274 | 1/1   | 0.94 | 0.28 | -    | 66,66,66,66                 | 0     |
| 56  | MG   | 2A    | 3067 | 1/1   | 0.93 | 0.09 | -    | 32,32,32,32                 | 0     |
| 56  | MG   | 2a    | 1718 | 1/1   | 0.91 | 0.09 | -    | 51,51,51,51                 | 0     |
| 56  | MG   | 1A    | 3130 | 1/1   | 0.94 | 0.12 | -    | 50,50,50,50                 | 0     |
| 56  | MG   | 1A    | 3150 | 1/1   | 0.90 | 0.29 | -    | 41,41,41,41                 | 0     |
| 56  | MG   | 2A    | 3362 | 1/1   | 0.98 | 0.19 | -    | 44,44,44,44                 | 0     |
| 56  | MG   | 1A    | 3798 | 1/1   | 0.92 | 0.11 | -    | 43,43,43,43                 | 0     |
| 56  | MG   | 1A    | 3052 | 1/1   | 0.93 | 0.21 | -    | 39,39,39,39                 | 0     |
| 56  | MG   | 1A    | 3761 | 1/1   | 0.83 | 0.13 | -    | 56,56,56,56                 | 0     |
| 56  | MG   | 1a    | 1811 | 1/1   | 0.95 | 0.22 | -    | 57,57,57,57                 | 0     |
| 56  | MG   | 1A    | 3541 | 1/1   | 0.96 | 0.08 | -    | 42,42,42,42                 | 0     |
| 56  | MG   | 1a    | 1714 | 1/1   | 0.97 | 0.23 | -    | 42,42,42,42                 | 0     |
| 56  | MG   | 1A    | 3355 | 1/1   | 0.97 | 0.22 | -    | 46,46,46,46                 | 0     |
| 56  | MG   | 1G    | 204  | 1/1   | 0.99 | 0.03 | -    | 48,48,48,48                 | 0     |
| 56  | MG   | 1A    | 3864 | 1/1   | 0.97 | 0.09 | -    | 38,38,38,38                 | 0     |
| 56  | MG   | 1A    | 3259 | 1/1   | 0.87 | 0.16 | -    | 61,61,61,61                 | 0     |
| 56  | MG   | 1A    | 3116 | 1/1   | 0.81 | 0.28 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | 1A    | 3831 | 1/1   | 0.95 | 0.25 | -    | 62,62,62,62                 | 0     |
| 56  | MG   | 1A    | 3640 | 1/1   | 0.93 | 0.20 | -    | 21,21,21,21                 | 0     |
| 56  | MG   | 2A    | 3227 | 1/1   | 0.84 | 0.16 | -    | 48,48,48,48                 | 0     |
| 56  | MG   | 2A    | 3320 | 1/1   | 0.89 | 0.13 | -    | 42,42,42,42                 | 0     |
| 56  | MG   | 1A    | 3304 | 1/1   | 0.96 | 0.12 | -    | 48,48,48,48                 | 0     |
| 56  | MG   | 1A    | 3455 | 1/1   | 0.94 | 0.14 | -    | 45,45,45,45                 | 0     |
| 56  | MG   | 2A    | 3547 | 1/1   | 0.90 | 0.17 | -    | 37,37,37,37                 | 0     |
| 56  | MG   | 1A    | 3239 | 1/1   | 0.85 | 0.13 | -    | 56,56,56,56                 | 0     |
| 56  | MG   | 2A    | 3500 | 1/1   | 0.96 | 0.11 | -    | 38,38,38,38                 | 0     |
| 56  | MG   | 1x    | 3007 | 1/1   | 0.96 | 0.28 | -    | 51,51,51,51                 | 0     |
| 56  | MG   | 2a    | 1636 | 1/1   | 0.97 | 0.08 | -    | 60,60,60,60                 | 0     |
| 56  | MG   | 2A    | 3507 | 1/1   | 0.96 | 0.16 | -    | 19,19,19,19                 | 0     |
| 56  | MG   | 2A    | 3408 | 1/1   | 0.94 | 0.08 | -    | 50,50,50,50                 | 0     |
| 56  | MG   | 2A    | 3214 | 1/1   | 0.88 | 0.23 | -    | 41,41,41,41                 | 0     |
| 56  | MG   | 2A    | 3161 | 1/1   | 0.96 | 0.25 | -    | 49,49,49,49                 | 0     |
| 56  | MG   | 1A    | 3545 | 1/1   | 0.98 | 0.08 | -    | 57,57,57,57                 | 0     |
| 56  | MG   | 1A    | 3818 | 1/1   | 0.95 | 0.16 | -    | 30,30,30,30                 | 0     |
| 56  | MG   | 2A    | 3454 | 1/1   | 0.99 | 0.09 | -    | 36,36,36,36                 | 0     |
| 56  | MG   | 2B    | 3003 | 1/1   | 0.86 | 0.17 | -    | 48,48,48,48                 | 0     |
| 56  | MG   | 1B    | 3010 | 1/1   | 0.83 | 0.11 | -    | 68,68,68,68                 | 0     |
| 56  | MG   | 2a    | 1764 | 1/1   | 0.92 | 0.17 | -    | 53,53,53,53                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56  | MG   | 2a    | 1684 | 1/1   | 0.95 | 0.31 | -    | 48,48,48,48                 | 0     |
| 56  | MG   | 1A    | 3904 | 1/1   | 0.87 | 0.13 | -    | 55,55,55,55                 | 0     |
| 56  | MG   | 2B    | 3001 | 1/1   | 0.78 | 0.27 | -    | 69,69,69,69                 | 0     |
| 56  | MG   | 1A    | 3437 | 1/1   | 0.92 | 0.15 | -    | 28,28,28,28                 | 0     |
| 56  | MG   | 2A    | 3562 | 1/1   | 0.98 | 0.14 | -    | 42,42,42,42                 | 0     |
| 56  | MG   | 2A    | 3266 | 1/1   | 0.93 | 0.13 | -    | 34,34,34,34                 | 0     |
| 56  | MG   | 1F    | 306  | 1/1   | 0.79 | 0.18 | -    | 46,46,46,46                 | 0     |
| 56  | MG   | 1A    | 3448 | 1/1   | 0.96 | 0.11 | -    | 57,57,57,57                 | 0     |
| 56  | MG   | 1A    | 3843 | 1/1   | 0.95 | 0.17 | -    | 33,33,33,33                 | 0     |
| 56  | MG   | 2A    | 3336 | 1/1   | 0.99 | 0.09 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | 2A    | 3247 | 1/1   | 0.94 | 0.12 | -    | 51,51,51,51                 | 0     |
| 56  | MG   | 2E    | 305  | 1/1   | 0.98 | 0.13 | -    | 39,39,39,39                 | 0     |
| 56  | MG   | 1A    | 3542 | 1/1   | 0.94 | 0.14 | -    | 52,52,52,52                 | 0     |
| 56  | MG   | 2a    | 1630 | 1/1   | 0.98 | 0.21 | -    | 55,55,55,55                 | 0     |
| 56  | MG   | 1l    | 203  | 1/1   | 0.87 | 0.17 | -    | 58,58,58,58                 | 0     |
| 56  | MG   | 2a    | 1673 | 1/1   | 0.90 | 0.26 | -    | 60,60,60,60                 | 0     |
| 56  | MG   | 2A    | 3625 | 1/1   | 0.92 | 0.08 | -    | 56,56,56,56                 | 0     |
| 56  | MG   | 2a    | 1602 | 1/1   | 0.98 | 0.25 | -    | 60,60,60,60                 | 0     |
| 56  | MG   | 1A    | 3538 | 1/1   | 0.97 | 0.14 | -    | 40,40,40,40                 | 0     |
| 56  | MG   | 2A    | 3529 | 1/1   | 0.89 | 0.22 | -    | 57,57,57,57                 | 0     |
| 56  | MG   | 1A    | 3078 | 1/1   | 0.97 | 0.25 | -    | 38,38,38,38                 | 0     |
| 56  | MG   | 1B    | 3016 | 1/1   | 0.93 | 0.19 | -    | 61,61,61,61                 | 0     |
| 56  | MG   | 1A    | 3874 | 1/1   | 0.86 | 0.19 | -    | 63,63,63,63                 | 0     |
| 56  | MG   | 1A    | 3211 | 1/1   | 0.93 | 0.17 | -    | 38,38,38,38                 | 0     |
| 56  | MG   | 2A    | 3582 | 1/1   | 0.93 | 0.14 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | 1A    | 3820 | 1/1   | 0.98 | 0.21 | -    | 45,45,45,45                 | 0     |
| 56  | MG   | 1A    | 3742 | 1/1   | 0.85 | 0.22 | -    | 37,37,37,37                 | 0     |
| 56  | MG   | 1A    | 3196 | 1/1   | 0.89 | 0.15 | -    | 52,52,52,52                 | 0     |
| 56  | MG   | 1A    | 3806 | 1/1   | 0.87 | 0.12 | -    | 73,73,73,73                 | 0     |
| 56  | MG   | 1A    | 3307 | 1/1   | 0.94 | 0.17 | -    | 55,55,55,55                 | 0     |
| 56  | MG   | 1U    | 204  | 1/1   | 0.94 | 0.20 | -    | 44,44,44,44                 | 0     |
| 56  | MG   | 2A    | 3036 | 1/1   | 0.95 | 0.20 | -    | 43,43,43,43                 | 0     |
| 56  | MG   | 2a    | 1680 | 1/1   | 0.82 | 0.15 | -    | 73,73,73,73                 | 0     |
| 56  | MG   | 1A    | 3278 | 1/1   | 0.91 | 0.18 | -    | 60,60,60,60                 | 0     |
| 56  | MG   | 2A    | 3384 | 1/1   | 0.97 | 0.10 | -    | 39,39,39,39                 | 0     |
| 56  | MG   | 1a    | 1764 | 1/1   | 0.93 | 0.12 | -    | 38,38,38,38                 | 0     |
| 56  | MG   | 2O    | 8002 | 1/1   | 0.68 | 1.29 | -    | 112,112,112,112             | 0     |
| 56  | MG   | 2A    | 3444 | 1/1   | 0.96 | 0.21 | -    | 50,50,50,50                 | 0     |
| 56  | MG   | 1A    | 3551 | 1/1   | 0.98 | 0.18 | -    | 26,26,26,26                 | 0     |
| 56  | MG   | 1A    | 3232 | 1/1   | 0.94 | 0.12 | -    | 49,49,49,49                 | 0     |
| 56  | MG   | 1A    | 3581 | 1/1   | 0.93 | 0.21 | -    | 50,50,50,50                 | 0     |
| 56  | MG   | 2A    | 3612 | 1/1   | 0.96 | 0.13 | -    | 57,57,57,57                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56  | MG   | 1a    | 1825 | 1/1   | 0.96 | 0.11 | -    | 46,46,46,46                 | 0     |
| 56  | MG   | 2A    | 3260 | 1/1   | 0.94 | 0.10 | -    | 52,52,52,52                 | 0     |
| 56  | MG   | 1A    | 3230 | 1/1   | 0.87 | 0.17 | -    | 39,39,39,39                 | 0     |
| 56  | MG   | 2A    | 3630 | 1/1   | 0.97 | 0.12 | -    | 41,41,41,41                 | 0     |
| 56  | MG   | 1a    | 1662 | 1/1   | 0.98 | 0.22 | -    | 51,51,51,51                 | 0     |
| 56  | MG   | 1A    | 3568 | 1/1   | 0.95 | 0.21 | -    | 53,53,53,53                 | 0     |
| 56  | MG   | 1a    | 1823 | 1/1   | 0.95 | 0.10 | -    | 58,58,58,58                 | 0     |
| 56  | MG   | 2A    | 3514 | 1/1   | 0.78 | 0.17 | -    | 59,59,59,59                 | 0     |
| 56  | MG   | 2A    | 3593 | 1/1   | 0.91 | 0.28 | -    | 56,56,56,56                 | 0     |
| 56  | MG   | 1A    | 3716 | 1/1   | 0.95 | 0.36 | -    | 59,59,59,59                 | 0     |
| 56  | MG   | 1A    | 3069 | 1/1   | 0.96 | 0.13 | -    | 27,27,27,27                 | 0     |
| 56  | MG   | 1A    | 3771 | 1/1   | 0.95 | 0.20 | -    | 39,39,39,39                 | 0     |
| 56  | MG   | 2A    | 3399 | 1/1   | 0.87 | 0.16 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | 1A    | 3059 | 1/1   | 0.93 | 0.18 | -    | 50,50,50,50                 | 0     |
| 56  | MG   | 2a    | 1676 | 1/1   | 0.97 | 0.21 | -    | 40,40,40,40                 | 0     |
| 56  | MG   | 1A    | 3186 | 1/1   | 0.98 | 0.35 | -    | 56,56,56,56                 | 0     |
| 56  | MG   | 2A    | 3503 | 1/1   | 0.94 | 0.11 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | 1A    | 3361 | 1/1   | 0.96 | 0.11 | -    | 33,33,33,33                 | 0     |
| 56  | MG   | 1A    | 3053 | 1/1   | 0.87 | 0.23 | -    | 52,52,52,52                 | 0     |
| 56  | MG   | 2A    | 3651 | 1/1   | 0.81 | 0.14 | -    | 55,55,55,55                 | 0     |
| 56  | MG   | 2a    | 1736 | 1/1   | 0.83 | 0.10 | -    | 68,68,68,68                 | 0     |
| 56  | MG   | 1A    | 3724 | 1/1   | 0.97 | 0.18 | -    | 23,23,23,23                 | 0     |
| 56  | MG   | 1A    | 3366 | 1/1   | 0.94 | 0.14 | -    | 61,61,61,61                 | 0     |
| 56  | MG   | 2A    | 3209 | 1/1   | 0.93 | 0.08 | -    | 41,41,41,41                 | 0     |
| 56  | MG   | 13    | 103  | 1/1   | 0.92 | 0.15 | -    | 50,50,50,50                 | 0     |
| 56  | MG   | 2A    | 3555 | 1/1   | 0.95 | 0.12 | -    | 53,53,53,53                 | 0     |
| 56  | MG   | 2a    | 1748 | 1/1   | 0.90 | 0.12 | -    | 77,77,77,77                 | 0     |
| 56  | MG   | 2A    | 3135 | 1/1   | 0.94 | 0.17 | -    | 33,33,33,33                 | 0     |
| 56  | MG   | 2a    | 1624 | 1/1   | 0.89 | 0.26 | -    | 54,54,54,54                 | 0     |
| 56  | MG   | 1A    | 3332 | 1/1   | 0.94 | 0.17 | -    | 31,31,31,31                 | 0     |
| 56  | MG   | 1A    | 3270 | 1/1   | 0.92 | 0.18 | -    | 57,57,57,57                 | 0     |
| 56  | MG   | 1a    | 1759 | 1/1   | 0.90 | 0.13 | -    | 57,57,57,57                 | 0     |
| 56  | MG   | 1A    | 3638 | 1/1   | 0.93 | 0.18 | -    | 27,27,27,27                 | 0     |
| 56  | MG   | 1d    | 502  | 1/1   | 0.92 | 0.18 | -    | 51,51,51,51                 | 0     |
| 56  | MG   | 1A    | 3880 | 1/1   | 0.83 | 0.12 | -    | 37,37,37,37                 | 0     |
| 56  | MG   | 1A    | 3733 | 1/1   | 0.96 | 0.15 | -    | 25,25,25,25                 | 0     |
| 56  | MG   | 1A    | 3661 | 1/1   | 0.97 | 0.20 | -    | 45,45,45,45                 | 0     |
| 56  | MG   | 2A    | 3367 | 1/1   | 0.94 | 0.22 | -    | 42,42,42,42                 | 0     |
| 56  | MG   | 1A    | 3749 | 1/1   | 0.94 | 0.14 | -    | 52,52,52,52                 | 0     |
| 56  | MG   | 2A    | 3075 | 1/1   | 0.77 | 0.27 | -    | 41,41,41,41                 | 0     |
| 56  | MG   | 2A    | 3003 | 1/1   | 0.93 | 0.10 | -    | 43,43,43,43                 | 0     |
| 56  | MG   | 2A    | 3493 | 1/1   | 0.84 | 0.12 | -    | 62,62,62,62                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56  | MG   | 1A    | 3450 | 1/1   | 0.97 | 0.13 | -    | 42,42,42,42                 | 0     |
| 56  | MG   | 1a    | 1710 | 1/1   | 0.91 | 0.16 | -    | 61,61,61,61                 | 0     |
| 56  | MG   | 2A    | 3410 | 1/1   | 0.98 | 0.10 | -    | 43,43,43,43                 | 0     |
| 56  | MG   | 1A    | 3310 | 1/1   | 0.95 | 0.13 | -    | 54,54,54,54                 | 0     |
| 56  | MG   | 1A    | 3725 | 1/1   | 0.95 | 0.15 | -    | 28,28,28,28                 | 0     |
| 56  | MG   | 1A    | 3136 | 1/1   | 0.96 | 0.12 | -    | 39,39,39,39                 | 0     |
| 56  | MG   | 2A    | 3438 | 1/1   | 0.90 | 0.15 | -    | 44,44,44,44                 | 0     |
| 56  | MG   | 1A    | 3872 | 1/1   | 0.79 | 0.11 | -    | 50,50,50,50                 | 0     |
| 56  | MG   | 1x    | 3006 | 1/1   | 0.93 | 0.13 | -    | 51,51,51,51                 | 0     |
| 56  | MG   | 20    | 103  | 1/1   | 0.91 | 0.08 | -    | 49,49,49,49                 | 0     |
| 56  | MG   | 2A    | 3667 | 1/1   | 0.83 | 0.14 | -    | 53,53,53,53                 | 0     |
| 56  | MG   | 1a    | 1635 | 1/1   | 0.89 | 0.31 | -    | 50,50,50,50                 | 0     |
| 56  | MG   | 1A    | 3627 | 1/1   | 0.94 | 0.07 | -    | 44,44,44,44                 | 0     |
| 56  | MG   | 2A    | 3230 | 1/1   | 0.87 | 0.22 | -    | 57,57,57,57                 | 0     |
| 56  | MG   | 1A    | 3364 | 1/1   | 0.96 | 0.16 | -    | 55,55,55,55                 | 0     |
| 56  | MG   | 2a    | 1642 | 1/1   | 0.74 | 0.16 | -    | 66,66,66,66                 | 0     |
| 56  | MG   | 1A    | 3260 | 1/1   | 0.89 | 0.15 | -    | 40,40,40,40                 | 0     |
| 56  | MG   | 2B    | 3002 | 1/1   | 0.89 | 0.17 | -    | 55,55,55,55                 | 0     |
| 56  | MG   | 2A    | 3595 | 1/1   | 0.98 | 0.08 | -    | 57,57,57,57                 | 0     |
| 56  | MG   | 2A    | 3020 | 1/1   | 0.97 | 0.08 | -    | 43,43,43,43                 | 0     |
| 56  | MG   | 1A    | 3349 | 1/1   | 0.91 | 0.30 | -    | 38,38,38,38                 | 0     |
| 56  | MG   | 2A    | 3156 | 1/1   | 0.98 | 0.24 | -    | 31,31,31,31                 | 0     |
| 56  | MG   | 1A    | 3867 | 1/1   | 0.97 | 0.09 | -    | 31,31,31,31                 | 0     |
| 56  | MG   | 1W    | 3002 | 1/1   | 0.94 | 0.17 | -    | 49,49,49,49                 | 0     |
| 56  | MG   | 2w    | 3001 | 1/1   | 0.88 | 0.20 | -    | 67,67,67,67                 | 0     |
| 56  | MG   | 1A    | 3079 | 1/1   | 0.97 | 0.35 | -    | 30,30,30,30                 | 0     |
| 56  | MG   | 1A    | 3303 | 1/1   | 0.91 | 0.15 | -    | 34,34,34,34                 | 0     |
| 56  | MG   | 1A    | 3681 | 1/1   | 0.94 | 0.11 | -    | 32,32,32,32                 | 0     |
| 56  | MG   | 2A    | 3262 | 1/1   | 0.96 | 0.14 | -    | 41,41,41,41                 | 0     |
| 56  | MG   | 2a    | 1744 | 1/1   | 0.97 | 0.11 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | 1A    | 3072 | 1/1   | 0.96 | 0.17 | -    | 40,40,40,40                 | 0     |
| 56  | MG   | 1a    | 1824 | 1/1   | 0.94 | 0.17 | -    | 48,48,48,48                 | 0     |
| 56  | MG   | 1a    | 1746 | 1/1   | 0.64 | 0.12 | -    | 85,85,85,85                 | 0     |
| 56  | MG   | 2A    | 3329 | 1/1   | 0.98 | 0.07 | -    | 43,43,43,43                 | 0     |
| 56  | MG   | 1a    | 1702 | 1/1   | 0.89 | 0.26 | -    | 60,60,60,60                 | 0     |
| 56  | MG   | 18    | 102  | 1/1   | 0.96 | 0.17 | -    | 33,33,33,33                 | 0     |
| 56  | MG   | 1A    | 3387 | 1/1   | 0.96 | 0.13 | -    | 38,38,38,38                 | 0     |
| 56  | MG   | 1A    | 3371 | 1/1   | 0.94 | 0.21 | -    | 56,56,56,56                 | 0     |
| 56  | MG   | 1A    | 3042 | 1/1   | 0.92 | 0.16 | -    | 27,27,27,27                 | 0     |
| 56  | MG   | 2A    | 3564 | 1/1   | 0.89 | 0.17 | -    | 45,45,45,45                 | 0     |
| 56  | MG   | 1A    | 3218 | 1/1   | 0.94 | 0.12 | -    | 51,51,51,51                 | 0     |
| 56  | MG   | 2A    | 3235 | 1/1   | 0.94 | 0.20 | -    | 49,49,49,49                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56  | MG   | 2a    | 1637 | 1/1   | 0.93 | 0.14 | -    | 60,60,60,60                 | 0     |
| 56  | MG   | 1A    | 3659 | 1/1   | 0.92 | 0.06 | -    | 64,64,64,64                 | 0     |
| 56  | MG   | 1A    | 3275 | 1/1   | 0.87 | 0.14 | -    | 39,39,39,39                 | 0     |
| 56  | MG   | 1A    | 3596 | 1/1   | 0.99 | 0.16 | -    | 32,32,32,32                 | 0     |
| 56  | MG   | 1A    | 3666 | 1/1   | 0.95 | 0.28 | -    | 44,44,44,44                 | 0     |
| 56  | MG   | 2A    | 3097 | 1/1   | 0.92 | 0.14 | -    | 57,57,57,57                 | 0     |
| 56  | MG   | 1A    | 3208 | 1/1   | 0.98 | 0.24 | -    | 24,24,24,24                 | 0     |
| 56  | MG   | 2A    | 3617 | 1/1   | 0.83 | 0.09 | -    | 54,54,54,54                 | 0     |
| 56  | MG   | 2A    | 3219 | 1/1   | 0.97 | 0.24 | -    | 45,45,45,45                 | 0     |
| 56  | MG   | 1A    | 3836 | 1/1   | 0.73 | 0.29 | -    | 54,54,54,54                 | 0     |
| 56  | MG   | 1A    | 3144 | 1/1   | 0.93 | 0.29 | -    | 40,40,40,40                 | 0     |
| 56  | MG   | 2A    | 3038 | 1/1   | 0.97 | 0.23 | -    | 48,48,48,48                 | 0     |
| 56  | MG   | 1a    | 1667 | 1/1   | 0.77 | 0.17 | -    | 68,68,68,68                 | 0     |
| 56  | MG   | 2a    | 1708 | 1/1   | 0.97 | 0.07 | -    | 52,52,52,52                 | 0     |
| 56  | MG   | 2A    | 3316 | 1/1   | 0.94 | 0.17 | -    | 25,25,25,25                 | 0     |
| 56  | MG   | 2A    | 3558 | 1/1   | 0.90 | 0.13 | -    | 54,54,54,54                 | 0     |
| 56  | MG   | 1a    | 1614 | 1/1   | 0.95 | 0.19 | -    | 37,37,37,37                 | 0     |
| 56  | MG   | 1A    | 3451 | 1/1   | 0.97 | 0.15 | -    | 40,40,40,40                 | 0     |
| 56  | MG   | 2A    | 3130 | 1/1   | 0.94 | 0.30 | -    | 54,54,54,54                 | 0     |
| 56  | MG   | 1a    | 1637 | 1/1   | 0.92 | 0.10 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | 1A    | 3334 | 1/1   | 0.90 | 0.23 | -    | 54,54,54,54                 | 0     |
| 56  | MG   | 1A    | 3391 | 1/1   | 0.95 | 0.17 | -    | 18,18,18,18                 | 0     |
| 56  | MG   | 1A    | 3675 | 1/1   | 0.95 | 0.17 | -    | 56,56,56,56                 | 0     |
| 56  | MG   | 1A    | 3151 | 1/1   | 0.96 | 0.22 | -    | 34,34,34,34                 | 0     |
| 56  | MG   | 1A    | 3197 | 1/1   | 0.93 | 0.22 | -    | 51,51,51,51                 | 0     |
| 56  | MG   | 1B    | 3018 | 1/1   | 0.97 | 0.20 | -    | 41,41,41,41                 | 0     |
| 56  | MG   | 2a    | 1761 | 1/1   | 0.96 | 0.09 | -    | 82,82,82,82                 | 0     |
| 56  | MG   | 2A    | 3101 | 1/1   | 0.94 | 0.21 | -    | 53,53,53,53                 | 0     |
| 56  | MG   | 1A    | 3441 | 1/1   | 0.84 | 0.15 | -    | 48,48,48,48                 | 0     |
| 56  | MG   | 23    | 3001 | 1/1   | 0.92 | 0.20 | -    | 54,54,54,54                 | 0     |
| 56  | MG   | 1A    | 3074 | 1/1   | 0.82 | 0.18 | -    | 45,45,45,45                 | 0     |
| 56  | MG   | 1A    | 3605 | 1/1   | 0.78 | 0.09 | -    | 74,74,74,74                 | 0     |
| 56  | MG   | 2a    | 1693 | 1/1   | 0.91 | 0.23 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | 2a    | 1629 | 1/1   | 0.79 | 0.19 | -    | 55,55,55,55                 | 0     |
| 56  | MG   | 2a    | 1743 | 1/1   | 0.92 | 0.10 | -    | 54,54,54,54                 | 0     |
| 56  | MG   | 2A    | 3374 | 1/1   | 0.95 | 0.17 | -    | 54,54,54,54                 | 0     |
| 56  | MG   | 1A    | 3498 | 1/1   | 0.86 | 0.14 | -    | 50,50,50,50                 | 0     |
| 56  | MG   | 2A    | 3536 | 1/1   | 0.97 | 0.11 | -    | 46,46,46,46                 | 0     |
| 56  | MG   | 1A    | 3672 | 1/1   | 0.98 | 0.08 | -    | 57,57,57,57                 | 0     |
| 56  | MG   | 1A    | 3149 | 1/1   | 0.99 | 0.30 | -    | 30,30,30,30                 | 0     |
| 56  | MG   | 2A    | 3054 | 1/1   | 0.96 | 0.09 | -    | 41,41,41,41                 | 0     |
| 56  | MG   | 1A    | 3726 | 1/1   | 0.87 | 0.15 | -    | 62,62,62,62                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56  | MG   | 2A    | 3272 | 1/1   | 0.94 | 0.15 | -    | 42,42,42,42                 | 0     |
| 56  | MG   | 2A    | 3047 | 1/1   | 0.94 | 0.10 | -    | 22,22,22,22                 | 0     |
| 56  | MG   | 1A    | 3122 | 1/1   | 0.98 | 0.29 | -    | 40,40,40,40                 | 0     |
| 56  | MG   | 1A    | 3378 | 1/1   | 0.96 | 0.21 | -    | 43,43,43,43                 | 0     |
| 56  | MG   | 2A    | 3477 | 1/1   | 0.97 | 0.16 | -    | 44,44,44,44                 | 0     |
| 56  | MG   | 1A    | 3420 | 1/1   | 0.95 | 0.08 | -    | 59,59,59,59                 | 0     |
| 56  | MG   | 1F    | 305  | 1/1   | 0.89 | 0.16 | -    | 46,46,46,46                 | 0     |
| 56  | MG   | 1A    | 3633 | 1/1   | 0.92 | 0.20 | -    | 40,40,40,40                 | 0     |
| 56  | MG   | 1A    | 3787 | 1/1   | 0.95 | 0.09 | -    | 34,34,34,34                 | 0     |
| 56  | MG   | 1X    | 3002 | 1/1   | 0.94 | 0.17 | -    | 45,45,45,45                 | 0     |
| 56  | MG   | 1A    | 3411 | 1/1   | 0.93 | 0.15 | -    | 51,51,51,51                 | 0     |
| 56  | MG   | 1A    | 3344 | 1/1   | 0.96 | 0.23 | -    | 48,48,48,48                 | 0     |
| 56  | MG   | 2A    | 3162 | 1/1   | 0.86 | 0.10 | -    | 45,45,45,45                 | 0     |
| 56  | MG   | 1A    | 3280 | 1/1   | 0.80 | 0.20 | -    | 50,50,50,50                 | 0     |
| 56  | MG   | 1a    | 1810 | 1/1   | 0.42 | 0.14 | -    | 90,90,90,90                 | 0     |
| 56  | MG   | 1A    | 3636 | 1/1   | 0.97 | 0.17 | -    | 53,53,53,53                 | 0     |
| 56  | MG   | 1A    | 3324 | 1/1   | 0.96 | 0.12 | -    | 43,43,43,43                 | 0     |
| 56  | MG   | 1B    | 3007 | 1/1   | 0.84 | 0.20 | -    | 53,53,53,53                 | 0     |
| 56  | MG   | 1A    | 3185 | 1/1   | 0.95 | 0.20 | -    | 50,50,50,50                 | 0     |
| 56  | MG   | 2A    | 3251 | 1/1   | 0.95 | 0.18 | -    | 27,27,27,27                 | 0     |
| 56  | MG   | 2A    | 3466 | 1/1   | 0.95 | 0.11 | -    | 50,50,50,50                 | 0     |
| 56  | MG   | 1A    | 3137 | 1/1   | 0.94 | 0.21 | -    | 32,32,32,32                 | 0     |
| 56  | MG   | 1A    | 3335 | 1/1   | 0.92 | 0.26 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | 1A    | 3616 | 1/1   | 0.95 | 0.22 | -    | 55,55,55,55                 | 0     |
| 56  | MG   | 2A    | 3290 | 1/1   | 0.97 | 0.12 | -    | 40,40,40,40                 | 0     |
| 56  | MG   | 2A    | 3437 | 1/1   | 0.98 | 0.13 | -    | 34,34,34,34                 | 0     |
| 56  | MG   | 1a    | 1655 | 1/1   | 0.93 | 0.20 | -    | 63,63,63,63                 | 0     |
| 56  | MG   | 1A    | 3184 | 1/1   | 0.96 | 0.14 | -    | 34,34,34,34                 | 0     |
| 56  | MG   | 2a    | 1699 | 1/1   | 0.96 | 0.12 | -    | 38,38,38,38                 | 0     |
| 56  | MG   | 2A    | 3096 | 1/1   | 0.90 | 0.17 | -    | 56,56,56,56                 | 0     |
| 56  | MG   | 1A    | 3888 | 1/1   | 0.44 | 0.14 | -    | 89,89,89,89                 | 0     |
| 56  | MG   | 2A    | 3049 | 1/1   | 0.93 | 0.12 | -    | 42,42,42,42                 | 0     |
| 56  | MG   | 2A    | 3645 | 1/1   | 0.91 | 0.14 | -    | 41,41,41,41                 | 0     |
| 56  | MG   | 2A    | 3218 | 1/1   | 0.93 | 0.29 | -    | 49,49,49,49                 | 0     |
| 56  | MG   | 1A    | 3943 | 1/1   | 0.85 | 0.17 | -    | 42,42,42,42                 | 0     |
| 56  | MG   | 1A    | 3063 | 1/1   | 0.90 | 0.22 | -    | 36,36,36,36                 | 0     |
| 56  | MG   | 2A    | 3305 | 1/1   | 0.89 | 0.17 | -    | 37,37,37,37                 | 0     |
| 56  | MG   | 1A    | 3509 | 1/1   | 0.96 | 0.13 | -    | 31,31,31,31                 | 0     |
| 56  | MG   | 1A    | 3007 | 1/1   | 0.95 | 0.21 | -    | 29,29,29,29                 | 0     |
| 56  | MG   | 1a    | 1648 | 1/1   | 0.97 | 0.24 | -    | 43,43,43,43                 | 0     |
| 56  | MG   | 2A    | 3499 | 1/1   | 0.91 | 0.09 | -    | 52,52,52,52                 | 0     |
| 56  | MG   | 1A    | 3446 | 1/1   | 0.96 | 0.03 | -    | 48,48,48,48                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 57  | K    | 2A    | 3207 | 1/1   | 0.86 | 0.26 | -    | 75,75,75,75                 | 0     |
| 56  | MG   | 2A    | 3158 | 1/1   | 0.96 | 0.14 | -    | 49,49,49,49                 | 0     |
| 56  | MG   | 1y    | 101  | 1/1   | 0.97 | 0.29 | -    | 38,38,38,38                 | 0     |
| 56  | MG   | 1A    | 3306 | 1/1   | 0.96 | 0.30 | -    | 55,55,55,55                 | 0     |
| 56  | MG   | 1a    | 1827 | 1/1   | 0.80 | 0.13 | -    | 55,55,55,55                 | 0     |
| 56  | MG   | 2A    | 3065 | 1/1   | 0.88 | 0.19 | -    | 43,43,43,43                 | 0     |
| 56  | MG   | 1A    | 3696 | 1/1   | 0.91 | 0.28 | -    | 38,38,38,38                 | 0     |
| 56  | MG   | 2a    | 1728 | 1/1   | 0.93 | 0.13 | -    | 52,52,52,52                 | 0     |
| 56  | MG   | 1A    | 3426 | 1/1   | 0.90 | 0.16 | -    | 51,51,51,51                 | 0     |
| 56  | MG   | 1A    | 3215 | 1/1   | 0.97 | 0.19 | -    | 56,56,56,56                 | 0     |
| 56  | MG   | 2A    | 3441 | 1/1   | 0.80 | 0.17 | -    | 33,33,33,33                 | 0     |
| 56  | MG   | 2A    | 3618 | 1/1   | 0.94 | 0.12 | -    | 44,44,44,44                 | 0     |
| 56  | MG   | 2a    | 1601 | 1/1   | 0.97 | 0.25 | -    | 45,45,45,45                 | 0     |
| 56  | MG   | 1A    | 3683 | 1/1   | 0.93 | 0.15 | -    | 50,50,50,50                 | 0     |
| 56  | MG   | 2A    | 3276 | 1/1   | 0.93 | 0.09 | -    | 48,48,48,48                 | 0     |
| 56  | MG   | 2a    | 1675 | 1/1   | 0.94 | 0.05 | -    | 66,66,66,66                 | 0     |
| 56  | MG   | 1a    | 1692 | 1/1   | 0.85 | 0.17 | -    | 60,60,60,60                 | 0     |
| 56  | MG   | 1A    | 3766 | 1/1   | 0.88 | 0.10 | -    | 57,57,57,57                 | 0     |
| 56  | MG   | 1A    | 3673 | 1/1   | 0.94 | 0.12 | -    | 59,59,59,59                 | 0     |
| 56  | MG   | 2a    | 1789 | 1/1   | 0.87 | 0.17 | -    | 58,58,58,58                 | 0     |
| 56  | MG   | 2a    | 1656 | 1/1   | 0.95 | 0.16 | -    | 62,62,62,62                 | 0     |
| 56  | MG   | 1a    | 1627 | 1/1   | 0.95 | 0.20 | -    | 58,58,58,58                 | 0     |
| 56  | MG   | 1A    | 3883 | 1/1   | 0.94 | 0.09 | -    | 60,60,60,60                 | 0     |
| 56  | MG   | 1A    | 3639 | 1/1   | 0.85 | 0.16 | -    | 39,39,39,39                 | 0     |
| 56  | MG   | 1A    | 3625 | 1/1   | 0.92 | 0.10 | -    | 51,51,51,51                 | 0     |
| 56  | MG   | 2a    | 1778 | 1/1   | 0.98 | 0.05 | -    | 51,51,51,51                 | 0     |
| 56  | MG   | 1A    | 3273 | 1/1   | 0.90 | 0.20 | -    | 42,42,42,42                 | 0     |
| 56  | MG   | 1a    | 1736 | 1/1   | 0.92 | 0.07 | -    | 58,58,58,58                 | 0     |
| 56  | MG   | 2A    | 3116 | 1/1   | 0.80 | 0.19 | -    | 56,56,56,56                 | 0     |
| 56  | MG   | 1A    | 3597 | 1/1   | 0.79 | 0.18 | -    | 50,50,50,50                 | 0     |
| 56  | MG   | 1A    | 3550 | 1/1   | 0.96 | 0.16 | -    | 40,40,40,40                 | 0     |
| 56  | MG   | 2A    | 3535 | 1/1   | 0.80 | 0.07 | -    | 62,62,62,62                 | 0     |
| 56  | MG   | 1a    | 1709 | 1/1   | 0.94 | 0.23 | -    | 60,60,60,60                 | 0     |
| 56  | MG   | 2a    | 1661 | 1/1   | 0.81 | 0.28 | -    | 65,65,65,65                 | 0     |
| 56  | MG   | 2A    | 3639 | 1/1   | 0.92 | 0.11 | -    | 52,52,52,52                 | 0     |
| 56  | MG   | 2F    | 304  | 1/1   | 0.82 | 0.14 | -    | 54,54,54,54                 | 0     |
| 56  | MG   | 1A    | 3503 | 1/1   | 0.90 | 0.18 | -    | 33,33,33,33                 | 0     |
| 56  | MG   | 2A    | 3671 | 1/1   | 0.97 | 0.05 | -    | 51,51,51,51                 | 0     |
| 56  | MG   | 2A    | 3027 | 1/1   | 0.92 | 0.11 | -    | 44,44,44,44                 | 0     |
| 56  | MG   | 2a    | 1682 | 1/1   | 0.94 | 0.29 | -    | 64,64,64,64                 | 0     |
| 56  | MG   | 2A    | 3236 | 1/1   | 0.91 | 0.16 | -    | 55,55,55,55                 | 0     |
| 56  | MG   | 2A    | 3644 | 1/1   | 0.89 | 0.40 | -    | 42,42,42,42                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56  | MG   | 1A    | 3424 | 1/1   | 0.94 | 0.18 | -    | 14,14,14,14                 | 0     |
| 56  | MG   | 1A    | 3267 | 1/1   | 0.85 | 0.15 | -    | 53,53,53,53                 | 0     |
| 56  | MG   | 1a    | 1724 | 1/1   | 0.95 | 0.15 | -    | 52,52,52,52                 | 0     |
| 56  | MG   | 2A    | 3079 | 1/1   | 0.93 | 0.17 | -    | 49,49,49,49                 | 0     |
| 56  | MG   | 1A    | 3098 | 1/1   | 0.82 | 0.17 | -    | 56,56,56,56                 | 0     |
| 56  | MG   | 1a    | 1800 | 1/1   | 0.88 | 0.13 | -    | 50,50,50,50                 | 0     |
| 56  | MG   | 1A    | 3343 | 1/1   | 0.92 | 0.20 | -    | 54,54,54,54                 | 0     |
| 56  | MG   | 1a    | 1798 | 1/1   | 0.77 | 0.13 | -    | 71,71,71,71                 | 0     |
| 56  | MG   | 1a    | 1821 | 1/1   | 0.95 | 0.09 | -    | 68,68,68,68                 | 0     |
| 56  | MG   | 1A    | 3656 | 1/1   | 0.97 | 0.12 | -    | 48,48,48,48                 | 0     |
| 56  | MG   | 1A    | 3453 | 1/1   | 0.96 | 0.10 | -    | 31,31,31,31                 | 0     |
| 56  | MG   | 1A    | 3773 | 1/1   | 0.82 | 0.25 | -    | 41,41,41,41                 | 0     |
| 56  | MG   | 1a    | 1658 | 1/1   | 0.98 | 0.30 | -    | 51,51,51,51                 | 0     |
| 56  | MG   | 2A    | 3463 | 1/1   | 0.96 | 0.09 | -    | 45,45,45,45                 | 0     |
| 56  | MG   | 1A    | 3289 | 1/1   | 0.94 | 0.13 | -    | 29,29,29,29                 | 0     |
| 56  | MG   | 1E    | 304  | 1/1   | 0.93 | 0.06 | -    | 57,57,57,57                 | 0     |
| 56  | MG   | 1A    | 3839 | 1/1   | 0.94 | 0.12 | -    | 70,70,70,70                 | 0     |
| 56  | MG   | 1A    | 3221 | 1/1   | 0.87 | 0.16 | -    | 48,48,48,48                 | 0     |
| 56  | MG   | 1a    | 1790 | 1/1   | 0.92 | 0.13 | -    | 46,46,46,46                 | 0     |
| 56  | MG   | 2a    | 1655 | 1/1   | 0.70 | 0.24 | -    | 64,64,64,64                 | 0     |
| 56  | MG   | 2A    | 3452 | 1/1   | 0.94 | 0.30 | -    | 54,54,54,54                 | 0     |
| 56  | MG   | 1a    | 1773 | 1/1   | 0.81 | 0.10 | -    | 64,64,64,64                 | 0     |
| 56  | MG   | 2a    | 1786 | 1/1   | 0.92 | 0.10 | -    | 59,59,59,59                 | 0     |
| 56  | MG   | 1A    | 3266 | 1/1   | 0.78 | 0.18 | -    | 61,61,61,61                 | 0     |
| 56  | MG   | 1T    | 202  | 1/1   | 0.97 | 0.09 | -    | 46,46,46,46                 | 0     |
| 56  | MG   | 2a    | 1712 | 1/1   | 0.97 | 0.21 | -    | 58,58,58,58                 | 0     |
| 56  | MG   | 1a    | 1803 | 1/1   | 0.95 | 0.06 | -    | 64,64,64,64                 | 0     |
| 56  | MG   | 1A    | 3329 | 1/1   | 0.94 | 0.20 | -    | 38,38,38,38                 | 0     |
| 56  | MG   | 1A    | 3768 | 1/1   | 0.94 | 0.23 | -    | 50,50,50,50                 | 0     |
| 56  | MG   | 1A    | 3790 | 1/1   | 0.89 | 0.15 | -    | 49,49,49,49                 | 0     |
| 56  | MG   | 1A    | 3840 | 1/1   | 0.97 | 0.26 | -    | 36,36,36,36                 | 0     |
| 56  | MG   | 2A    | 3583 | 1/1   | 0.94 | 0.13 | -    | 41,41,41,41                 | 0     |
| 56  | MG   | 2A    | 3353 | 1/1   | 0.94 | 0.10 | -    | 49,49,49,49                 | 0     |
| 56  | MG   | 1A    | 3413 | 1/1   | 0.97 | 0.13 | -    | 30,30,30,30                 | 0     |
| 56  | MG   | 1A    | 3560 | 1/1   | 0.92 | 0.16 | -    | 49,49,49,49                 | 0     |
| 56  | MG   | 2A    | 3069 | 1/1   | 0.95 | 0.16 | -    | 30,30,30,30                 | 0     |
| 56  | MG   | 2A    | 3287 | 1/1   | 0.95 | 0.07 | -    | 31,31,31,31                 | 0     |
| 56  | MG   | 2A    | 3519 | 1/1   | 0.93 | 0.15 | -    | 43,43,43,43                 | 0     |
| 56  | MG   | 2A    | 3084 | 1/1   | 0.90 | 0.10 | -    | 40,40,40,40                 | 0     |
| 56  | MG   | 1P    | 201  | 1/1   | 0.95 | 0.07 | -    | 50,50,50,50                 | 0     |
| 56  | MG   | 1a    | 1604 | 1/1   | 0.90 | 0.11 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | 1A    | 3285 | 1/1   | 0.81 | 0.18 | -    | 49,49,49,49                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56  | MG   | 1A    | 3118 | 1/1   | 0.95 | 0.18 | -    | 30,30,30,30                 | 0     |
| 56  | MG   | 2A    | 3492 | 1/1   | 0.79 | 0.14 | -    | 50,50,50,50                 | 0     |
| 56  | MG   | 1A    | 3516 | 1/1   | 0.96 | 0.16 | -    | 25,25,25,25                 | 0     |
| 56  | MG   | 1A    | 3406 | 1/1   | 0.96 | 0.18 | -    | 23,23,23,23                 | 0     |
| 56  | MG   | 1A    | 3539 | 1/1   | 0.97 | 0.25 | -    | 51,51,51,51                 | 0     |
| 56  | MG   | 28    | 101  | 1/1   | 0.86 | 0.20 | -    | 57,57,57,57                 | 0     |
| 56  | MG   | 2A    | 3114 | 1/1   | 0.95 | 0.25 | -    | 51,51,51,51                 | 0     |
| 56  | MG   | 1A    | 3410 | 1/1   | 0.96 | 0.21 | -    | 42,42,42,42                 | 0     |
| 56  | MG   | 2A    | 3404 | 1/1   | 0.90 | 0.14 | -    | 37,37,37,37                 | 0     |
| 56  | MG   | 1A    | 3255 | 1/1   | 0.97 | 0.21 | -    | 50,50,50,50                 | 0     |
| 56  | MG   | 1a    | 1654 | 1/1   | 0.89 | 0.09 | -    | 54,54,54,54                 | 0     |
| 56  | MG   | 2A    | 3326 | 1/1   | 0.98 | 0.06 | -    | 42,42,42,42                 | 0     |
| 56  | MG   | 1a    | 1755 | 1/1   | 0.89 | 0.13 | -    | 57,57,57,57                 | 0     |
| 56  | MG   | 2A    | 3237 | 1/1   | 0.84 | 0.18 | -    | 57,57,57,57                 | 0     |
| 56  | MG   | 1E    | 306  | 1/1   | 0.97 | 0.16 | -    | 56,56,56,56                 | 0     |
| 56  | MG   | 10    | 104  | 1/1   | 0.98 | 0.04 | -    | 55,55,55,55                 | 0     |
| 56  | MG   | 1a    | 1809 | 1/1   | 0.88 | 0.10 | -    | 83,83,83,83                 | 0     |
| 56  | MG   | 1A    | 3100 | 1/1   | 0.94 | 0.11 | -    | 57,57,57,57                 | 0     |
| 56  | MG   | 1A    | 3527 | 1/1   | 0.96 | 0.11 | -    | 41,41,41,41                 | 0     |
| 56  | MG   | 2A    | 3074 | 1/1   | 0.61 | 0.18 | -    | 54,54,54,54                 | 0     |
| 56  | MG   | 2A    | 3665 | 1/1   | 0.96 | 0.09 | -    | 57,57,57,57                 | 0     |
| 56  | MG   | 1A    | 3028 | 1/1   | 0.95 | 0.17 | -    | 20,20,20,20                 | 0     |
| 56  | MG   | 1A    | 3693 | 1/1   | 0.92 | 0.21 | -    | 48,48,48,48                 | 0     |
| 56  | MG   | 1a    | 1729 | 1/1   | 0.94 | 0.16 | -    | 53,53,53,53                 | 0     |
| 56  | MG   | 1A    | 3728 | 1/1   | 0.96 | 0.20 | -    | 50,50,50,50                 | 0     |
| 56  | MG   | 1A    | 3287 | 1/1   | 0.87 | 0.17 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | 1A    | 3821 | 1/1   | 0.92 | 0.22 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | 1A    | 3167 | 1/1   | 0.94 | 0.38 | -    | 42,42,42,42                 | 0     |
| 56  | MG   | 1A    | 3279 | 1/1   | 0.89 | 0.12 | -    | 52,52,52,52                 | 0     |
| 56  | MG   | 2A    | 3155 | 1/1   | 0.90 | 0.22 | -    | 43,43,43,43                 | 0     |
| 56  | MG   | 2a    | 1695 | 1/1   | 0.86 | 0.18 | -    | 54,54,54,54                 | 0     |
| 56  | MG   | 1A    | 3679 | 1/1   | 0.95 | 0.15 | -    | 52,52,52,52                 | 0     |
| 56  | MG   | 1w    | 3006 | 1/1   | 0.94 | 0.06 | -    | 67,67,67,67                 | 0     |
| 56  | MG   | 2A    | 3487 | 1/1   | 0.92 | 0.09 | -    | 56,56,56,56                 | 0     |
| 56  | MG   | 1a    | 1817 | 1/1   | 0.96 | 0.19 | -    | 48,48,48,48                 | 0     |
| 56  | MG   | 2A    | 3439 | 1/1   | 0.96 | 0.12 | -    | 36,36,36,36                 | 0     |
| 56  | MG   | 2B    | 3016 | 1/1   | 0.92 | 0.27 | -    | 66,66,66,66                 | 0     |
| 56  | MG   | 2A    | 3269 | 1/1   | 0.92 | 0.15 | -    | 38,38,38,38                 | 0     |
| 56  | MG   | 2A    | 3476 | 1/1   | 0.98 | 0.13 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | 1A    | 3589 | 1/1   | 0.92 | 0.17 | -    | 29,29,29,29                 | 0     |
| 56  | MG   | 1A    | 3795 | 1/1   | 0.98 | 0.13 | -    | 20,20,20,20                 | 0     |
| 56  | MG   | 2a    | 1649 | 1/1   | 0.62 | 0.21 | -    | 71,71,71,71                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56  | MG   | 1A    | 3226 | 1/1   | 0.87 | 0.37 | -    | 35,35,35,35                 | 0     |
| 56  | MG   | 1a    | 1657 | 1/1   | 0.73 | 0.26 | -    | 56,56,56,56                 | 0     |
| 56  | MG   | 1A    | 3824 | 1/1   | 0.92 | 0.16 | -    | 36,36,36,36                 | 0     |
| 56  | MG   | 1A    | 3648 | 1/1   | 0.88 | 0.10 | -    | 46,46,46,46                 | 0     |
| 56  | MG   | 2A    | 3486 | 1/1   | 0.95 | 0.06 | -    | 54,54,54,54                 | 0     |
| 56  | MG   | 2A    | 3525 | 1/1   | 0.93 | 0.10 | -    | 52,52,52,52                 | 0     |
| 56  | MG   | 1A    | 3102 | 1/1   | 0.96 | 0.28 | -    | 44,44,44,44                 | 0     |
| 56  | MG   | 1A    | 3891 | 1/1   | 0.89 | 0.26 | -    | 76,76,76,76                 | 0     |
| 56  | MG   | 2A    | 3131 | 1/1   | 0.90 | 0.22 | -    | 49,49,49,49                 | 0     |
| 56  | MG   | 2A    | 3565 | 1/1   | 0.97 | 0.15 | -    | 50,50,50,50                 | 0     |
| 56  | MG   | 1A    | 3808 | 1/1   | 0.96 | 0.23 | -    | 41,41,41,41                 | 0     |
| 56  | MG   | 2a    | 1735 | 1/1   | 0.96 | 0.22 | -    | 42,42,42,42                 | 0     |
| 56  | MG   | 1A    | 3261 | 1/1   | 0.94 | 0.74 | -    | 51,51,51,51                 | 0     |
| 56  | MG   | 2A    | 3198 | 1/1   | 0.89 | 0.13 | -    | 42,42,42,42                 | 0     |
| 56  | MG   | 1A    | 3408 | 1/1   | 0.95 | 0.15 | -    | 43,43,43,43                 | 0     |
| 56  | MG   | 2A    | 3211 | 1/1   | 0.96 | 0.13 | -    | 43,43,43,43                 | 0     |
| 56  | MG   | 1A    | 3556 | 1/1   | 0.94 | 0.13 | -    | 43,43,43,43                 | 0     |
| 56  | MG   | 2A    | 3183 | 1/1   | 0.98 | 0.08 | -    | 44,44,44,44                 | 0     |
| 56  | MG   | 1A    | 3088 | 1/1   | 0.90 | 0.24 | -    | 54,54,54,54                 | 0     |
| 56  | MG   | 2A    | 3018 | 1/1   | 0.98 | 0.26 | -    | 52,52,52,52                 | 0     |
| 56  | MG   | 1A    | 3893 | 1/1   | 0.79 | 0.08 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | 2A    | 3425 | 1/1   | 0.84 | 0.16 | -    | 38,38,38,38                 | 0     |
| 56  | MG   | 1A    | 3117 | 1/1   | 0.87 | 0.26 | -    | 38,38,38,38                 | 0     |
| 56  | MG   | 1A    | 3141 | 1/1   | 0.99 | 0.25 | -    | 27,27,27,27                 | 0     |
| 56  | MG   | 1A    | 3825 | 1/1   | 0.97 | 0.17 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | 2x    | 101  | 1/1   | 0.93 | 0.22 | -    | 56,56,56,56                 | 0     |
| 56  | MG   | 1A    | 3003 | 1/1   | 0.95 | 0.14 | -    | 32,32,32,32                 | 0     |
| 56  | MG   | 1Z    | 3003 | 1/1   | 0.88 | 0.18 | -    | 61,61,61,61                 | 0     |
| 56  | MG   | 2A    | 3473 | 1/1   | 0.92 | 0.08 | -    | 51,51,51,51                 | 0     |
| 56  | MG   | 1A    | 3205 | 1/1   | 0.96 | 0.15 | -    | 33,33,33,33                 | 0     |
| 56  | MG   | 1A    | 3018 | 1/1   | 0.87 | 0.21 | -    | 52,52,52,52                 | 0     |
| 56  | MG   | 1A    | 3511 | 1/1   | 0.96 | 0.15 | -    | 49,49,49,49                 | 0     |
| 56  | MG   | 1a    | 1617 | 1/1   | 0.89 | 0.17 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | 1A    | 3326 | 1/1   | 0.95 | 0.23 | -    | 43,43,43,43                 | 0     |
| 56  | MG   | 1A    | 3380 | 1/1   | 0.86 | 0.20 | -    | 30,30,30,30                 | 0     |
| 56  | MG   | 2A    | 3255 | 1/1   | 0.93 | 0.15 | -    | 43,43,43,43                 | 0     |
| 56  | MG   | 1A    | 3811 | 1/1   | 0.87 | 0.12 | -    | 64,64,64,64                 | 0     |
| 56  | MG   | 1A    | 3701 | 1/1   | 0.88 | 0.14 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | 2A    | 3333 | 1/1   | 0.91 | 0.20 | -    | 35,35,35,35                 | 0     |
| 56  | MG   | 1A    | 3549 | 1/1   | 0.97 | 0.17 | -    | 41,41,41,41                 | 0     |
| 56  | MG   | 1a    | 1772 | 1/1   | 0.96 | 0.10 | -    | 60,60,60,60                 | 0     |
| 56  | MG   | 15    | 102  | 1/1   | 0.96 | 0.10 | -    | 37,37,37,37                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56  | MG   | 1A    | 3333 | 1/1   | 0.76 | 0.17 | -    | 51,51,51,51                 | 0     |
| 56  | MG   | 1a    | 1606 | 1/1   | 0.91 | 0.18 | -    | 54,54,54,54                 | 0     |
| 56  | MG   | 2A    | 3343 | 1/1   | 0.89 | 0.10 | -    | 33,33,33,33                 | 0     |
| 56  | MG   | 1a    | 1659 | 1/1   | 0.97 | 0.23 | -    | 55,55,55,55                 | 0     |
| 56  | MG   | 1f    | 3001 | 1/1   | 0.95 | 0.18 | -    | 38,38,38,38                 | 0     |
| 56  | MG   | 1A    | 3846 | 1/1   | 0.94 | 0.17 | -    | 51,51,51,51                 | 0     |
| 56  | MG   | 2a    | 1689 | 1/1   | 0.91 | 0.12 | -    | 61,61,61,61                 | 0     |
| 56  | MG   | 2A    | 3217 | 1/1   | 0.86 | 0.23 | -    | 60,60,60,60                 | 0     |
| 56  | MG   | 1A    | 3859 | 1/1   | 0.93 | 0.14 | -    | 53,53,53,53                 | 0     |
| 56  | MG   | 1A    | 3210 | 1/1   | 0.78 | 0.12 | -    | 55,55,55,55                 | 0     |
| 56  | MG   | 1a    | 1703 | 1/1   | 0.97 | 0.15 | -    | 50,50,50,50                 | 0     |
| 56  | MG   | 2A    | 3292 | 1/1   | 0.94 | 0.15 | -    | 45,45,45,45                 | 0     |
| 56  | MG   | 2A    | 3377 | 1/1   | 0.95 | 0.08 | -    | 43,43,43,43                 | 0     |
| 56  | MG   | 1A    | 3405 | 1/1   | 0.97 | 0.16 | -    | 40,40,40,40                 | 0     |
| 56  | MG   | 1A    | 3288 | 1/1   | 0.97 | 0.18 | -    | 36,36,36,36                 | 0     |
| 56  | MG   | 2A    | 3467 | 1/1   | 0.95 | 0.09 | -    | 65,65,65,65                 | 0     |
| 56  | MG   | 1O    | 205  | 1/1   | 0.85 | 0.15 | -    | 55,55,55,55                 | 0     |
| 56  | MG   | 1A    | 3823 | 1/1   | 0.87 | 0.13 | -    | 67,67,67,67                 | 0     |
| 56  | MG   | 2A    | 3241 | 1/1   | 0.90 | 0.08 | -    | 42,42,42,42                 | 0     |
| 56  | MG   | 1a    | 1779 | 1/1   | 0.95 | 0.14 | -    | 36,36,36,36                 | 0     |
| 56  | MG   | 1A    | 3292 | 1/1   | 0.80 | 0.14 | -    | 49,49,49,49                 | 0     |
| 56  | MG   | 1A    | 3284 | 1/1   | 0.93 | 0.22 | -    | 42,42,42,42                 | 0     |
| 56  | MG   | 1A    | 3090 | 1/1   | 0.93 | 0.18 | -    | 39,39,39,39                 | 0     |
| 56  | MG   | 1A    | 3006 | 1/1   | 0.93 | 0.13 | -    | 53,53,53,53                 | 0     |
| 56  | MG   | 2A    | 3394 | 1/1   | 0.91 | 0.15 | -    | 45,45,45,45                 | 0     |
| 56  | MG   | 2A    | 3107 | 1/1   | 0.93 | 0.13 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | 1A    | 3372 | 1/1   | 0.91 | 0.17 | -    | 52,52,52,52                 | 0     |
| 56  | MG   | 1a    | 1732 | 1/1   | 0.98 | 0.26 | -    | 42,42,42,42                 | 0     |
| 56  | MG   | 2Z    | 8001 | 1/1   | 0.94 | 0.13 | -    | 70,70,70,70                 | 0     |
| 56  | MG   | 1A    | 3513 | 1/1   | 0.98 | 0.23 | -    | 29,29,29,29                 | 0     |
| 56  | MG   | 2a    | 1605 | 1/1   | 0.92 | 0.12 | -    | 81,81,81,81                 | 0     |
| 56  | MG   | 2Q    | 203  | 1/1   | 0.96 | 0.16 | -    | 37,37,37,37                 | 0     |
| 56  | MG   | 1A    | 3713 | 1/1   | 0.95 | 0.13 | -    | 36,36,36,36                 | 0     |
| 56  | MG   | 1A    | 3353 | 1/1   | 0.94 | 0.26 | -    | 36,36,36,36                 | 0     |
| 56  | MG   | 1A    | 3309 | 1/1   | 0.98 | 0.19 | -    | 36,36,36,36                 | 0     |
| 56  | MG   | 1A    | 3807 | 1/1   | 0.97 | 0.21 | -    | 49,49,49,49                 | 0     |
| 56  | MG   | 2a    | 1706 | 1/1   | 0.63 | 0.14 | -    | 75,75,75,75                 | 0     |
| 56  | MG   | 2A    | 3357 | 1/1   | 0.85 | 0.16 | -    | 49,49,49,49                 | 0     |
| 56  | MG   | 1A    | 3105 | 1/1   | 0.95 | 0.20 | -    | 31,31,31,31                 | 0     |
| 56  | MG   | 2A    | 3340 | 1/1   | 0.94 | 0.10 | -    | 27,27,27,27                 | 0     |
| 56  | MG   | 1A    | 3890 | 1/1   | 0.98 | 0.16 | -    | 38,38,38,38                 | 0     |
| 56  | MG   | 2A    | 3592 | 1/1   | 0.80 | 0.14 | -    | 57,57,57,57                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56  | MG   | 2a    | 1614 | 1/1   | 0.91 | 0.15 | -    | 71,71,71,71                 | 0     |
| 56  | MG   | 1A    | 3704 | 1/1   | 0.94 | 0.10 | -    | 43,43,43,43                 | 0     |
| 56  | MG   | 1A    | 3336 | 1/1   | 0.97 | 0.17 | -    | 40,40,40,40                 | 0     |
| 56  | MG   | 1A    | 3286 | 1/1   | 0.94 | 0.40 | -    | 41,41,41,41                 | 0     |
| 56  | MG   | 1A    | 3849 | 1/1   | 0.98 | 0.20 | -    | 29,29,29,29                 | 0     |
| 56  | MG   | 2B    | 3006 | 1/1   | 0.89 | 0.14 | -    | 51,51,51,51                 | 0     |
| 56  | MG   | 1A    | 3524 | 1/1   | 0.94 | 0.16 | -    | 50,50,50,50                 | 0     |
| 56  | MG   | 2A    | 3546 | 1/1   | 0.96 | 0.14 | -    | 33,33,33,33                 | 0     |
| 56  | MG   | 2A    | 3177 | 1/1   | 0.91 | 0.11 | -    | 37,37,37,37                 | 0     |
| 56  | MG   | 1A    | 3906 | 1/1   | 0.96 | 0.15 | -    | 42,42,42,42                 | 0     |
| 56  | MG   | 2A    | 3637 | 1/1   | 0.94 | 0.13 | -    | 41,41,41,41                 | 0     |
| 56  | MG   | 2P    | 201  | 1/1   | 0.87 | 0.12 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | 1A    | 3056 | 1/1   | 0.77 | 0.19 | -    | 48,48,48,48                 | 0     |
| 56  | MG   | 1a    | 1733 | 1/1   | 0.91 | 0.11 | -    | 33,33,33,33                 | 0     |
| 56  | MG   | 1A    | 3213 | 1/1   | 0.83 | 0.24 | -    | 42,42,42,42                 | 0     |
| 56  | MG   | 1A    | 3161 | 1/1   | 0.97 | 0.20 | -    | 41,41,41,41                 | 0     |
| 56  | MG   | 1w    | 3002 | 1/1   | 0.87 | 0.09 | -    | 56,56,56,56                 | 0     |
| 56  | MG   | 1A    | 3376 | 1/1   | 0.77 | 0.15 | -    | 42,42,42,42                 | 0     |
| 56  | MG   | 2A    | 3187 | 1/1   | 0.86 | 0.14 | -    | 60,60,60,60                 | 0     |
| 56  | MG   | 2a    | 1722 | 1/1   | 0.91 | 0.21 | -    | 57,57,57,57                 | 0     |
| 56  | MG   | 20    | 102  | 1/1   | 0.69 | 0.23 | -    | 57,57,57,57                 | 0     |
| 56  | MG   | 1A    | 3635 | 1/1   | 0.81 | 0.09 | -    | 49,49,49,49                 | 0     |
| 56  | MG   | 2a    | 1677 | 1/1   | 0.95 | 0.18 | -    | 51,51,51,51                 | 0     |
| 56  | MG   | 2A    | 3184 | 1/1   | 0.91 | 0.17 | -    | 46,46,46,46                 | 0     |
| 56  | MG   | 1A    | 3783 | 1/1   | 0.78 | 0.15 | -    | 27,27,27,27                 | 0     |
| 56  | MG   | 2A    | 3111 | 1/1   | 0.93 | 0.15 | -    | 43,43,43,43                 | 0     |
| 56  | MG   | 1A    | 3168 | 1/1   | 0.95 | 0.23 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | 2a    | 1726 | 1/1   | 0.94 | 0.11 | -    | 64,64,64,64                 | 0     |
| 56  | MG   | 10    | 103  | 1/1   | 0.94 | 0.10 | -    | 60,60,60,60                 | 0     |
| 56  | MG   | 2A    | 3590 | 1/1   | 0.95 | 0.21 | -    | 41,41,41,41                 | 0     |
| 56  | MG   | 1A    | 3272 | 1/1   | 0.93 | 0.17 | -    | 38,38,38,38                 | 0     |
| 56  | MG   | 2A    | 3080 | 1/1   | 0.96 | 0.17 | -    | 50,50,50,50                 | 0     |
| 56  | MG   | 2A    | 3573 | 1/1   | 0.93 | 0.08 | -    | 54,54,54,54                 | 0     |
| 56  | MG   | 2A    | 3488 | 1/1   | 0.95 | 0.10 | -    | 52,52,52,52                 | 0     |
| 56  | MG   | 1A    | 3628 | 1/1   | 0.94 | 0.19 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | 2A    | 3300 | 1/1   | 0.87 | 0.13 | -    | 29,29,29,29                 | 0     |
| 56  | MG   | 1A    | 3293 | 1/1   | 0.89 | 0.17 | -    | 26,26,26,26                 | 0     |
| 56  | MG   | 1A    | 3444 | 1/1   | 0.96 | 0.10 | -    | 37,37,37,37                 | 0     |
| 56  | MG   | 2a    | 1760 | 1/1   | 0.91 | 0.10 | -    | 54,54,54,54                 | 0     |
| 56  | MG   | 1A    | 3182 | 1/1   | 0.78 | 0.24 | -    | 65,65,65,65                 | 0     |
| 56  | MG   | 1A    | 3179 | 1/1   | 0.96 | 0.22 | -    | 31,31,31,31                 | 0     |
| 56  | MG   | 1A    | 3886 | 1/1   | 0.90 | 0.16 | -    | 50,50,50,50                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56  | MG   | 1A    | 3756 | 1/1   | 0.95 | 0.14 | -    | 39,39,39,39                 | 0     |
| 56  | MG   | 2A    | 3458 | 1/1   | 0.97 | 0.17 | -    | 57,57,57,57                 | 0     |
| 56  | MG   | 1A    | 3619 | 1/1   | 0.93 | 0.20 | -    | 53,53,53,53                 | 0     |
| 56  | MG   | 1A    | 3860 | 1/1   | 0.98 | 0.14 | -    | 38,38,38,38                 | 0     |
| 56  | MG   | 1A    | 3083 | 1/1   | 0.89 | 0.24 | -    | 27,27,27,27                 | 0     |
| 56  | MG   | 1A    | 3459 | 1/1   | 0.99 | 0.15 | -    | 40,40,40,40                 | 0     |
| 56  | MG   | 1A    | 3486 | 1/1   | 0.84 | 0.17 | -    | 46,46,46,46                 | 0     |
| 56  | MG   | 2A    | 3034 | 1/1   | 0.96 | 0.15 | -    | 40,40,40,40                 | 0     |
| 56  | MG   | 2V    | 201  | 1/1   | 0.90 | 0.11 | -    | 44,44,44,44                 | 0     |
| 56  | MG   | 1A    | 3483 | 1/1   | 0.88 | 0.17 | -    | 29,29,29,29                 | 0     |
| 56  | MG   | 1A    | 3295 | 1/1   | 0.96 | 0.15 | -    | 43,43,43,43                 | 0     |
| 56  | MG   | 1a    | 1638 | 1/1   | 0.95 | 0.24 | -    | 42,42,42,42                 | 0     |
| 56  | MG   | 2A    | 3455 | 1/1   | 0.97 | 0.20 | -    | 44,44,44,44                 | 0     |
| 56  | MG   | 2A    | 3277 | 1/1   | 0.98 | 0.17 | -    | 35,35,35,35                 | 0     |
| 56  | MG   | 2A    | 3346 | 1/1   | 0.97 | 0.07 | -    | 36,36,36,36                 | 0     |
| 56  | MG   | 2A    | 3318 | 1/1   | 0.96 | 0.19 | -    | 38,38,38,38                 | 0     |
| 56  | MG   | 2A    | 3520 | 1/1   | 0.83 | 0.11 | -    | 51,51,51,51                 | 0     |
| 56  | MG   | 1A    | 3066 | 1/1   | 0.95 | 0.39 | -    | 31,31,31,31                 | 0     |
| 56  | MG   | 1A    | 3546 | 1/1   | 0.95 | 0.13 | -    | 45,45,45,45                 | 0     |
| 56  | MG   | 2A    | 3212 | 1/1   | 0.86 | 0.18 | -    | 55,55,55,55                 | 0     |
| 56  | MG   | 2A    | 3501 | 1/1   | 0.84 | 0.07 | -    | 46,46,46,46                 | 0     |
| 56  | MG   | 1a    | 1682 | 1/1   | 0.91 | 0.22 | -    | 57,57,57,57                 | 0     |
| 56  | MG   | 1A    | 3322 | 1/1   | 0.89 | 0.34 | -    | 55,55,55,55                 | 0     |
| 56  | MG   | 1A    | 3740 | 1/1   | 0.97 | 0.06 | -    | 39,39,39,39                 | 0     |
| 56  | MG   | 1a    | 1775 | 1/1   | 0.96 | 0.07 | -    | 52,52,52,52                 | 0     |
| 56  | MG   | 1A    | 3737 | 1/1   | 0.97 | 0.19 | -    | 50,50,50,50                 | 0     |
| 56  | MG   | 2a    | 1626 | 1/1   | 0.89 | 0.24 | -    | 50,50,50,50                 | 0     |
| 56  | MG   | 2w    | 3003 | 1/1   | 0.75 | 0.10 | -    | 70,70,70,70                 | 0     |
| 56  | MG   | 1A    | 3027 | 1/1   | 0.97 | 0.28 | -    | 33,33,33,33                 | 0     |
| 56  | MG   | 1A    | 3514 | 1/1   | 0.92 | 0.16 | -    | 40,40,40,40                 | 0     |
| 56  | MG   | 1a    | 1650 | 1/1   | 0.91 | 0.21 | -    | 55,55,55,55                 | 0     |
| 56  | MG   | 1A    | 3879 | 1/1   | 0.90 | 0.21 | -    | 54,54,54,54                 | 0     |
| 56  | MG   | 1a    | 1816 | 1/1   | 0.95 | 0.17 | -    | 49,49,49,49                 | 0     |
| 56  | MG   | 1A    | 3438 | 1/1   | 0.94 | 0.14 | -    | 30,30,30,30                 | 0     |
| 56  | MG   | 1A    | 3195 | 1/1   | 0.97 | 0.10 | -    | 39,39,39,39                 | 0     |
| 56  | MG   | 2A    | 3040 | 1/1   | 0.95 | 0.13 | -    | 43,43,43,43                 | 0     |
| 56  | MG   | 2a    | 1683 | 1/1   | 0.95 | 0.25 | -    | 57,57,57,57                 | 0     |
| 56  | MG   | 1A    | 3863 | 1/1   | 0.92 | 0.12 | -    | 31,31,31,31                 | 0     |
| 56  | MG   | 1A    | 3091 | 1/1   | 0.92 | 0.15 | -    | 48,48,48,48                 | 0     |
| 56  | MG   | 1A    | 3075 | 1/1   | 0.84 | 0.25 | -    | 43,43,43,43                 | 0     |
| 56  | MG   | 2A    | 3025 | 1/1   | 0.79 | 0.20 | -    | 61,61,61,61                 | 0     |
| 56  | MG   | 1A    | 3236 | 1/1   | 0.82 | 0.17 | -    | 52,52,52,52                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56  | MG   | 1A    | 3423 | 1/1   | 0.93 | 0.13 | -    | 42,42,42,42                 | 0     |
| 56  | MG   | 2a    | 1701 | 1/1   | 0.94 | 0.15 | -    | 62,62,62,62                 | 0     |
| 56  | MG   | 1A    | 3016 | 1/1   | 0.94 | 0.12 | -    | 34,34,34,34                 | 0     |
| 56  | MG   | 2A    | 3574 | 1/1   | 0.91 | 0.14 | -    | 43,43,43,43                 | 0     |
| 56  | MG   | 2A    | 3540 | 1/1   | 0.91 | 0.17 | -    | 43,43,43,43                 | 0     |
| 56  | MG   | 1A    | 3258 | 1/1   | 0.98 | 0.17 | -    | 32,32,32,32                 | 0     |
| 56  | MG   | 1A    | 3623 | 1/1   | 0.95 | 0.18 | -    | 53,53,53,53                 | 0     |
| 56  | MG   | 2A    | 3139 | 1/1   | 0.97 | 0.22 | -    | 38,38,38,38                 | 0     |
| 56  | MG   | 1A    | 3032 | 1/1   | 0.99 | 0.21 | -    | 41,41,41,41                 | 0     |
| 56  | MG   | 1A    | 3562 | 1/1   | 0.94 | 0.10 | -    | 42,42,42,42                 | 0     |
| 56  | MG   | 1B    | 3015 | 1/1   | 0.98 | 0.15 | -    | 31,31,31,31                 | 0     |
| 56  | MG   | 1A    | 3870 | 1/1   | 0.91 | 0.12 | -    | 44,44,44,44                 | 0     |
| 56  | MG   | 10    | 102  | 1/1   | 0.98 | 0.20 | -    | 62,62,62,62                 | 0     |
| 56  | MG   | 1A    | 3531 | 1/1   | 0.94 | 0.14 | -    | 53,53,53,53                 | 0     |
| 56  | MG   | 1A    | 3852 | 1/1   | 0.90 | 0.15 | -    | 38,38,38,38                 | 0     |
| 56  | MG   | 2A    | 3052 | 1/1   | 0.87 | 0.19 | -    | 50,50,50,50                 | 0     |
| 56  | MG   | 1a    | 1634 | 1/1   | 0.85 | 0.17 | -    | 61,61,61,61                 | 0     |
| 56  | MG   | 1A    | 3365 | 1/1   | 0.93 | 0.17 | -    | 48,48,48,48                 | 0     |
| 56  | MG   | 1A    | 3784 | 1/1   | 0.73 | 0.14 | -    | 63,63,63,63                 | 0     |
| 56  | MG   | 2A    | 3070 | 1/1   | 0.93 | 0.15 | -    | 28,28,28,28                 | 0     |
| 56  | MG   | 1A    | 3128 | 1/1   | 0.97 | 0.27 | -    | 49,49,49,49                 | 0     |
| 56  | MG   | 1A    | 3346 | 1/1   | 0.98 | 0.20 | -    | 41,41,41,41                 | 0     |
| 56  | MG   | 1A    | 3643 | 1/1   | 0.93 | 0.19 | -    | 30,30,30,30                 | 0     |
| 56  | MG   | 10    | 101  | 1/1   | 0.74 | 0.31 | -    | 59,59,59,59                 | 0     |
| 56  | MG   | 1A    | 3802 | 1/1   | 0.97 | 0.10 | -    | 60,60,60,60                 | 0     |
| 56  | MG   | 1A    | 3884 | 1/1   | 0.93 | 0.13 | -    | 52,52,52,52                 | 0     |
| 56  | MG   | 1A    | 3081 | 1/1   | 0.89 | 0.20 | -    | 43,43,43,43                 | 0     |
| 56  | MG   | 1A    | 3492 | 1/1   | 0.93 | 0.11 | -    | 49,49,49,49                 | 0     |
| 56  | MG   | 2a    | 1620 | 1/1   | 0.96 | 0.09 | -    | 58,58,58,58                 | 0     |
| 56  | MG   | 1A    | 3135 | 1/1   | 0.87 | 0.14 | -    | 49,49,49,49                 | 0     |
| 56  | MG   | 2A    | 3331 | 1/1   | 0.98 | 0.20 | -    | 39,39,39,39                 | 0     |
| 56  | MG   | 2A    | 3105 | 1/1   | 0.93 | 0.19 | -    | 49,49,49,49                 | 0     |
| 56  | MG   | 2q    | 3001 | 1/1   | 0.91 | 0.05 | -    | 66,66,66,66                 | 0     |
| 56  | MG   | 1A    | 3757 | 1/1   | 0.77 | 0.09 | -    | 44,44,44,44                 | 0     |
| 56  | MG   | 1A    | 3708 | 1/1   | 0.96 | 0.20 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | 1D    | 303  | 1/1   | 0.97 | 0.30 | -    | 25,25,25,25                 | 0     |
| 56  | MG   | 2a    | 1654 | 1/1   | 0.94 | 0.13 | -    | 64,64,64,64                 | 0     |
| 56  | MG   | 2A    | 3248 | 1/1   | 0.83 | 0.12 | -    | 52,52,52,52                 | 0     |
| 56  | MG   | 1a    | 1807 | 1/1   | 0.88 | 0.15 | -    | 84,84,84,84                 | 0     |
| 56  | MG   | 2A    | 3002 | 1/1   | 0.89 | 0.23 | -    | 53,53,53,53                 | 0     |
| 56  | MG   | 2a    | 1765 | 1/1   | 0.95 | 0.10 | -    | 53,53,53,53                 | 0     |
| 56  | MG   | 1A    | 3552 | 1/1   | 0.97 | 0.16 | -    | 22,22,22,22                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56  | MG   | 2A    | 3370 | 1/1   | 0.94 | 0.11 | -    | 42,42,42,42                 | 0     |
| 56  | MG   | 1A    | 3588 | 1/1   | 0.97 | 0.29 | -    | 39,39,39,39                 | 0     |
| 56  | MG   | 1A    | 3961 | 1/1   | 0.93 | 0.34 | -    | 45,45,45,45                 | 0     |
| 56  | MG   | 2A    | 3600 | 1/1   | 0.97 | 0.10 | -    | 42,42,42,42                 | 0     |
| 56  | MG   | 1A    | 3799 | 1/1   | 0.86 | 0.36 | -    | 55,55,55,55                 | 0     |
| 56  | MG   | 1a    | 1749 | 1/1   | 0.95 | 0.09 | -    | 56,56,56,56                 | 0     |
| 56  | MG   | 2A    | 3274 | 1/1   | 0.94 | 0.15 | -    | 48,48,48,48                 | 0     |
| 56  | MG   | 1A    | 3180 | 1/1   | 0.94 | 0.13 | -    | 56,56,56,56                 | 0     |
| 56  | MG   | 1R    | 202  | 1/1   | 0.97 | 0.22 | -    | 36,36,36,36                 | 0     |
| 56  | MG   | 1A    | 3025 | 1/1   | 0.80 | 0.12 | -    | 44,44,44,44                 | 0     |
| 56  | MG   | 2a    | 1751 | 1/1   | 0.95 | 0.15 | -    | 65,65,65,65                 | 0     |
| 56  | MG   | 2A    | 3532 | 1/1   | 0.76 | 0.11 | -    | 69,69,69,69                 | 0     |
| 56  | MG   | 1a    | 1739 | 1/1   | 0.92 | 0.11 | -    | 51,51,51,51                 | 0     |
| 56  | MG   | 1a    | 1828 | 1/1   | 0.83 | 0.12 | -    | 62,62,62,62                 | 0     |
| 56  | MG   | 2A    | 3626 | 1/1   | 0.93 | 0.12 | -    | 49,49,49,49                 | 0     |
| 56  | MG   | 1A    | 3537 | 1/1   | 0.95 | 0.14 | -    | 40,40,40,40                 | 0     |
| 56  | MG   | 1A    | 3889 | 1/1   | 0.94 | 0.13 | -    | 36,36,36,36                 | 0     |
| 56  | MG   | 1A    | 3360 | 1/1   | 0.86 | 0.21 | -    | 50,50,50,50                 | 0     |
| 56  | MG   | 2a    | 1678 | 1/1   | 0.90 | 0.12 | -    | 64,64,64,64                 | 0     |
| 56  | MG   | 1A    | 3558 | 1/1   | 0.71 | 0.12 | -    | 51,51,51,51                 | 0     |
| 56  | MG   | 2A    | 3077 | 1/1   | 0.90 | 0.12 | -    | 43,43,43,43                 | 0     |
| 56  | MG   | 2E    | 303  | 1/1   | 0.90 | 0.13 | -    | 42,42,42,42                 | 0     |
| 56  | MG   | 2A    | 3063 | 1/1   | 0.93 | 0.16 | -    | 43,43,43,43                 | 0     |
| 56  | MG   | 1A    | 3745 | 1/1   | 0.95 | 0.14 | -    | 61,61,61,61                 | 0     |
| 56  | MG   | 1B    | 3013 | 1/1   | 0.94 | 0.09 | -    | 53,53,53,53                 | 0     |
| 56  | MG   | 1A    | 3370 | 1/1   | 0.88 | 0.21 | -    | 42,42,42,42                 | 0     |
| 56  | MG   | 1A    | 3375 | 1/1   | 0.96 | 0.16 | -    | 32,32,32,32                 | 0     |
| 56  | MG   | 2a    | 1664 | 1/1   | 0.84 | 0.15 | -    | 71,71,71,71                 | 0     |
| 56  | MG   | 2A    | 3506 | 1/1   | 0.94 | 0.12 | -    | 50,50,50,50                 | 0     |
| 56  | MG   | 1a    | 1784 | 1/1   | 0.94 | 0.08 | -    | 58,58,58,58                 | 0     |
| 56  | MG   | 2A    | 3386 | 1/1   | 0.80 | 0.11 | -    | 50,50,50,50                 | 0     |
| 56  | MG   | 2A    | 3411 | 1/1   | 0.98 | 0.23 | -    | 50,50,50,50                 | 0     |
| 56  | MG   | 1a    | 1758 | 1/1   | 0.89 | 0.14 | -    | 55,55,55,55                 | 0     |
| 56  | MG   | 1A    | 3951 | 1/1   | 0.97 | 0.22 | -    | 33,33,33,33                 | 0     |
| 56  | MG   | 2a    | 1753 | 1/1   | 0.89 | 0.07 | -    | 80,80,80,80                 | 0     |
| 56  | MG   | 2A    | 3628 | 1/1   | 0.94 | 0.16 | -    | 46,46,46,46                 | 0     |
| 56  | MG   | 1A    | 3711 | 1/1   | 0.97 | 0.17 | -    | 41,41,41,41                 | 0     |
| 56  | MG   | 1A    | 3014 | 1/1   | 0.95 | 0.18 | -    | 32,32,32,32                 | 0     |
| 56  | MG   | 2A    | 3136 | 1/1   | 0.92 | 0.20 | -    | 45,45,45,45                 | 0     |
| 56  | MG   | 2a    | 1709 | 1/1   | 0.85 | 0.12 | -    | 68,68,68,68                 | 0     |
| 56  | MG   | 1A    | 3140 | 1/1   | 0.97 | 0.22 | -    | 41,41,41,41                 | 0     |
| 56  | MG   | 17    | 102  | 1/1   | 0.87 | 0.11 | -    | 50,50,50,50                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56  | MG   | 1A    | 3797 | 1/1   | 0.92 | 0.15 | -    | 57,57,57,57                 | 0     |
| 56  | MG   | 2A    | 3259 | 1/1   | 0.94 | 0.15 | -    | 43,43,43,43                 | 0     |
| 56  | MG   | 1A    | 3534 | 1/1   | 0.94 | 0.08 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | 15    | 103  | 1/1   | 0.97 | 0.09 | -    | 53,53,53,53                 | 0     |
| 56  | MG   | 1A    | 3543 | 1/1   | 0.92 | 0.17 | -    | 55,55,55,55                 | 0     |
| 56  | MG   | 1A    | 3023 | 1/1   | 0.82 | 0.36 | -    | 57,57,57,57                 | 0     |
| 56  | MG   | 1A    | 3037 | 1/1   | 0.96 | 0.09 | -    | 38,38,38,38                 | 0     |
| 56  | MG   | 1A    | 3263 | 1/1   | 0.96 | 0.23 | -    | 41,41,41,41                 | 0     |
| 56  | MG   | 1A    | 3147 | 1/1   | 0.92 | 0.18 | -    | 34,34,34,34                 | 0     |
| 56  | MG   | 1a    | 1774 | 1/1   | 0.90 | 0.09 | -    | 48,48,48,48                 | 0     |
| 56  | MG   | 2A    | 3062 | 1/1   | 0.97 | 0.16 | -    | 42,42,42,42                 | 0     |
| 56  | MG   | 1A    | 3662 | 1/1   | 0.79 | 0.20 | -    | 55,55,55,55                 | 0     |
| 56  | MG   | 2A    | 3178 | 1/1   | 0.97 | 0.20 | -    | 43,43,43,43                 | 0     |
| 56  | MG   | 1a    | 1751 | 1/1   | 0.93 | 0.18 | -    | 45,45,45,45                 | 0     |
| 56  | MG   | 2A    | 3636 | 1/1   | 0.81 | 0.17 | -    | 55,55,55,55                 | 0     |
| 56  | MG   | 1a    | 1721 | 1/1   | 0.82 | 0.17 | -    | 66,66,66,66                 | 0     |
| 56  | MG   | 1A    | 3776 | 1/1   | 0.96 | 0.21 | -    | 45,45,45,45                 | 0     |
| 56  | MG   | 2a    | 1791 | 1/1   | 0.81 | 0.13 | -    | 63,63,63,63                 | 0     |
| 56  | MG   | 1x    | 3008 | 1/1   | 0.89 | 0.22 | -    | 61,61,61,61                 | 0     |
| 56  | MG   | 1A    | 3490 | 1/1   | 0.87 | 0.10 | -    | 53,53,53,53                 | 0     |
| 56  | MG   | 1a    | 1609 | 1/1   | 0.90 | 0.12 | -    | 54,54,54,54                 | 0     |
| 56  | MG   | 2a    | 1691 | 1/1   | 0.94 | 0.14 | -    | 57,57,57,57                 | 0     |
| 56  | MG   | 1a    | 1685 | 1/1   | 0.90 | 0.07 | -    | 66,66,66,66                 | 0     |
| 56  | MG   | 1A    | 3155 | 1/1   | 0.96 | 0.14 | -    | 48,48,48,48                 | 0     |
| 56  | MG   | 1a    | 1728 | 1/1   | 0.98 | 0.15 | -    | 49,49,49,49                 | 0     |
| 56  | MG   | 2a    | 1770 | 1/1   | 0.96 | 0.20 | -    | 41,41,41,41                 | 0     |
| 56  | MG   | 1a    | 1647 | 1/1   | 0.92 | 0.16 | -    | 60,60,60,60                 | 0     |
| 56  | MG   | 1A    | 3649 | 1/1   | 0.62 | 0.15 | -    | 58,58,58,58                 | 0     |
| 56  | MG   | 2A    | 3544 | 1/1   | 0.97 | 0.10 | -    | 53,53,53,53                 | 0     |
| 56  | MG   | 2a    | 1625 | 1/1   | 0.79 | 0.15 | -    | 71,71,71,71                 | 0     |
| 56  | MG   | 2A    | 3244 | 1/1   | 0.85 | 0.14 | -    | 43,43,43,43                 | 0     |
| 56  | MG   | 1A    | 3034 | 1/1   | 0.95 | 0.25 | -    | 35,35,35,35                 | 0     |
| 56  | MG   | 2a    | 1783 | 1/1   | 0.86 | 0.18 | -    | 60,60,60,60                 | 0     |
| 56  | MG   | 2A    | 3213 | 1/1   | 0.94 | 0.14 | -    | 45,45,45,45                 | 0     |
| 56  | MG   | 2A    | 3100 | 1/1   | 0.87 | 0.10 | -    | 52,52,52,52                 | 0     |
| 56  | MG   | 1A    | 3418 | 1/1   | 0.93 | 0.20 | -    | 34,34,34,34                 | 0     |
| 56  | MG   | 1A    | 3626 | 1/1   | 0.90 | 0.12 | -    | 56,56,56,56                 | 0     |
| 56  | MG   | 1A    | 3385 | 1/1   | 0.86 | 0.18 | -    | 42,42,42,42                 | 0     |
| 56  | MG   | 1A    | 3415 | 1/1   | 0.94 | 0.16 | -    | 28,28,28,28                 | 0     |
| 56  | MG   | 2A    | 3141 | 1/1   | 0.91 | 0.12 | -    | 29,29,29,29                 | 0     |
| 56  | MG   | 1A    | 3099 | 1/1   | 0.82 | 0.17 | -    | 51,51,51,51                 | 0     |
| 56  | MG   | 1A    | 3763 | 1/1   | 0.97 | 0.19 | -    | 39,39,39,39                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56  | MG   | 1A    | 3800 | 1/1   | 0.87 | 0.19 | -    | 54,54,54,54                 | 0     |
| 56  | MG   | 1A    | 3254 | 1/1   | 0.89 | 0.26 | -    | 58,58,58,58                 | 0     |
| 56  | MG   | 1a    | 1783 | 1/1   | 0.94 | 0.12 | -    | 63,63,63,63                 | 0     |
| 56  | MG   | 2A    | 3422 | 1/1   | 0.96 | 0.12 | -    | 43,43,43,43                 | 0     |
| 56  | MG   | 2A    | 3480 | 1/1   | 0.94 | 0.19 | -    | 72,72,72,72                 | 0     |
| 56  | MG   | 1a    | 1668 | 1/1   | 0.89 | 0.12 | -    | 52,52,52,52                 | 0     |
| 56  | MG   | 1A    | 3338 | 1/1   | 0.96 | 0.08 | -    | 36,36,36,36                 | 0     |
| 56  | MG   | 2a    | 1627 | 1/1   | 0.97 | 0.08 | -    | 46,46,46,46                 | 0     |
| 56  | MG   | 2A    | 3350 | 1/1   | 0.96 | 0.12 | -    | 38,38,38,38                 | 0     |
| 56  | MG   | 2A    | 3427 | 1/1   | 0.97 | 0.14 | -    | 42,42,42,42                 | 0     |
| 56  | MG   | 2a    | 1604 | 1/1   | 0.93 | 0.08 | -    | 60,60,60,60                 | 0     |
| 56  | MG   | 2A    | 3584 | 1/1   | 0.90 | 0.27 | -    | 58,58,58,58                 | 0     |
| 56  | MG   | 12    | 3001 | 1/1   | 0.93 | 0.17 | -    | 53,53,53,53                 | 0     |
| 56  | MG   | 1A    | 3709 | 1/1   | 0.89 | 0.16 | -    | 43,43,43,43                 | 0     |
| 56  | MG   | 1A    | 3201 | 1/1   | 0.96 | 0.20 | -    | 39,39,39,39                 | 0     |
| 56  | MG   | 1a    | 1716 | 1/1   | 0.95 | 0.14 | -    | 62,62,62,62                 | 0     |
| 56  | MG   | 1A    | 3225 | 1/1   | 0.82 | 0.23 | -    | 55,55,55,55                 | 0     |
| 56  | MG   | 1A    | 3277 | 1/1   | 0.93 | 0.22 | -    | 57,57,57,57                 | 0     |
| 56  | MG   | 1A    | 3510 | 1/1   | 0.94 | 0.17 | -    | 25,25,25,25                 | 0     |
| 56  | MG   | 1A    | 3157 | 1/1   | 0.89 | 0.18 | -    | 39,39,39,39                 | 0     |
| 56  | MG   | 2a    | 1724 | 1/1   | 0.78 | 0.16 | -    | 83,83,83,83                 | 0     |
| 56  | MG   | 1A    | 3302 | 1/1   | 0.93 | 0.28 | -    | 30,30,30,30                 | 0     |
| 56  | MG   | 2A    | 3170 | 1/1   | 0.92 | 0.13 | -    | 58,58,58,58                 | 0     |
| 56  | MG   | 2A    | 3186 | 1/1   | 0.95 | 0.19 | -    | 43,43,43,43                 | 0     |
| 56  | MG   | 2a    | 1759 | 1/1   | 0.93 | 0.10 | -    | 76,76,76,76                 | 0     |
| 56  | MG   | 1w    | 3003 | 1/1   | 0.85 | 0.32 | -    | 78,78,78,78                 | 0     |
| 56  | MG   | 1A    | 3689 | 1/1   | 0.94 | 0.16 | -    | 35,35,35,35                 | 0     |
| 56  | MG   | 2a    | 1713 | 1/1   | 0.97 | 0.11 | -    | 49,49,49,49                 | 0     |
| 56  | MG   | 2A    | 3577 | 1/1   | 0.81 | 0.23 | -    | 61,61,61,61                 | 0     |
| 56  | MG   | 2a    | 1769 | 1/1   | 0.83 | 0.11 | -    | 73,73,73,73                 | 0     |
| 56  | MG   | 2B    | 3017 | 1/1   | 0.95 | 0.31 | -    | 63,63,63,63                 | 0     |
| 56  | MG   | 1a    | 1694 | 1/1   | 0.96 | 0.20 | -    | 66,66,66,66                 | 0     |
| 56  | MG   | 1A    | 3504 | 1/1   | 0.95 | 0.17 | -    | 50,50,50,50                 | 0     |
| 56  | MG   | 2A    | 3554 | 1/1   | 0.94 | 0.07 | -    | 45,45,45,45                 | 0     |
| 56  | MG   | 2A    | 3364 | 1/1   | 0.96 | 0.14 | -    | 31,31,31,31                 | 0     |
| 56  | MG   | 2a    | 1660 | 1/1   | 0.95 | 0.09 | -    | 61,61,61,61                 | 0     |
| 56  | MG   | 2A    | 3392 | 1/1   | 0.95 | 0.17 | -    | 55,55,55,55                 | 0     |
| 56  | MG   | 2A    | 3312 | 1/1   | 0.93 | 0.16 | -    | 48,48,48,48                 | 0     |
| 56  | MG   | 2A    | 3344 | 1/1   | 0.97 | 0.10 | -    | 30,30,30,30                 | 0     |
| 56  | MG   | 2a    | 1788 | 1/1   | 0.93 | 0.16 | -    | 68,68,68,68                 | 0     |
| 56  | MG   | 1w    | 3004 | 1/1   | 0.86 | 0.16 | -    | 51,51,51,51                 | 0     |
| 56  | MG   | 2A    | 3014 | 1/1   | 0.94 | 0.12 | -    | 38,38,38,38                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56  | MG   | 2a    | 1670 | 1/1   | 0.88 | 0.19 | -    | 53,53,53,53                 | 0     |
| 56  | MG   | 1a    | 1785 | 1/1   | 0.97 | 0.20 | -    | 41,41,41,41                 | 0     |
| 56  | MG   | 2A    | 3129 | 1/1   | 0.96 | 0.23 | -    | 41,41,41,41                 | 0     |
| 56  | MG   | 1x    | 3005 | 1/1   | 0.81 | 0.20 | -    | 66,66,66,66                 | 0     |
| 56  | MG   | 2A    | 3137 | 1/1   | 0.89 | 0.34 | -    | 42,42,42,42                 | 0     |
| 56  | MG   | 2A    | 3634 | 1/1   | 0.92 | 0.17 | -    | 38,38,38,38                 | 0     |
| 56  | MG   | 1a    | 1630 | 1/1   | 0.86 | 0.19 | -    | 57,57,57,57                 | 0     |
| 56  | MG   | 1a    | 1782 | 1/1   | 0.92 | 0.17 | -    | 44,44,44,44                 | 0     |
| 56  | MG   | 1a    | 1688 | 1/1   | 0.93 | 0.12 | -    | 44,44,44,44                 | 0     |
| 56  | MG   | 2A    | 3672 | 1/1   | 0.98 | 0.25 | -    | 41,41,41,41                 | 0     |
| 56  | MG   | 1Q    | 206  | 1/1   | 0.74 | 0.22 | -    | 54,54,54,54                 | 0     |
| 56  | MG   | 2A    | 3635 | 1/1   | 0.96 | 0.11 | -    | 38,38,38,38                 | 0     |
| 56  | MG   | 1A    | 3907 | 1/1   | 0.92 | 0.24 | -    | 40,40,40,40                 | 0     |
| 56  | MG   | 2A    | 3602 | 1/1   | 0.94 | 0.07 | -    | 50,50,50,50                 | 0     |
| 56  | MG   | 2A    | 3372 | 1/1   | 0.98 | 0.22 | -    | 41,41,41,41                 | 0     |
| 56  | MG   | 2A    | 3445 | 1/1   | 0.96 | 0.08 | -    | 39,39,39,39                 | 0     |
| 56  | MG   | 2a    | 1686 | 1/1   | 0.94 | 0.32 | -    | 66,66,66,66                 | 0     |
| 56  | MG   | 1a    | 1766 | 1/1   | 0.94 | 0.16 | -    | 59,59,59,59                 | 0     |
| 56  | MG   | 1A    | 3544 | 1/1   | 0.95 | 0.09 | -    | 54,54,54,54                 | 0     |
| 56  | MG   | 1A    | 3730 | 1/1   | 0.95 | 0.12 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | 1A    | 3224 | 1/1   | 0.89 | 0.17 | -    | 51,51,51,51                 | 0     |
| 56  | MG   | 1A    | 3022 | 1/1   | 0.95 | 0.15 | -    | 27,27,27,27                 | 0     |
| 56  | MG   | 2A    | 3530 | 1/1   | 0.78 | 0.10 | -    | 52,52,52,52                 | 0     |
| 56  | MG   | 1A    | 3495 | 1/1   | 0.95 | 0.20 | -    | 43,43,43,43                 | 0     |
| 56  | MG   | 1S    | 3002 | 1/1   | 0.95 | 0.13 | -    | 53,53,53,53                 | 0     |
| 56  | MG   | 1A    | 3393 | 1/1   | 0.93 | 0.14 | -    | 35,35,35,35                 | 0     |
| 56  | MG   | 1a    | 1776 | 1/1   | 0.90 | 0.14 | -    | 63,63,63,63                 | 0     |
| 56  | MG   | 2A    | 3462 | 1/1   | 0.95 | 0.13 | -    | 57,57,57,57                 | 0     |
| 56  | MG   | 1A    | 3563 | 1/1   | 0.95 | 0.09 | -    | 33,33,33,33                 | 0     |
| 56  | MG   | 2A    | 3234 | 1/1   | 0.79 | 0.11 | -    | 54,54,54,54                 | 0     |
| 56  | MG   | 1A    | 3786 | 1/1   | 0.98 | 0.16 | -    | 36,36,36,36                 | 0     |
| 56  | MG   | 1A    | 3054 | 1/1   | 0.91 | 0.22 | -    | 54,54,54,54                 | 0     |
| 56  | MG   | 1A    | 3694 | 1/1   | 0.95 | 0.17 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | 2A    | 3334 | 1/1   | 0.94 | 0.12 | -    | 44,44,44,44                 | 0     |
| 56  | MG   | 2E    | 304  | 1/1   | 0.95 | 0.12 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | 1A    | 3667 | 1/1   | 0.75 | 0.11 | -    | 45,45,45,45                 | 0     |
| 56  | MG   | 1A    | 3298 | 1/1   | 0.98 | 0.21 | -    | 33,33,33,33                 | 0     |
| 56  | MG   | 1A    | 3047 | 1/1   | 0.97 | 0.16 | -    | 35,35,35,35                 | 0     |
| 56  | MG   | 1I    | 3001 | 1/1   | 0.91 | 0.09 | -    | 58,58,58,58                 | 0     |
| 56  | MG   | 1v    | 3001 | 1/1   | 0.92 | 0.12 | -    | 56,56,56,56                 | 0     |
| 56  | MG   | 1A    | 3706 | 1/1   | 0.88 | 0.13 | -    | 51,51,51,51                 | 0     |
| 56  | MG   | 2a    | 1666 | 1/1   | 0.95 | 0.13 | -    | 49,49,49,49                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56  | MG   | 1A    | 3194 | 1/1   | 0.94 | 0.18 | -    | 38,38,38,38                 | 0     |
| 56  | MG   | 1A    | 3739 | 1/1   | 0.95 | 0.09 | -    | 48,48,48,48                 | 0     |
| 56  | MG   | 1A    | 3404 | 1/1   | 0.98 | 0.14 | -    | 44,44,44,44                 | 0     |
| 56  | MG   | 2B    | 3010 | 1/1   | 0.95 | 0.10 | -    | 50,50,50,50                 | 0     |
| 56  | MG   | 1A    | 3699 | 1/1   | 0.88 | 0.16 | -    | 66,66,66,66                 | 0     |
| 56  | MG   | 1A    | 3382 | 1/1   | 0.96 | 0.18 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | 2A    | 3351 | 1/1   | 0.92 | 0.12 | -    | 46,46,46,46                 | 0     |
| 56  | MG   | 1A    | 3529 | 1/1   | 0.89 | 0.21 | -    | 54,54,54,54                 | 0     |
| 56  | MG   | 2A    | 3528 | 1/1   | 0.95 | 0.10 | -    | 55,55,55,55                 | 0     |
| 56  | MG   | 1a    | 1613 | 1/1   | 0.86 | 0.20 | -    | 62,62,62,62                 | 0     |
| 56  | MG   | 2A    | 3059 | 1/1   | 0.98 | 0.10 | -    | 46,46,46,46                 | 0     |
| 56  | MG   | 1A    | 3427 | 1/1   | 0.92 | 0.16 | -    | 39,39,39,39                 | 0     |
| 56  | MG   | 2B    | 3012 | 1/1   | 0.98 | 0.19 | -    | 51,51,51,51                 | 0     |
| 56  | MG   | 1A    | 3341 | 1/1   | 0.74 | 0.22 | -    | 60,60,60,60                 | 0     |
| 56  | MG   | 1a    | 1740 | 1/1   | 0.96 | 0.11 | -    | 45,45,45,45                 | 0     |
| 56  | MG   | 2A    | 3271 | 1/1   | 0.87 | 0.14 | -    | 34,34,34,34                 | 0     |
| 56  | MG   | 2a    | 1603 | 1/1   | 0.90 | 0.20 | -    | 65,65,65,65                 | 0     |
| 56  | MG   | 2A    | 3175 | 1/1   | 0.94 | 0.24 | -    | 54,54,54,54                 | 0     |
| 56  | MG   | 1A    | 3109 | 1/1   | 0.96 | 0.56 | -    | 34,34,34,34                 | 0     |
| 56  | MG   | 2a    | 1777 | 1/1   | 0.83 | 0.18 | -    | 77,77,77,77                 | 0     |
| 56  | MG   | 2A    | 3160 | 1/1   | 0.94 | 0.12 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | 2a    | 1749 | 1/1   | 0.96 | 0.19 | -    | 58,58,58,58                 | 0     |
| 56  | MG   | 1A    | 3055 | 1/1   | 0.92 | 0.18 | -    | 50,50,50,50                 | 0     |
| 56  | MG   | 1P    | 204  | 1/1   | 0.90 | 0.27 | -    | 42,42,42,42                 | 0     |
| 56  | MG   | 2A    | 3126 | 1/1   | 0.86 | 0.21 | -    | 53,53,53,53                 | 0     |
| 56  | MG   | 1A    | 3847 | 1/1   | 0.78 | 0.52 | -    | 74,74,74,74                 | 0     |
| 56  | MG   | 2A    | 3322 | 1/1   | 0.97 | 0.13 | -    | 49,49,49,49                 | 0     |
| 56  | MG   | 2a    | 1771 | 1/1   | 0.85 | 0.23 | -    | 63,63,63,63                 | 0     |
| 56  | MG   | 2a    | 1610 | 1/1   | 0.96 | 0.33 | -    | 52,52,52,52                 | 0     |
| 56  | MG   | 2A    | 3446 | 1/1   | 0.92 | 0.10 | -    | 43,43,43,43                 | 0     |
| 56  | MG   | 1a    | 1814 | 1/1   | 0.93 | 0.19 | -    | 57,57,57,57                 | 0     |
| 56  | MG   | 2A    | 3221 | 1/1   | 0.96 | 0.20 | -    | 43,43,43,43                 | 0     |
| 56  | MG   | 1A    | 3216 | 1/1   | 0.97 | 0.41 | -    | 36,36,36,36                 | 0     |
| 56  | MG   | 2A    | 3403 | 1/1   | 0.97 | 0.17 | -    | 37,37,37,37                 | 0     |
| 56  | MG   | 1a    | 1675 | 1/1   | 0.98 | 0.08 | -    | 40,40,40,40                 | 0     |
| 56  | MG   | 1a    | 1697 | 1/1   | 0.79 | 0.14 | -    | 63,63,63,63                 | 0     |
| 56  | MG   | 2a    | 1796 | 1/1   | 0.94 | 0.15 | -    | 60,60,60,60                 | 0     |
| 56  | MG   | 2A    | 3122 | 1/1   | 0.93 | 0.19 | -    | 60,60,60,60                 | 0     |
| 56  | MG   | 1a    | 1748 | 1/1   | 0.90 | 0.10 | -    | 58,58,58,58                 | 0     |
| 56  | MG   | 1A    | 3101 | 1/1   | 0.92 | 0.29 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | 1A    | 3124 | 1/1   | 0.91 | 0.17 | -    | 51,51,51,51                 | 0     |
| 56  | MG   | 1A    | 3557 | 1/1   | 0.94 | 0.11 | -    | 44,44,44,44                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56  | MG   | 1A    | 3788 | 1/1   | 0.84 | 0.16 | -    | 24,24,24,24                 | 0     |
| 56  | MG   | 1e    | 201  | 1/1   | 0.93 | 0.30 | -    | 60,60,60,60                 | 0     |
| 56  | MG   | 2a    | 1694 | 1/1   | 0.96 | 0.21 | -    | 62,62,62,62                 | 0     |
| 56  | MG   | 2A    | 3460 | 1/1   | 0.98 | 0.12 | -    | 40,40,40,40                 | 0     |
| 56  | MG   | 2A    | 3670 | 1/1   | 0.97 | 0.16 | -    | 57,57,57,57                 | 0     |
| 56  | MG   | 1A    | 3755 | 1/1   | 0.79 | 0.13 | -    | 55,55,55,55                 | 0     |
| 56  | MG   | 1A    | 3177 | 1/1   | 0.92 | 0.13 | -    | 44,44,44,44                 | 0     |
| 56  | MG   | 1A    | 3526 | 1/1   | 0.92 | 0.11 | -    | 49,49,49,49                 | 0     |
| 56  | MG   | 1A    | 3646 | 1/1   | 0.95 | 0.24 | -    | 36,36,36,36                 | 0     |
| 56  | MG   | 1A    | 3096 | 1/1   | 0.96 | 0.15 | -    | 22,22,22,22                 | 0     |
| 56  | MG   | 2A    | 3490 | 1/1   | 0.95 | 0.22 | -    | 48,48,48,48                 | 0     |
| 56  | MG   | 2A    | 3208 | 1/1   | 0.81 | 0.14 | -    | 45,45,45,45                 | 0     |
| 56  | MG   | 1A    | 3082 | 1/1   | 0.94 | 0.16 | -    | 41,41,41,41                 | 0     |
| 56  | MG   | 1A    | 3439 | 1/1   | 0.94 | 0.17 | -    | 43,43,43,43                 | 0     |
| 56  | MG   | 2a    | 1698 | 1/1   | 0.95 | 0.16 | -    | 57,57,57,57                 | 0     |
| 56  | MG   | 1A    | 3243 | 1/1   | 0.80 | 0.12 | -    | 56,56,56,56                 | 0     |
| 56  | MG   | 2A    | 3246 | 1/1   | 0.95 | 0.11 | -    | 56,56,56,56                 | 0     |
| 56  | MG   | 2A    | 3243 | 1/1   | 0.89 | 0.22 | -    | 53,53,53,53                 | 0     |
| 56  | MG   | 2x    | 102  | 1/1   | 0.87 | 0.11 | -    | 58,58,58,58                 | 0     |
| 56  | MG   | 1A    | 3803 | 1/1   | 0.81 | 0.15 | -    | 60,60,60,60                 | 0     |
| 56  | MG   | 2A    | 3379 | 1/1   | 0.93 | 0.15 | -    | 42,42,42,42                 | 0     |
| 56  | MG   | 1A    | 3937 | 1/1   | 0.96 | 0.25 | -    | 39,39,39,39                 | 0     |
| 56  | MG   | 1a    | 1691 | 1/1   | 0.67 | 0.21 | -    | 66,66,66,66                 | 0     |
| 56  | MG   | 1E    | 302  | 1/1   | 0.85 | 0.26 | -    | 43,43,43,43                 | 0     |
| 56  | MG   | 2A    | 3174 | 1/1   | 0.98 | 0.08 | -    | 42,42,42,42                 | 0     |
| 56  | MG   | 2A    | 3249 | 1/1   | 0.91 | 0.17 | -    | 30,30,30,30                 | 0     |
| 56  | MG   | 2a    | 1755 | 1/1   | 0.97 | 0.12 | -    | 61,61,61,61                 | 0     |
| 56  | MG   | 2A    | 3289 | 1/1   | 0.95 | 0.12 | -    | 60,60,60,60                 | 0     |
| 56  | MG   | 2a    | 1772 | 1/1   | 0.95 | 0.11 | -    | 52,52,52,52                 | 0     |
| 56  | MG   | 1A    | 3048 | 1/1   | 0.96 | 0.23 | -    | 32,32,32,32                 | 0     |
| 56  | MG   | 1B    | 3005 | 1/1   | 0.82 | 0.18 | -    | 58,58,58,58                 | 0     |
| 56  | MG   | 1x    | 3004 | 1/1   | 0.93 | 0.26 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | 1B    | 3001 | 1/1   | 0.98 | 0.25 | -    | 39,39,39,39                 | 0     |
| 56  | MG   | 2A    | 3335 | 1/1   | 0.99 | 0.09 | -    | 25,25,25,25                 | 0     |
| 56  | MG   | 2E    | 301  | 1/1   | 0.87 | 0.11 | -    | 36,36,36,36                 | 0     |
| 56  | MG   | 1a    | 1777 | 1/1   | 0.95 | 0.14 | -    | 47,47,47,47                 | 0     |
| 57  | K    | 1A    | 3321 | 1/1   | 0.93 | 0.14 | -    | 84,84,84,84                 | 0     |
| 56  | MG   | 1a    | 1643 | 1/1   | 0.95 | 0.33 | -    | 51,51,51,51                 | 0     |
| 56  | MG   | 2A    | 3232 | 1/1   | 0.94 | 0.12 | -    | 41,41,41,41                 | 0     |
| 56  | MG   | 1A    | 3294 | 1/1   | 0.97 | 0.17 | -    | 32,32,32,32                 | 0     |
| 56  | MG   | 1A    | 3189 | 1/1   | 0.97 | 0.15 | -    | 32,32,32,32                 | 0     |
| 56  | MG   | 2a    | 1663 | 1/1   | 0.96 | 0.24 | -    | 62,62,62,62                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56  | MG   | 2A    | 3591 | 1/1   | 0.95 | 0.20 | -    | 45,45,45,45                 | 0     |
| 56  | MG   | 1A    | 3830 | 1/1   | 0.91 | 0.14 | -    | 53,53,53,53                 | 0     |
| 56  | MG   | 2a    | 1608 | 1/1   | 0.76 | 0.14 | -    | 65,65,65,65                 | 0     |
| 56  | MG   | 1a    | 1665 | 1/1   | 0.77 | 0.25 | -    | 56,56,56,56                 | 0     |
| 56  | MG   | 1A    | 3523 | 1/1   | 0.92 | 0.15 | -    | 57,57,57,57                 | 0     |
| 56  | MG   | 1A    | 3348 | 1/1   | 0.92 | 0.23 | -    | 54,54,54,54                 | 0     |
| 56  | MG   | 2A    | 3053 | 1/1   | 0.89 | 0.18 | -    | 44,44,44,44                 | 0     |
| 56  | MG   | 1B    | 3021 | 1/1   | 0.86 | 0.10 | -    | 48,48,48,48                 | 0     |
| 56  | MG   | 2a    | 1711 | 1/1   | 0.94 | 0.18 | -    | 57,57,57,57                 | 0     |
| 56  | MG   | 2A    | 3268 | 1/1   | 0.96 | 0.12 | -    | 37,37,37,37                 | 0     |
| 56  | MG   | 2A    | 3019 | 1/1   | 0.94 | 0.17 | -    | 52,52,52,52                 | 0     |
| 56  | MG   | 1a    | 1769 | 1/1   | 0.93 | 0.15 | -    | 69,69,69,69                 | 0     |
| 56  | MG   | 2A    | 3220 | 1/1   | 0.94 | 0.20 | -    | 55,55,55,55                 | 0     |
| 56  | MG   | 2A    | 3032 | 1/1   | 0.92 | 0.15 | -    | 35,35,35,35                 | 0     |
| 56  | MG   | 13    | 102  | 1/1   | 0.88 | 0.16 | -    | 52,52,52,52                 | 0     |
| 56  | MG   | 2A    | 3557 | 1/1   | 0.94 | 0.14 | -    | 49,49,49,49                 | 0     |
| 56  | MG   | 1A    | 3676 | 1/1   | 0.98 | 0.25 | -    | 50,50,50,50                 | 0     |
| 56  | MG   | 1O    | 204  | 1/1   | 0.89 | 0.14 | -    | 52,52,52,52                 | 0     |
| 56  | MG   | 2A    | 3225 | 1/1   | 0.91 | 0.22 | -    | 53,53,53,53                 | 0     |
| 56  | MG   | 2a    | 1767 | 1/1   | 0.76 | 0.15 | -    | 74,74,74,74                 | 0     |
| 56  | MG   | 1A    | 3463 | 1/1   | 0.92 | 0.16 | -    | 25,25,25,25                 | 0     |
| 56  | MG   | 11    | 103  | 1/1   | 0.95 | 0.25 | -    | 45,45,45,45                 | 0     |
| 56  | MG   | 1A    | 3695 | 1/1   | 0.98 | 0.26 | -    | 42,42,42,42                 | 0     |
| 56  | MG   | 2A    | 3082 | 1/1   | 0.81 | 0.25 | -    | 45,45,45,45                 | 0     |
| 56  | MG   | 2A    | 3164 | 1/1   | 0.89 | 0.15 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | 1A    | 3318 | 1/1   | 0.99 | 0.18 | -    | 53,53,53,53                 | 0     |
| 56  | MG   | 2A    | 3231 | 1/1   | 0.91 | 0.14 | -    | 49,49,49,49                 | 0     |
| 56  | MG   | 2a    | 1742 | 1/1   | 0.94 | 0.16 | -    | 62,62,62,62                 | 0     |
| 56  | MG   | 2A    | 3675 | 1/1   | 0.93 | 0.26 | -    | 55,55,55,55                 | 0     |
| 56  | MG   | 2g    | 8001 | 1/1   | 0.94 | 0.10 | -    | 57,57,57,57                 | 0     |
| 56  | MG   | 2A    | 3409 | 1/1   | 0.97 | 0.24 | -    | 42,42,42,42                 | 0     |
| 56  | MG   | 2A    | 3288 | 1/1   | 0.96 | 0.10 | -    | 44,44,44,44                 | 0     |
| 56  | MG   | 1A    | 3460 | 1/1   | 0.86 | 0.15 | -    | 37,37,37,37                 | 0     |
| 56  | MG   | 1a    | 1711 | 1/1   | 0.87 | 0.11 | -    | 49,49,49,49                 | 0     |
| 56  | MG   | 2A    | 3352 | 1/1   | 0.96 | 0.20 | -    | 55,55,55,55                 | 0     |
| 56  | MG   | 1A    | 3813 | 1/1   | 0.95 | 0.31 | -    | 40,40,40,40                 | 0     |
| 56  | MG   | 1A    | 3214 | 1/1   | 0.72 | 0.18 | -    | 59,59,59,59                 | 0     |
| 56  | MG   | 1A    | 3002 | 1/1   | 0.96 | 0.31 | -    | 61,61,61,61                 | 0     |
| 56  | MG   | 1A    | 3250 | 1/1   | 0.94 | 0.36 | -    | 30,30,30,30                 | 0     |
| 56  | MG   | 1a    | 1699 | 1/1   | 0.94 | 0.08 | -    | 46,46,46,46                 | 0     |
| 56  | MG   | 1A    | 3618 | 1/1   | 0.88 | 0.07 | -    | 70,70,70,70                 | 0     |
| 56  | MG   | 2A    | 3433 | 1/1   | 0.97 | 0.16 | -    | 41,41,41,41                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56  | MG   | 1a    | 1820 | 1/1   | 0.88 | 0.15 | -    | 62,62,62,62                 | 0     |
| 56  | MG   | 2l    | 202  | 1/1   | 0.86 | 0.19 | -    | 62,62,62,62                 | 0     |
| 56  | MG   | 2A    | 3087 | 1/1   | 0.85 | 0.16 | -    | 55,55,55,55                 | 0     |
| 56  | MG   | 1A    | 3156 | 1/1   | 0.98 | 0.24 | -    | 34,34,34,34                 | 0     |
| 56  | MG   | 1Q    | 204  | 1/1   | 0.97 | 0.12 | -    | 55,55,55,55                 | 0     |
| 56  | MG   | 2A    | 3383 | 1/1   | 0.98 | 0.11 | -    | 46,46,46,46                 | 0     |
| 56  | MG   | 1A    | 3163 | 1/1   | 0.93 | 0.14 | -    | 41,41,41,41                 | 0     |
| 56  | MG   | 1A    | 3655 | 1/1   | 0.97 | 0.17 | -    | 52,52,52,52                 | 0     |
| 56  | MG   | 1A    | 3631 | 1/1   | 0.91 | 0.09 | -    | 67,67,67,67                 | 0     |
| 56  | MG   | 2A    | 3614 | 1/1   | 0.97 | 0.10 | -    | 54,54,54,54                 | 0     |
| 56  | MG   | 1A    | 3717 | 1/1   | 0.87 | 0.19 | -    | 60,60,60,60                 | 0     |
| 56  | MG   | 2A    | 3580 | 1/1   | 0.94 | 0.12 | -    | 38,38,38,38                 | 0     |
| 56  | MG   | 1A    | 3131 | 1/1   | 0.91 | 0.16 | -    | 44,44,44,44                 | 0     |
| 56  | MG   | 2A    | 3430 | 1/1   | 0.96 | 0.14 | -    | 56,56,56,56                 | 0     |
| 56  | MG   | 2a    | 1618 | 1/1   | 0.91 | 0.26 | -    | 67,67,67,67                 | 0     |
| 56  | MG   | 2a    | 1756 | 1/1   | 0.75 | 0.12 | -    | 49,49,49,49                 | 0     |
| 56  | MG   | 1A    | 3428 | 1/1   | 0.93 | 0.13 | -    | 43,43,43,43                 | 0     |
| 56  | MG   | 2A    | 3106 | 1/1   | 0.96 | 0.13 | -    | 28,28,28,28                 | 0     |
| 56  | MG   | 1A    | 3829 | 1/1   | 0.95 | 0.24 | -    | 59,59,59,59                 | 0     |
| 56  | MG   | 2A    | 3041 | 1/1   | 0.89 | 0.10 | -    | 59,59,59,59                 | 0     |
| 56  | MG   | 2a    | 1730 | 1/1   | 0.74 | 0.17 | -    | 71,71,71,71                 | 0     |
| 56  | MG   | 2A    | 3328 | 1/1   | 0.79 | 0.12 | -    | 39,39,39,39                 | 0     |
| 56  | MG   | 1B    | 3012 | 1/1   | 0.76 | 0.16 | -    | 66,66,66,66                 | 0     |
| 56  | MG   | 1a    | 1705 | 1/1   | 0.87 | 0.13 | -    | 56,56,56,56                 | 0     |
| 56  | MG   | 1A    | 3142 | 1/1   | 0.95 | 0.26 | -    | 17,17,17,17                 | 0     |
| 56  | MG   | 2A    | 3204 | 1/1   | 0.93 | 0.23 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | 2A    | 3261 | 1/1   | 0.93 | 0.19 | -    | 34,34,34,34                 | 0     |
| 56  | MG   | 1a    | 1676 | 1/1   | 0.74 | 0.17 | -    | 64,64,64,64                 | 0     |
| 56  | MG   | 2F    | 303  | 1/1   | 0.86 | 0.19 | -    | 58,58,58,58                 | 0     |
| 56  | MG   | 2a    | 1635 | 1/1   | 0.92 | 0.15 | -    | 49,49,49,49                 | 0     |
| 56  | MG   | 2A    | 3521 | 1/1   | 0.86 | 0.16 | -    | 63,63,63,63                 | 0     |
| 56  | MG   | 1A    | 3169 | 1/1   | 0.80 | 0.15 | -    | 44,44,44,44                 | 0     |
| 56  | MG   | 1a    | 1819 | 1/1   | 0.91 | 0.14 | -    | 61,61,61,61                 | 0     |
| 56  | MG   | 1a    | 1750 | 1/1   | 0.89 | 0.11 | -    | 41,41,41,41                 | 0     |
| 56  | MG   | 1T    | 201  | 1/1   | 0.94 | 0.19 | -    | 43,43,43,43                 | 0     |
| 56  | MG   | 1W    | 3006 | 1/1   | 0.93 | 0.15 | -    | 46,46,46,46                 | 0     |
| 56  | MG   | 2a    | 1646 | 1/1   | 0.91 | 0.14 | -    | 55,55,55,55                 | 0     |
| 56  | MG   | 1a    | 1787 | 1/1   | 0.98 | 0.14 | -    | 48,48,48,48                 | 0     |
| 56  | MG   | 1A    | 3262 | 1/1   | 0.89 | 0.23 | -    | 48,48,48,48                 | 0     |
| 56  | MG   | 1D    | 301  | 1/1   | 0.91 | 0.22 | -    | 46,46,46,46                 | 0     |
| 56  | MG   | 2A    | 3397 | 1/1   | 0.97 | 0.14 | -    | 36,36,36,36                 | 0     |
| 56  | MG   | 1F    | 301  | 1/1   | 0.96 | 0.15 | -    | 51,51,51,51                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56  | MG   | 1A    | 3166 | 1/1   | 0.95 | 0.25 | -    | 44,44,44,44                 | 0     |
| 56  | MG   | 1a    | 1663 | 1/1   | 0.97 | 0.10 | -    | 59,59,59,59                 | 0     |
| 56  | MG   | 1A    | 3107 | 1/1   | 0.94 | 0.12 | -    | 26,26,26,26                 | 0     |
| 56  | MG   | 1A    | 3758 | 1/1   | 0.72 | 0.14 | -    | 40,40,40,40                 | 0     |
| 56  | MG   | 1R    | 203  | 1/1   | 0.85 | 0.19 | -    | 44,44,44,44                 | 0     |
| 56  | MG   | 1A    | 3611 | 1/1   | 0.95 | 0.18 | -    | 46,46,46,46                 | 0     |
| 56  | MG   | 1a    | 1744 | 1/1   | 0.89 | 0.09 | -    | 53,53,53,53                 | 0     |
| 56  | MG   | 1A    | 3764 | 1/1   | 0.87 | 0.10 | -    | 40,40,40,40                 | 0     |
| 56  | MG   | 1W    | 3001 | 1/1   | 0.91 | 0.24 | -    | 43,43,43,43                 | 0     |
| 56  | MG   | 2A    | 3601 | 1/1   | 0.93 | 0.14 | -    | 49,49,49,49                 | 0     |
| 56  | MG   | 1A    | 3617 | 1/1   | 0.98 | 0.17 | -    | 26,26,26,26                 | 0     |
| 56  | MG   | 1A    | 3276 | 1/1   | 0.87 | 0.24 | -    | 51,51,51,51                 | 0     |
| 56  | MG   | 1A    | 3833 | 1/1   | 0.98 | 0.13 | -    | 54,54,54,54                 | 0     |
| 56  | MG   | 2a    | 1741 | 1/1   | 0.96 | 0.25 | -    | 48,48,48,48                 | 0     |
| 56  | MG   | 1a    | 1768 | 1/1   | 0.91 | 0.13 | -    | 56,56,56,56                 | 0     |
| 56  | MG   | 1A    | 3881 | 1/1   | 0.94 | 0.10 | -    | 48,48,48,48                 | 0     |
| 56  | MG   | 1A    | 3674 | 1/1   | 0.88 | 0.12 | -    | 53,53,53,53                 | 0     |
| 56  | MG   | 1a    | 1633 | 1/1   | 0.98 | 0.24 | -    | 52,52,52,52                 | 0     |
| 56  | MG   | 2A    | 3594 | 1/1   | 0.95 | 0.06 | -    | 48,48,48,48                 | 0     |
| 56  | MG   | 1a    | 1826 | 1/1   | 0.78 | 0.20 | -    | 72,72,72,72                 | 0     |
| 56  | MG   | 2A    | 3518 | 1/1   | 0.95 | 0.07 | -    | 50,50,50,50                 | 0     |
| 56  | MG   | 1A    | 3240 | 1/1   | 0.97 | 0.19 | -    | 40,40,40,40                 | 0     |
| 56  | MG   | 2A    | 3361 | 1/1   | 0.91 | 0.07 | -    | 58,58,58,58                 | 0     |
| 56  | MG   | 1A    | 3844 | 1/1   | 0.90 | 0.16 | -    | 64,64,64,64                 | 0     |
| 56  | MG   | 2a    | 1651 | 1/1   | 0.76 | 0.25 | -    | 70,70,70,70                 | 0     |
| 56  | MG   | 2A    | 3154 | 1/1   | 0.98 | 0.22 | -    | 41,41,41,41                 | 0     |
| 56  | MG   | 2A    | 3200 | 1/1   | 0.90 | 0.10 | -    | 46,46,46,46                 | 0     |
| 56  | MG   | 2A    | 3607 | 1/1   | 0.95 | 0.17 | -    | 60,60,60,60                 | 0     |
| 56  | MG   | 1A    | 3356 | 1/1   | 0.88 | 0.13 | -    | 35,35,35,35                 | 0     |
| 56  | MG   | 1A    | 3017 | 1/1   | 0.88 | 0.23 | -    | 31,31,31,31                 | 0     |
| 56  | MG   | 1A    | 3815 | 1/1   | 0.91 | 0.14 | -    | 60,60,60,60                 | 0     |
| 56  | MG   | 1a    | 1640 | 1/1   | 0.95 | 0.21 | -    | 41,41,41,41                 | 0     |
| 56  | MG   | 1a    | 1683 | 1/1   | 0.93 | 0.25 | -    | 64,64,64,64                 | 0     |
| 56  | MG   | 2A    | 3613 | 1/1   | 0.95 | 0.15 | -    | 64,64,64,64                 | 0     |
| 56  | MG   | 1G    | 202  | 1/1   | 0.96 | 0.15 | -    | 45,45,45,45                 | 0     |
| 56  | MG   | 1a    | 1742 | 1/1   | 0.86 | 0.16 | -    | 68,68,68,68                 | 0     |
| 56  | MG   | 1A    | 3119 | 1/1   | 0.96 | 0.43 | -    | 36,36,36,36                 | 0     |
| 56  | MG   | 1Q    | 202  | 1/1   | 0.94 | 0.26 | -    | 41,41,41,41                 | 0     |
| 56  | MG   | 2A    | 3369 | 1/1   | 0.93 | 0.10 | -    | 50,50,50,50                 | 0     |
| 56  | MG   | 2A    | 3138 | 1/1   | 0.94 | 0.14 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | 1A    | 3895 | 1/1   | 0.88 | 0.19 | -    | 40,40,40,40                 | 0     |
| 56  | MG   | 1a    | 1743 | 1/1   | 0.84 | 0.25 | -    | 63,63,63,63                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56  | MG   | 16    | 502  | 1/1   | 0.94 | 0.19 | -    | 51,51,51,51                 | 0     |
| 56  | MG   | 1x    | 3009 | 1/1   | 0.90 | 0.12 | -    | 58,58,58,58                 | 0     |
| 56  | MG   | 2A    | 3098 | 1/1   | 0.98 | 0.07 | -    | 37,37,37,37                 | 0     |
| 56  | MG   | 1A    | 3571 | 1/1   | 0.96 | 0.19 | -    | 39,39,39,39                 | 0     |
| 56  | MG   | 1Q    | 203  | 1/1   | 0.97 | 0.22 | -    | 33,33,33,33                 | 0     |
| 56  | MG   | 2A    | 3619 | 1/1   | 0.91 | 0.12 | -    | 55,55,55,55                 | 0     |
| 56  | MG   | 2A    | 3566 | 1/1   | 0.91 | 0.11 | -    | 38,38,38,38                 | 0     |
| 56  | MG   | 2A    | 3596 | 1/1   | 0.96 | 0.10 | -    | 42,42,42,42                 | 0     |
| 56  | MG   | 1A    | 3407 | 1/1   | 0.93 | 0.09 | -    | 34,34,34,34                 | 0     |
| 56  | MG   | 1A    | 3569 | 1/1   | 0.92 | 0.14 | -    | 50,50,50,50                 | 0     |
| 56  | MG   | 1a    | 1664 | 1/1   | 0.85 | 0.10 | -    | 57,57,57,57                 | 0     |
| 56  | MG   | 2A    | 3324 | 1/1   | 0.95 | 0.15 | -    | 50,50,50,50                 | 0     |
| 56  | MG   | 1A    | 3752 | 1/1   | 0.97 | 0.10 | -    | 37,37,37,37                 | 0     |
| 56  | MG   | 2a    | 1734 | 1/1   | 0.88 | 0.13 | -    | 70,70,70,70                 | 0     |
| 56  | MG   | 1A    | 3345 | 1/1   | 0.91 | 0.20 | -    | 35,35,35,35                 | 0     |
| 56  | MG   | 2B    | 3014 | 1/1   | 0.89 | 0.26 | -    | 65,65,65,65                 | 0     |
| 56  | MG   | 2A    | 3210 | 1/1   | 0.87 | 0.14 | -    | 40,40,40,40                 | 0     |
| 56  | MG   | 2A    | 3102 | 1/1   | 0.83 | 0.15 | -    | 49,49,49,49                 | 0     |
| 56  | MG   | 1a    | 1626 | 1/1   | 0.95 | 0.28 | -    | 45,45,45,45                 | 0     |
| 56  | MG   | 2a    | 1716 | 1/1   | 0.94 | 0.07 | -    | 52,52,52,52                 | 0     |
| 56  | MG   | 2Q    | 204  | 1/1   | 0.85 | 0.29 | -    | 44,44,44,44                 | 0     |
| 56  | MG   | 1A    | 3697 | 1/1   | 0.90 | 0.12 | -    | 57,57,57,57                 | 0     |
| 56  | MG   | 1A    | 3412 | 1/1   | 0.92 | 0.13 | -    | 35,35,35,35                 | 0     |
| 56  | MG   | 1A    | 3271 | 1/1   | 0.70 | 0.14 | -    | 71,71,71,71                 | 0     |
| 56  | MG   | 2A    | 3606 | 1/1   | 0.96 | 0.06 | -    | 51,51,51,51                 | 0     |
| 56  | MG   | 2B    | 3011 | 1/1   | 0.95 | 0.20 | -    | 55,55,55,55                 | 0     |
| 56  | MG   | 2A    | 3648 | 1/1   | 0.95 | 0.27 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | 2A    | 3194 | 1/1   | 0.95 | 0.21 | -    | 40,40,40,40                 | 0     |
| 56  | MG   | 2A    | 3611 | 1/1   | 0.97 | 0.08 | -    | 60,60,60,60                 | 0     |
| 56  | MG   | 1A    | 3916 | 1/1   | 0.99 | 0.31 | -    | 34,34,34,34                 | 0     |
| 56  | MG   | 2A    | 3537 | 1/1   | 0.92 | 0.09 | -    | 57,57,57,57                 | 0     |
| 56  | MG   | 1A    | 3828 | 1/1   | 0.93 | 0.16 | -    | 58,58,58,58                 | 0     |
| 56  | MG   | 2A    | 3629 | 1/1   | 0.97 | 0.07 | -    | 56,56,56,56                 | 0     |
| 56  | MG   | 1A    | 3036 | 1/1   | 0.92 | 0.23 | -    | 49,49,49,49                 | 0     |
| 56  | MG   | 1A    | 3158 | 1/1   | 0.97 | 0.14 | -    | 49,49,49,49                 | 0     |
| 56  | MG   | 2A    | 3491 | 1/1   | 0.82 | 0.17 | -    | 49,49,49,49                 | 0     |
| 56  | MG   | 1A    | 3133 | 1/1   | 0.91 | 0.20 | -    | 44,44,44,44                 | 0     |
| 56  | MG   | 1A    | 3816 | 1/1   | 0.94 | 0.47 | -    | 62,62,62,62                 | 0     |
| 56  | MG   | 2A    | 3005 | 1/1   | 0.89 | 0.19 | -    | 50,50,50,50                 | 0     |
| 56  | MG   | 1a    | 1671 | 1/1   | 0.94 | 0.18 | -    | 42,42,42,42                 | 0     |
| 56  | MG   | 2a    | 1766 | 1/1   | 0.95 | 0.11 | -    | 56,56,56,56                 | 0     |
| 56  | MG   | 2A    | 3498 | 1/1   | 0.87 | 0.11 | -    | 37,37,37,37                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56  | MG   | 1A    | 3383 | 1/1   | 0.92 | 0.21 | -    | 33,33,33,33                 | 0     |
| 56  | MG   | 2A    | 3110 | 1/1   | 0.89 | 0.34 | -    | 46,46,46,46                 | 0     |
| 56  | MG   | 2A    | 3011 | 1/1   | 0.84 | 0.18 | -    | 41,41,41,41                 | 0     |
| 56  | MG   | 1A    | 3712 | 1/1   | 0.97 | 0.22 | -    | 50,50,50,50                 | 0     |
| 56  | MG   | 2A    | 3321 | 1/1   | 0.95 | 0.24 | -    | 53,53,53,53                 | 0     |
| 56  | MG   | 2A    | 3360 | 1/1   | 0.94 | 0.09 | -    | 35,35,35,35                 | 0     |
| 56  | MG   | 1A    | 3085 | 1/1   | 0.84 | 0.18 | -    | 51,51,51,51                 | 0     |
| 56  | MG   | 2a    | 1623 | 1/1   | 0.88 | 0.15 | -    | 65,65,65,65                 | 0     |
| 56  | MG   | 1E    | 301  | 1/1   | 0.87 | 0.19 | -    | 27,27,27,27                 | 0     |
| 56  | MG   | 2A    | 3551 | 1/1   | 0.80 | 0.17 | -    | 51,51,51,51                 | 0     |
| 56  | MG   | 2A    | 3128 | 1/1   | 0.91 | 0.12 | -    | 49,49,49,49                 | 0     |
| 56  | MG   | 2A    | 3527 | 1/1   | 0.89 | 0.08 | -    | 53,53,53,53                 | 0     |
| 56  | MG   | 1B    | 3026 | 1/1   | 0.92 | 0.10 | -    | 62,62,62,62                 | 0     |
| 56  | MG   | 1A    | 3148 | 1/1   | 0.94 | 0.32 | -    | 31,31,31,31                 | 0     |
| 56  | MG   | 2A    | 3072 | 1/1   | 0.93 | 0.12 | -    | 40,40,40,40                 | 0     |
| 56  | MG   | 1A    | 3507 | 1/1   | 0.91 | 0.19 | -    | 34,34,34,34                 | 0     |
| 56  | MG   | 2A    | 3363 | 1/1   | 0.90 | 0.14 | -    | 30,30,30,30                 | 0     |
| 56  | MG   | 1A    | 3475 | 1/1   | 0.90 | 0.15 | -    | 37,37,37,37                 | 0     |
| 56  | MG   | 1a    | 1726 | 1/1   | 0.88 | 0.06 | -    | 57,57,57,57                 | 0     |
| 56  | MG   | 2a    | 1784 | 1/1   | 0.98 | 0.11 | -    | 56,56,56,56                 | 0     |
| 56  | MG   | 2A    | 3330 | 1/1   | 0.88 | 0.14 | -    | 44,44,44,44                 | 0     |
| 56  | MG   | 1A    | 3610 | 1/1   | 0.85 | 0.08 | -    | 56,56,56,56                 | 0     |
| 56  | MG   | 2a    | 1721 | 1/1   | 0.91 | 0.13 | -    | 61,61,61,61                 | 0     |
| 56  | MG   | 1a    | 1770 | 1/1   | 0.99 | 0.14 | -    | 44,44,44,44                 | 0     |
| 56  | MG   | 1A    | 3743 | 1/1   | 0.93 | 0.17 | -    | 38,38,38,38                 | 0     |
| 56  | MG   | 2A    | 3229 | 1/1   | 0.92 | 0.19 | -    | 53,53,53,53                 | 0     |
| 56  | MG   | 1A    | 3647 | 1/1   | 0.93 | 0.07 | -    | 45,45,45,45                 | 0     |
| 56  | MG   | 1A    | 3004 | 1/1   | 0.92 | 0.17 | -    | 28,28,28,28                 | 0     |
| 56  | MG   | 1A    | 3663 | 1/1   | 0.88 | 0.14 | -    | 46,46,46,46                 | 0     |
| 56  | MG   | 1a    | 1781 | 1/1   | 0.96 | 0.17 | -    | 63,63,63,63                 | 0     |
| 56  | MG   | 1A    | 3746 | 1/1   | 0.94 | 0.07 | -    | 45,45,45,45                 | 0     |
| 56  | MG   | 1A    | 3853 | 1/1   | 0.94 | 0.07 | -    | 41,41,41,41                 | 0     |
| 56  | MG   | 1a    | 1707 | 1/1   | 0.80 | 0.20 | -    | 62,62,62,62                 | 0     |
| 56  | MG   | 1A    | 3465 | 1/1   | 0.89 | 0.12 | -    | 32,32,32,32                 | 0     |
| 56  | MG   | 1A    | 3219 | 1/1   | 0.93 | 0.22 | -    | 40,40,40,40                 | 0     |
| 56  | MG   | 2a    | 1645 | 1/1   | 0.99 | 0.15 | -    | 50,50,50,50                 | 0     |
| 56  | MG   | 2a    | 1782 | 1/1   | 0.95 | 0.23 | -    | 71,71,71,71                 | 0     |
| 56  | MG   | 2A    | 3176 | 1/1   | 0.80 | 0.24 | -    | 52,52,52,52                 | 0     |
| 56  | MG   | 2p    | 3001 | 1/1   | 0.95 | 0.13 | -    | 52,52,52,52                 | 0     |
| 56  | MG   | 2a    | 1652 | 1/1   | 0.88 | 0.14 | -    | 62,62,62,62                 | 0     |
| 56  | MG   | 2a    | 1653 | 1/1   | 0.91 | 0.13 | -    | 51,51,51,51                 | 0     |
| 56  | MG   | 1A    | 3152 | 1/1   | 0.92 | 0.19 | -    | 37,37,37,37                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56  | MG   | 1A    | 3501 | 1/1   | 0.94 | 0.18 | -    | 32,32,32,32                 | 0     |
| 56  | MG   | 1A    | 3810 | 1/1   | 0.93 | 0.13 | -    | 36,36,36,36                 | 0     |
| 56  | MG   | 1A    | 3041 | 1/1   | 0.97 | 0.16 | -    | 35,35,35,35                 | 0     |
| 56  | MG   | 2A    | 3193 | 1/1   | 0.96 | 0.11 | -    | 40,40,40,40                 | 0     |
| 56  | MG   | 2a    | 1681 | 1/1   | 0.92 | 0.26 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | 1A    | 3347 | 1/1   | 0.86 | 0.27 | -    | 54,54,54,54                 | 0     |
| 56  | MG   | 2A    | 3597 | 1/1   | 0.96 | 0.16 | -    | 46,46,46,46                 | 0     |
| 56  | MG   | 2a    | 1634 | 1/1   | 0.86 | 0.16 | -    | 53,53,53,53                 | 0     |
| 56  | MG   | 1a    | 1623 | 1/1   | 0.95 | 0.14 | -    | 59,59,59,59                 | 0     |
| 56  | MG   | 1A    | 3579 | 1/1   | 0.96 | 0.19 | -    | 21,21,21,21                 | 0     |
| 56  | MG   | 1A    | 3723 | 1/1   | 0.95 | 0.15 | -    | 62,62,62,62                 | 0     |
| 56  | MG   | 1A    | 3429 | 1/1   | 0.89 | 0.23 | -    | 53,53,53,53                 | 0     |
| 56  | MG   | 2a    | 1752 | 1/1   | 0.95 | 0.10 | -    | 68,68,68,68                 | 0     |
| 56  | MG   | 1A    | 3238 | 1/1   | 0.91 | 0.22 | -    | 28,28,28,28                 | 0     |
| 56  | MG   | 1a    | 1678 | 1/1   | 0.98 | 0.14 | -    | 57,57,57,57                 | 0     |
| 56  | MG   | 2A    | 3283 | 1/1   | 0.95 | 0.17 | -    | 51,51,51,51                 | 0     |
| 56  | MG   | 1a    | 1616 | 1/1   | 0.84 | 0.19 | -    | 62,62,62,62                 | 0     |
| 56  | MG   | 1A    | 3454 | 1/1   | 0.98 | 0.20 | -    | 35,35,35,35                 | 0     |
| 56  | MG   | 2B    | 3005 | 1/1   | 0.96 | 0.20 | -    | 54,54,54,54                 | 0     |
| 56  | MG   | 2a    | 1731 | 1/1   | 0.73 | 0.10 | -    | 65,65,65,65                 | 0     |
| 56  | MG   | 2A    | 3414 | 1/1   | 0.85 | 0.15 | -    | 40,40,40,40                 | 0     |
| 56  | MG   | 2A    | 3044 | 1/1   | 0.94 | 0.17 | -    | 36,36,36,36                 | 0     |
| 56  | MG   | 1A    | 3143 | 1/1   | 0.90 | 0.11 | -    | 30,30,30,30                 | 0     |
| 56  | MG   | 1A    | 3120 | 1/1   | 0.95 | 0.12 | -    | 38,38,38,38                 | 0     |
| 56  | MG   | 1A    | 3489 | 1/1   | 0.96 | 0.17 | -    | 40,40,40,40                 | 0     |
| 56  | MG   | 1B    | 3014 | 1/1   | 0.82 | 0.22 | -    | 63,63,63,63                 | 0     |
| 56  | MG   | 2A    | 3216 | 1/1   | 0.88 | 0.10 | -    | 43,43,43,43                 | 0     |
| 56  | MG   | 2a    | 1615 | 1/1   | 0.97 | 0.18 | -    | 63,63,63,63                 | 0     |
| 56  | MG   | 1A    | 3575 | 1/1   | 0.92 | 0.20 | -    | 38,38,38,38                 | 0     |
| 56  | MG   | 1A    | 3785 | 1/1   | 0.97 | 0.15 | -    | 37,37,37,37                 | 0     |
| 56  | MG   | 2A    | 3046 | 1/1   | 0.90 | 0.12 | -    | 38,38,38,38                 | 0     |
| 56  | MG   | 2A    | 3056 | 1/1   | 0.86 | 0.12 | -    | 54,54,54,54                 | 0     |
| 56  | MG   | 2a    | 1617 | 1/1   | 0.71 | 0.15 | -    | 52,52,52,52                 | 0     |
| 56  | MG   | 2A    | 3368 | 1/1   | 0.82 | 0.14 | -    | 38,38,38,38                 | 0     |
| 56  | MG   | 1A    | 3779 | 1/1   | 0.84 | 0.34 | -    | 44,44,44,44                 | 0     |
| 56  | MG   | 1A    | 3283 | 1/1   | 0.96 | 0.16 | -    | 37,37,37,37                 | 0     |
| 56  | MG   | 1A    | 3256 | 1/1   | 0.95 | 0.14 | -    | 49,49,49,49                 | 0     |
| 56  | MG   | 2A    | 3125 | 1/1   | 0.88 | 0.12 | -    | 56,56,56,56                 | 0     |
| 56  | MG   | 2a    | 1763 | 1/1   | 0.98 | 0.16 | -    | 46,46,46,46                 | 0     |
| 56  | MG   | 2a    | 1790 | 1/1   | 0.91 | 0.19 | -    | 66,66,66,66                 | 0     |
| 56  | MG   | 1A    | 3866 | 1/1   | 0.87 | 0.13 | -    | 44,44,44,44                 | 0     |
| 56  | MG   | 2a    | 1674 | 1/1   | 0.80 | 0.14 | -    | 58,58,58,58                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56  | MG   | 1A    | 3528 | 1/1   | 0.88 | 0.10 | -    | 64,64,64,64                 | 0     |
| 56  | MG   | 1A    | 3555 | 1/1   | 0.87 | 0.12 | -    | 55,55,55,55                 | 0     |
| 56  | MG   | 1A    | 3330 | 1/1   | 0.96 | 0.21 | -    | 42,42,42,42                 | 0     |
| 56  | MG   | 1A    | 3354 | 1/1   | 0.93 | 0.19 | -    | 45,45,45,45                 | 0     |
| 56  | MG   | 1Z    | 3002 | 1/1   | 0.91 | 0.24 | -    | 56,56,56,56                 | 0     |
| 56  | MG   | 1A    | 3092 | 1/1   | 0.95 | 0.16 | -    | 41,41,41,41                 | 0     |
| 56  | MG   | 1A    | 3574 | 1/1   | 0.96 | 0.16 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | 2U    | 202  | 1/1   | 0.97 | 0.09 | -    | 35,35,35,35                 | 0     |
| 56  | MG   | 1A    | 3220 | 1/1   | 0.86 | 0.36 | -    | 48,48,48,48                 | 0     |
| 56  | MG   | 1A    | 3301 | 1/1   | 0.91 | 0.44 | -    | 38,38,38,38                 | 0     |
| 56  | MG   | 2A    | 3534 | 1/1   | 0.95 | 0.06 | -    | 62,62,62,62                 | 0     |
| 56  | MG   | 1a    | 1796 | 1/1   | 0.91 | 0.13 | -    | 40,40,40,40                 | 0     |
| 56  | MG   | 1a    | 1624 | 1/1   | 0.72 | 0.11 | -    | 65,65,65,65                 | 0     |
| 56  | MG   | 1A    | 3598 | 1/1   | 0.91 | 0.19 | -    | 42,42,42,42                 | 0     |
| 56  | MG   | 1A    | 3320 | 1/1   | 0.93 | 0.23 | -    | 59,59,59,59                 | 0     |
| 56  | MG   | 2A    | 3166 | 1/1   | 0.88 | 0.17 | -    | 43,43,43,43                 | 0     |
| 56  | MG   | 1A    | 3851 | 1/1   | 0.86 | 0.23 | -    | 45,45,45,45                 | 0     |
| 56  | MG   | 1a    | 1795 | 1/1   | 0.91 | 0.07 | -    | 64,64,64,64                 | 0     |
| 56  | MG   | 1A    | 3308 | 1/1   | 0.84 | 0.21 | -    | 58,58,58,58                 | 0     |
| 56  | MG   | 1A    | 3909 | 1/1   | 0.97 | 0.13 | -    | 36,36,36,36                 | 0     |
| 56  | MG   | 1A    | 3791 | 1/1   | 0.99 | 0.18 | -    | 43,43,43,43                 | 0     |
| 56  | MG   | 2A    | 3382 | 1/1   | 0.87 | 0.10 | -    | 48,48,48,48                 | 0     |
| 56  | MG   | 2A    | 3172 | 1/1   | 0.85 | 0.11 | -    | 59,59,59,59                 | 0     |
| 56  | MG   | 1A    | 3494 | 1/1   | 0.84 | 0.10 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | 2A    | 3483 | 1/1   | 0.90 | 0.07 | -    | 61,61,61,61                 | 0     |
| 56  | MG   | 2A    | 3179 | 1/1   | 0.83 | 0.12 | -    | 45,45,45,45                 | 0     |
| 56  | MG   | 2A    | 3103 | 1/1   | 0.93 | 0.25 | -    | 49,49,49,49                 | 0     |
| 56  | MG   | 1A    | 3176 | 1/1   | 0.93 | 0.16 | -    | 27,27,27,27                 | 0     |
| 56  | MG   | 2A    | 3181 | 1/1   | 0.94 | 0.11 | -    | 44,44,44,44                 | 0     |
| 56  | MG   | 1A    | 3339 | 1/1   | 0.98 | 0.23 | -    | 46,46,46,46                 | 0     |
| 56  | MG   | 1A    | 3246 | 1/1   | 0.93 | 0.21 | -    | 48,48,48,48                 | 0     |
| 56  | MG   | 2A    | 3661 | 1/1   | 0.91 | 0.11 | -    | 41,41,41,41                 | 0     |
| 56  | MG   | 2A    | 3134 | 1/1   | 0.95 | 0.09 | -    | 44,44,44,44                 | 0     |
| 56  | MG   | 1A    | 3379 | 1/1   | 0.95 | 0.18 | -    | 52,52,52,52                 | 0     |
| 56  | MG   | 1A    | 3351 | 1/1   | 0.94 | 0.09 | -    | 51,51,51,51                 | 0     |
| 56  | MG   | 2a    | 1720 | 1/1   | 0.90 | 0.10 | -    | 53,53,53,53                 | 0     |
| 56  | MG   | 2a    | 1628 | 1/1   | 0.90 | 0.13 | -    | 65,65,65,65                 | 0     |
| 56  | MG   | 1a    | 1780 | 1/1   | 0.98 | 0.07 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | 2a    | 1754 | 1/1   | 0.98 | 0.08 | -    | 67,67,67,67                 | 0     |
| 56  | MG   | 2A    | 3641 | 1/1   | 0.91 | 0.10 | -    | 46,46,46,46                 | 0     |
| 56  | MG   | 1A    | 3181 | 1/1   | 0.92 | 0.22 | -    | 48,48,48,48                 | 0     |
| 56  | MG   | 2B    | 3009 | 1/1   | 0.80 | 0.19 | -    | 62,62,62,62                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56  | MG   | 2A    | 3464 | 1/1   | 0.92 | 0.09 | -    | 41,41,41,41                 | 0     |
| 56  | MG   | 1A    | 3024 | 1/1   | 0.99 | 0.17 | -    | 27,27,27,27                 | 0     |
| 56  | MG   | 1A    | 3311 | 1/1   | 0.96 | 0.26 | -    | 50,50,50,50                 | 0     |
| 56  | MG   | 1A    | 3923 | 1/1   | 0.92 | 0.21 | -    | 39,39,39,39                 | 0     |
| 56  | MG   | 1A    | 3809 | 1/1   | 0.92 | 0.14 | -    | 42,42,42,42                 | 0     |
| 56  | MG   | 2v    | 3001 | 1/1   | 0.93 | 0.12 | -    | 56,56,56,56                 | 0     |
| 56  | MG   | 2A    | 3605 | 1/1   | 0.93 | 0.11 | -    | 45,45,45,45                 | 0     |
| 56  | MG   | 1A    | 3778 | 1/1   | 0.84 | 0.10 | -    | 48,48,48,48                 | 0     |
| 56  | MG   | 2A    | 3051 | 1/1   | 0.81 | 0.15 | -    | 61,61,61,61                 | 0     |
| 56  | MG   | 1A    | 3390 | 1/1   | 0.93 | 0.15 | -    | 42,42,42,42                 | 0     |
| 56  | MG   | 2A    | 3286 | 1/1   | 0.97 | 0.18 | -    | 55,55,55,55                 | 0     |
| 56  | MG   | 2A    | 3008 | 1/1   | 0.97 | 0.20 | -    | 39,39,39,39                 | 0     |
| 56  | MG   | 1a    | 1802 | 1/1   | 0.91 | 0.10 | -    | 50,50,50,50                 | 0     |
| 56  | MG   | 1A    | 3080 | 1/1   | 0.90 | 0.24 | -    | 31,31,31,31                 | 0     |
| 56  | MG   | 1a    | 1687 | 1/1   | 0.96 | 0.11 | -    | 55,55,55,55                 | 0     |
| 56  | MG   | 2A    | 3143 | 1/1   | 0.97 | 0.13 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | 2A    | 3192 | 1/1   | 0.94 | 0.21 | -    | 51,51,51,51                 | 0     |
| 56  | MG   | 1A    | 3499 | 1/1   | 0.97 | 0.12 | -    | 34,34,34,34                 | 0     |
| 56  | MG   | 2A    | 3553 | 1/1   | 0.94 | 0.06 | -    | 53,53,53,53                 | 0     |
| 56  | MG   | 1A    | 3536 | 1/1   | 0.98 | 0.11 | -    | 48,48,48,48                 | 0     |
| 56  | MG   | 1A    | 3877 | 1/1   | 0.97 | 0.11 | -    | 49,49,49,49                 | 0     |
| 56  | MG   | 2a    | 1719 | 1/1   | 0.96 | 0.17 | -    | 44,44,44,44                 | 0     |
| 56  | MG   | 2A    | 3242 | 1/1   | 0.94 | 0.13 | -    | 54,54,54,54                 | 0     |
| 56  | MG   | 1A    | 3532 | 1/1   | 0.90 | 0.18 | -    | 59,59,59,59                 | 0     |
| 56  | MG   | 1A    | 3805 | 1/1   | 0.87 | 0.19 | -    | 64,64,64,64                 | 0     |
| 56  | MG   | 2A    | 3448 | 1/1   | 0.90 | 0.13 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | 1A    | 3138 | 1/1   | 0.98 | 0.26 | -    | 32,32,32,32                 | 0     |
| 56  | MG   | 1a    | 1698 | 1/1   | 0.97 | 0.18 | -    | 51,51,51,51                 | 0     |
| 56  | MG   | 1A    | 3264 | 1/1   | 0.82 | 0.15 | -    | 64,64,64,64                 | 0     |
| 56  | MG   | 1A    | 3603 | 1/1   | 0.94 | 0.13 | -    | 31,31,31,31                 | 0     |
| 56  | MG   | 2A    | 3471 | 1/1   | 0.93 | 0.10 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | 2a    | 1775 | 1/1   | 0.90 | 0.10 | -    | 71,71,71,71                 | 0     |
| 56  | MG   | 1B    | 3006 | 1/1   | 0.90 | 0.23 | -    | 44,44,44,44                 | 0     |
| 56  | MG   | 1O    | 201  | 1/1   | 0.96 | 0.15 | -    | 39,39,39,39                 | 0     |
| 56  | MG   | 1A    | 3086 | 1/1   | 0.93 | 0.15 | -    | 41,41,41,41                 | 0     |
| 56  | MG   | 1A    | 3660 | 1/1   | 0.76 | 0.14 | -    | 50,50,50,50                 | 0     |
| 56  | MG   | 1A    | 3227 | 1/1   | 0.95 | 0.10 | -    | 42,42,42,42                 | 0     |
| 56  | MG   | 1A    | 3719 | 1/1   | 0.93 | 0.17 | -    | 41,41,41,41                 | 0     |
| 56  | MG   | 2a    | 1669 | 1/1   | 0.95 | 0.16 | -    | 44,44,44,44                 | 0     |
| 56  | MG   | 2A    | 3147 | 1/1   | 0.98 | 0.12 | -    | 38,38,38,38                 | 0     |
| 56  | MG   | 2a    | 1785 | 1/1   | 0.93 | 0.14 | -    | 66,66,66,66                 | 0     |
| 56  | MG   | 2A    | 3073 | 1/1   | 0.88 | 0.14 | -    | 46,46,46,46                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56  | MG   | 1A    | 3067 | 1/1   | 0.97 | 0.16 | -    | 18,18,18,18                 | 0     |
| 56  | MG   | 1Q    | 205  | 1/1   | 0.82 | 0.24 | -    | 58,58,58,58                 | 0     |
| 56  | MG   | 1a    | 1812 | 1/1   | 0.93 | 0.16 | -    | 51,51,51,51                 | 0     |
| 56  | MG   | 1A    | 3223 | 1/1   | 0.93 | 0.29 | -    | 42,42,42,42                 | 0     |
| 56  | MG   | 1A    | 3582 | 1/1   | 0.93 | 0.16 | -    | 45,45,45,45                 | 0     |
| 56  | MG   | 1A    | 3422 | 1/1   | 0.96 | 0.14 | -    | 45,45,45,45                 | 0     |
| 56  | MG   | 2A    | 3037 | 1/1   | 0.91 | 0.13 | -    | 42,42,42,42                 | 0     |
| 56  | MG   | 2A    | 3252 | 1/1   | 0.89 | 0.09 | -    | 58,58,58,58                 | 0     |
| 56  | MG   | 1A    | 3005 | 1/1   | 0.98 | 0.15 | -    | 43,43,43,43                 | 0     |
| 56  | MG   | 2A    | 3588 | 1/1   | 0.93 | 0.09 | -    | 60,60,60,60                 | 0     |
| 56  | MG   | 2a    | 1762 | 1/1   | 0.94 | 0.13 | -    | 55,55,55,55                 | 0     |
| 56  | MG   | 2A    | 3515 | 1/1   | 0.96 | 0.12 | -    | 35,35,35,35                 | 0     |
| 56  | MG   | 1A    | 3731 | 1/1   | 0.96 | 0.15 | -    | 58,58,58,58                 | 0     |
| 56  | MG   | 2a    | 1690 | 1/1   | 0.94 | 0.26 | -    | 50,50,50,50                 | 0     |
| 56  | MG   | 1A    | 3011 | 1/1   | 0.93 | 0.21 | -    | 41,41,41,41                 | 0     |
| 56  | MG   | 2A    | 3624 | 1/1   | 0.94 | 0.08 | -    | 44,44,44,44                 | 0     |
| 56  | MG   | 1A    | 3634 | 1/1   | 0.92 | 0.14 | -    | 56,56,56,56                 | 0     |
| 56  | MG   | 1A    | 3359 | 1/1   | 0.94 | 0.09 | -    | 44,44,44,44                 | 0     |
| 56  | MG   | 1a    | 1645 | 1/1   | 0.84 | 0.14 | -    | 56,56,56,56                 | 0     |
| 56  | MG   | 2j    | 8001 | 1/1   | 0.97 | 0.13 | -    | 69,69,69,69                 | 0     |
| 56  | MG   | 1A    | 3727 | 1/1   | 0.96 | 0.16 | -    | 45,45,45,45                 | 0     |
| 56  | MG   | 1A    | 3228 | 1/1   | 0.88 | 0.17 | -    | 39,39,39,39                 | 0     |
| 56  | MG   | 1A    | 3231 | 1/1   | 0.92 | 0.20 | -    | 53,53,53,53                 | 0     |
| 56  | MG   | 2A    | 3378 | 1/1   | 0.95 | 0.16 | -    | 48,48,48,48                 | 0     |
| 56  | MG   | 1x    | 3010 | 1/1   | 0.94 | 0.07 | -    | 74,74,74,74                 | 0     |
| 56  | MG   | 1a    | 1693 | 1/1   | 0.72 | 0.16 | -    | 60,60,60,60                 | 0     |
| 56  | MG   | 2a    | 1658 | 1/1   | 0.91 | 0.09 | -    | 69,69,69,69                 | 0     |
| 56  | MG   | 2a    | 1607 | 1/1   | 0.95 | 0.18 | -    | 48,48,48,48                 | 0     |
| 56  | MG   | 2A    | 3638 | 1/1   | 0.98 | 0.10 | -    | 55,55,55,55                 | 0     |
| 56  | MG   | 2A    | 3545 | 1/1   | 0.95 | 0.24 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | 1A    | 3368 | 1/1   | 0.93 | 0.14 | -    | 41,41,41,41                 | 0     |
| 56  | MG   | 1A    | 3938 | 1/1   | 0.88 | 0.35 | -    | 43,43,43,43                 | 0     |
| 56  | MG   | 2B    | 3013 | 1/1   | 0.94 | 0.16 | -    | 45,45,45,45                 | 0     |
| 56  | MG   | 2A    | 3538 | 1/1   | 0.85 | 0.10 | -    | 53,53,53,53                 | 0     |
| 56  | MG   | 1A    | 3076 | 1/1   | 0.88 | 0.14 | -    | 43,43,43,43                 | 0     |
| 56  | MG   | 1A    | 3484 | 1/1   | 0.95 | 0.23 | -    | 30,30,30,30                 | 0     |
| 56  | MG   | 1A    | 3357 | 1/1   | 0.96 | 0.28 | -    | 52,52,52,52                 | 0     |
| 56  | MG   | 1A    | 3703 | 1/1   | 0.94 | 0.10 | -    | 50,50,50,50                 | 0     |
| 56  | MG   | 2a    | 1685 | 1/1   | 0.92 | 0.11 | -    | 53,53,53,53                 | 0     |
| 56  | MG   | 1A    | 3702 | 1/1   | 0.96 | 0.14 | -    | 45,45,45,45                 | 0     |
| 56  | MG   | 2A    | 3468 | 1/1   | 0.95 | 0.10 | -    | 38,38,38,38                 | 0     |
| 56  | MG   | 2A    | 3420 | 1/1   | 0.96 | 0.10 | -    | 43,43,43,43                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56  | MG   | 1B    | 3028 | 1/1   | 0.93 | 0.15 | -    | 39,39,39,39                 | 0     |
| 56  | MG   | 1A    | 3325 | 1/1   | 0.92 | 0.15 | -    | 38,38,38,38                 | 0     |
| 56  | MG   | 1A    | 3282 | 1/1   | 0.92 | 0.13 | -    | 53,53,53,53                 | 0     |
| 56  | MG   | 2A    | 3188 | 1/1   | 0.89 | 0.18 | -    | 50,50,50,50                 | 0     |
| 56  | MG   | 2A    | 3171 | 1/1   | 0.93 | 0.13 | -    | 43,43,43,43                 | 0     |
| 56  | MG   | 2A    | 3149 | 1/1   | 0.94 | 0.13 | -    | 49,49,49,49                 | 0     |
| 56  | MG   | 2A    | 3278 | 1/1   | 0.95 | 0.13 | -    | 31,31,31,31                 | 0     |
| 56  | MG   | 1A    | 3233 | 1/1   | 0.95 | 0.39 | -    | 35,35,35,35                 | 0     |
| 56  | MG   | 1A    | 3759 | 1/1   | 0.94 | 0.17 | -    | 45,45,45,45                 | 0     |
| 56  | MG   | 2A    | 3093 | 1/1   | 0.94 | 0.11 | -    | 51,51,51,51                 | 0     |
| 56  | MG   | 2A    | 3516 | 1/1   | 0.97 | 0.15 | -    | 46,46,46,46                 | 0     |
| 56  | MG   | 1A    | 3058 | 1/1   | 0.98 | 0.21 | -    | 44,44,44,44                 | 0     |
| 56  | MG   | 1A    | 3868 | 1/1   | 0.84 | 0.09 | -    | 48,48,48,48                 | 0     |
| 56  | MG   | 2A    | 3085 | 1/1   | 0.93 | 0.13 | -    | 37,37,37,37                 | 0     |
| 56  | MG   | 1A    | 3505 | 1/1   | 0.89 | 0.15 | -    | 28,28,28,28                 | 0     |
| 56  | MG   | 1A    | 3645 | 1/1   | 0.93 | 0.11 | -    | 23,23,23,23                 | 0     |
| 56  | MG   | 1A    | 3164 | 1/1   | 0.89 | 0.14 | -    | 51,51,51,51                 | 0     |
| 56  | MG   | 1Z    | 3004 | 1/1   | 0.91 | 0.17 | -    | 52,52,52,52                 | 0     |
| 56  | MG   | 2A    | 3524 | 1/1   | 0.90 | 0.09 | -    | 56,56,56,56                 | 0     |
| 56  | MG   | 1a    | 1695 | 1/1   | 0.92 | 0.09 | -    | 55,55,55,55                 | 0     |
| 56  | MG   | 2A    | 3109 | 1/1   | 0.94 | 0.09 | -    | 49,49,49,49                 | 0     |
| 56  | MG   | 2A    | 3604 | 1/1   | 0.89 | 0.12 | -    | 45,45,45,45                 | 0     |
| 56  | MG   | 1a    | 1641 | 1/1   | 0.87 | 0.16 | -    | 50,50,50,50                 | 0     |
| 56  | MG   | 2A    | 3539 | 1/1   | 0.97 | 0.10 | -    | 51,51,51,51                 | 0     |
| 56  | MG   | 2A    | 3440 | 1/1   | 0.95 | 0.20 | -    | 42,42,42,42                 | 0     |
| 56  | MG   | 1A    | 3624 | 1/1   | 0.88 | 0.16 | -    | 57,57,57,57                 | 0     |
| 56  | MG   | 1A    | 3677 | 1/1   | 0.85 | 0.13 | -    | 57,57,57,57                 | 0     |
| 56  | MG   | 1a    | 1618 | 1/1   | 0.89 | 0.13 | -    | 64,64,64,64                 | 0     |
| 56  | MG   | 1A    | 3894 | 1/1   | 0.93 | 0.15 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | 2A    | 3280 | 1/1   | 0.97 | 0.21 | -    | 42,42,42,42                 | 0     |
| 56  | MG   | 1A    | 3609 | 1/1   | 0.91 | 0.06 | -    | 43,43,43,43                 | 0     |
| 56  | MG   | 1A    | 3009 | 1/1   | 0.95 | 0.12 | -    | 30,30,30,30                 | 0     |
| 56  | MG   | 1A    | 3621 | 1/1   | 0.98 | 0.12 | -    | 48,48,48,48                 | 0     |
| 56  | MG   | 1A    | 3435 | 1/1   | 0.95 | 0.14 | -    | 35,35,35,35                 | 0     |
| 56  | MG   | 2A    | 3313 | 1/1   | 0.97 | 0.11 | -    | 37,37,37,37                 | 0     |
| 56  | MG   | 1A    | 3669 | 1/1   | 0.93 | 0.18 | -    | 34,34,34,34                 | 0     |
| 56  | MG   | 1a    | 1681 | 1/1   | 0.83 | 0.27 | -    | 54,54,54,54                 | 0     |
| 56  | MG   | 1a    | 1791 | 1/1   | 0.93 | 0.16 | -    | 62,62,62,62                 | 0     |
| 56  | MG   | 1a    | 1737 | 1/1   | 0.97 | 0.14 | -    | 33,33,33,33                 | 0     |
| 56  | MG   | 2A    | 3029 | 1/1   | 0.90 | 0.18 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | 1a    | 1788 | 1/1   | 0.92 | 0.13 | -    | 64,64,64,64                 | 0     |
| 56  | MG   | 1A    | 3146 | 1/1   | 0.99 | 0.22 | -    | 31,31,31,31                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56  | MG   | 1A    | 3114 | 1/1   | 0.92 | 0.26 | -    | 32,32,32,32                 | 0     |
| 56  | MG   | 2A    | 3484 | 1/1   | 0.95 | 0.11 | -    | 53,53,53,53                 | 0     |
| 56  | MG   | 2A    | 3623 | 1/1   | 0.95 | 0.09 | -    | 46,46,46,46                 | 0     |
| 56  | MG   | 2r    | 101  | 1/1   | 0.84 | 0.14 | -    | 66,66,66,66                 | 0     |
| 56  | MG   | 1a    | 1686 | 1/1   | 0.87 | 0.16 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | 1A    | 3399 | 1/1   | 0.96 | 0.16 | -    | 42,42,42,42                 | 0     |
| 56  | MG   | 1A    | 3026 | 1/1   | 0.95 | 0.19 | -    | 29,29,29,29                 | 0     |
| 56  | MG   | 1A    | 3850 | 1/1   | 0.89 | 0.25 | -    | 60,60,60,60                 | 0     |
| 56  | MG   | 2A    | 3416 | 1/1   | 0.90 | 0.20 | -    | 44,44,44,44                 | 0     |
| 56  | MG   | 2a    | 1746 | 1/1   | 0.97 | 0.11 | -    | 59,59,59,59                 | 0     |
| 56  | MG   | 1A    | 3153 | 1/1   | 0.96 | 0.18 | -    | 31,31,31,31                 | 0     |
| 56  | MG   | 1A    | 3547 | 1/1   | 0.98 | 0.08 | -    | 36,36,36,36                 | 0     |
| 56  | MG   | 1A    | 3845 | 1/1   | 0.99 | 0.25 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | 2A    | 3086 | 1/1   | 0.83 | 0.13 | -    | 43,43,43,43                 | 0     |
| 56  | MG   | 1A    | 3241 | 1/1   | 0.95 | 0.13 | -    | 51,51,51,51                 | 0     |
| 56  | MG   | 1A    | 3570 | 1/1   | 0.92 | 0.14 | -    | 43,43,43,43                 | 0     |
| 56  | MG   | 2A    | 3185 | 1/1   | 0.97 | 0.25 | -    | 55,55,55,55                 | 0     |
| 56  | MG   | 1a    | 1799 | 1/1   | 0.90 | 0.33 | -    | 85,85,85,85                 | 0     |
| 56  | MG   | 1a    | 1700 | 1/1   | 0.93 | 0.28 | -    | 51,51,51,51                 | 0     |
| 56  | MG   | 1A    | 3331 | 1/1   | 0.94 | 0.25 | -    | 53,53,53,53                 | 0     |
| 56  | MG   | 2T    | 3001 | 1/1   | 0.97 | 0.14 | -    | 50,50,50,50                 | 0     |
| 56  | MG   | 2a    | 1612 | 1/1   | 0.93 | 0.14 | -    | 54,54,54,54                 | 0     |
| 56  | MG   | 2A    | 3426 | 1/1   | 0.93 | 0.12 | -    | 38,38,38,38                 | 0     |
| 56  | MG   | 2A    | 3449 | 1/1   | 0.97 | 0.12 | -    | 42,42,42,42                 | 0     |
| 56  | MG   | 2B    | 3015 | 1/1   | 0.96 | 0.17 | -    | 48,48,48,48                 | 0     |
| 56  | MG   | 1a    | 1636 | 1/1   | 0.90 | 0.11 | -    | 53,53,53,53                 | 0     |
| 56  | MG   | 1A    | 3855 | 1/1   | 0.98 | 0.17 | -    | 23,23,23,23                 | 0     |
| 56  | MG   | 1A    | 3665 | 1/1   | 0.90 | 0.09 | -    | 53,53,53,53                 | 0     |
| 56  | MG   | 1A    | 3352 | 1/1   | 0.91 | 0.20 | -    | 58,58,58,58                 | 0     |
| 56  | MG   | 1A    | 3578 | 1/1   | 0.76 | 0.12 | -    | 39,39,39,39                 | 0     |
| 56  | MG   | 2A    | 3513 | 1/1   | 0.89 | 0.07 | -    | 50,50,50,50                 | 0     |
| 56  | MG   | 1y    | 102  | 1/1   | 0.96 | 0.12 | -    | 63,63,63,63                 | 0     |
| 56  | MG   | 1A    | 3959 | 1/1   | 0.96 | 0.38 | -    | 53,53,53,53                 | 0     |
| 56  | MG   | 1A    | 3925 | 1/1   | 0.99 | 0.07 | -    | 59,59,59,59                 | 0     |
| 56  | MG   | 1A    | 3832 | 1/1   | 0.98 | 0.10 | -    | 57,57,57,57                 | 0     |
| 56  | MG   | 2A    | 3517 | 1/1   | 0.97 | 0.11 | -    | 54,54,54,54                 | 0     |
| 56  | MG   | 1A    | 3299 | 1/1   | 0.96 | 0.25 | -    | 40,40,40,40                 | 0     |
| 56  | MG   | 2A    | 3068 | 1/1   | 0.90 | 0.12 | -    | 39,39,39,39                 | 0     |
| 56  | MG   | 2A    | 3115 | 1/1   | 0.88 | 0.15 | -    | 38,38,38,38                 | 0     |
| 56  | MG   | 1A    | 3878 | 1/1   | 0.97 | 0.13 | -    | 40,40,40,40                 | 0     |
| 56  | MG   | 1A    | 3734 | 1/1   | 0.86 | 0.17 | -    | 48,48,48,48                 | 0     |
| 56  | MG   | 1A    | 3754 | 1/1   | 0.97 | 0.11 | -    | 53,53,53,53                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56  | MG   | 1a    | 1797 | 1/1   | 0.98 | 0.19 | -    | 52,52,52,52                 | 0     |
| 56  | MG   | 2A    | 3127 | 1/1   | 0.87 | 0.12 | -    | 50,50,50,50                 | 0     |
| 56  | MG   | 2A    | 3182 | 1/1   | 0.81 | 0.10 | -    | 53,53,53,53                 | 0     |
| 56  | MG   | 1A    | 3328 | 1/1   | 0.98 | 0.12 | -    | 27,27,27,27                 | 0     |
| 56  | MG   | 2a    | 1740 | 1/1   | 0.81 | 0.14 | -    | 82,82,82,82                 | 0     |
| 56  | MG   | 1B    | 3020 | 1/1   | 0.97 | 0.15 | -    | 48,48,48,48                 | 0     |
| 56  | MG   | 1A    | 3964 | 1/1   | 0.90 | 0.18 | -    | 26,26,26,26                 | 0     |
| 56  | MG   | 1a    | 1792 | 1/1   | 0.95 | 0.11 | -    | 75,75,75,75                 | 0     |
| 56  | MG   | 2A    | 3121 | 1/1   | 0.92 | 0.16 | -    | 41,41,41,41                 | 0     |
| 56  | MG   | 1Z    | 3005 | 1/1   | 0.88 | 0.26 | -    | 56,56,56,56                 | 0     |
| 56  | MG   | 1A    | 3112 | 1/1   | 0.93 | 0.26 | -    | 43,43,43,43                 | 0     |
| 56  | MG   | 1a    | 1835 | 1/1   | 0.88 | 0.15 | -    | 57,57,57,57                 | 0     |
| 56  | MG   | 1a    | 1605 | 1/1   | 0.94 | 0.11 | -    | 50,50,50,50                 | 0     |
| 56  | MG   | 1A    | 3657 | 1/1   | 0.96 | 0.09 | -    | 29,29,29,29                 | 0     |
| 56  | MG   | 1a    | 1718 | 1/1   | 0.91 | 0.16 | -    | 54,54,54,54                 | 0     |
| 56  | MG   | 1A    | 3519 | 1/1   | 0.94 | 0.08 | -    | 41,41,41,41                 | 0     |
| 56  | MG   | 1A    | 3057 | 1/1   | 0.83 | 0.12 | -    | 44,44,44,44                 | 0     |
| 56  | MG   | 1A    | 3115 | 1/1   | 0.94 | 0.12 | -    | 37,37,37,37                 | 0     |
| 56  | MG   | 1a    | 1720 | 1/1   | 0.98 | 0.17 | -    | 64,64,64,64                 | 0     |
| 56  | MG   | 2A    | 3148 | 1/1   | 0.96 | 0.21 | -    | 43,43,43,43                 | 0     |
| 56  | MG   | 2A    | 3239 | 1/1   | 0.96 | 0.10 | -    | 43,43,43,43                 | 0     |
| 56  | MG   | 2A    | 3603 | 1/1   | 0.79 | 0.18 | -    | 65,65,65,65                 | 0     |
| 56  | MG   | 1A    | 3440 | 1/1   | 0.90 | 0.16 | -    | 72,72,72,72                 | 0     |
| 56  | MG   | 1A    | 3337 | 1/1   | 0.91 | 0.15 | -    | 39,39,39,39                 | 0     |
| 56  | MG   | 1A    | 3077 | 1/1   | 0.96 | 0.15 | -    | 39,39,39,39                 | 0     |
| 56  | MG   | 1a    | 1701 | 1/1   | 0.87 | 0.11 | -    | 52,52,52,52                 | 0     |
| 56  | MG   | 1A    | 3777 | 1/1   | 0.85 | 0.10 | -    | 42,42,42,42                 | 0     |
| 56  | MG   | 2a    | 1665 | 1/1   | 0.93 | 0.14 | -    | 55,55,55,55                 | 0     |
| 56  | MG   | 1A    | 3409 | 1/1   | 0.86 | 0.08 | -    | 34,34,34,34                 | 0     |
| 56  | MG   | 2A    | 3270 | 1/1   | 0.68 | 0.08 | -    | 38,38,38,38                 | 0     |
| 56  | MG   | 2A    | 3407 | 1/1   | 0.80 | 0.11 | -    | 44,44,44,44                 | 0     |
| 56  | MG   | 1A    | 3741 | 1/1   | 0.92 | 0.14 | -    | 58,58,58,58                 | 0     |
| 56  | MG   | 2B    | 3018 | 1/1   | 0.94 | 0.06 | -    | 57,57,57,57                 | 0     |
| 56  | MG   | 2a    | 1703 | 1/1   | 0.95 | 0.18 | -    | 61,61,61,61                 | 0     |
| 56  | MG   | 2A    | 3475 | 1/1   | 0.94 | 0.06 | -    | 52,52,52,52                 | 0     |
| 56  | MG   | 2F    | 301  | 1/1   | 0.79 | 0.23 | -    | 37,37,37,37                 | 0     |
| 56  | MG   | 1A    | 3812 | 1/1   | 0.94 | 0.15 | -    | 41,41,41,41                 | 0     |
| 56  | MG   | 1w    | 3005 | 1/1   | 0.92 | 0.18 | -    | 82,82,82,82                 | 0     |
| 56  | MG   | 2a    | 1729 | 1/1   | 0.82 | 0.12 | -    | 65,65,65,65                 | 0     |
| 56  | MG   | 1a    | 1801 | 1/1   | 0.89 | 0.16 | -    | 54,54,54,54                 | 0     |
| 56  | MG   | 1A    | 3753 | 1/1   | 0.97 | 0.05 | -    | 49,49,49,49                 | 0     |
| 56  | MG   | 2A    | 3050 | 1/1   | 0.94 | 0.18 | -    | 43,43,43,43                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56  | MG   | 1a    | 1719 | 1/1   | 0.94 | 0.14 | -    | 45,45,45,45                 | 0     |
| 56  | MG   | 1A    | 3607 | 1/1   | 0.95 | 0.21 | -    | 30,30,30,30                 | 0     |
| 56  | MG   | 1A    | 3191 | 1/1   | 0.95 | 0.06 | -    | 38,38,38,38                 | 0     |
| 56  | MG   | 1B    | 3023 | 1/1   | 0.98 | 0.19 | -    | 51,51,51,51                 | 0     |
| 56  | MG   | 2A    | 3376 | 1/1   | 0.85 | 0.12 | -    | 41,41,41,41                 | 0     |
| 56  | MG   | 2A    | 3657 | 1/1   | 0.95 | 0.06 | -    | 36,36,36,36                 | 0     |
| 56  | MG   | 2A    | 3633 | 1/1   | 0.95 | 0.11 | -    | 49,49,49,49                 | 0     |
| 56  | MG   | 2A    | 3496 | 1/1   | 0.95 | 0.13 | -    | 53,53,53,53                 | 0     |
| 56  | MG   | 1a    | 1822 | 1/1   | 0.97 | 0.14 | -    | 62,62,62,62                 | 0     |
| 56  | MG   | 1A    | 3671 | 1/1   | 0.93 | 0.14 | -    | 38,38,38,38                 | 0     |
| 56  | MG   | 1A    | 3170 | 1/1   | 0.87 | 0.20 | -    | 39,39,39,39                 | 0     |
| 56  | MG   | 1a    | 1731 | 1/1   | 0.97 | 0.15 | -    | 61,61,61,61                 | 0     |
| 56  | MG   | 2A    | 3485 | 1/1   | 0.94 | 0.10 | -    | 59,59,59,59                 | 0     |
| 56  | MG   | 1A    | 3470 | 1/1   | 0.96 | 0.17 | -    | 27,27,27,27                 | 0     |
| 56  | MG   | 1A    | 3154 | 1/1   | 0.97 | 0.35 | -    | 36,36,36,36                 | 0     |
| 56  | MG   | 2A    | 3083 | 1/1   | 0.91 | 0.14 | -    | 48,48,48,48                 | 0     |
| 56  | MG   | 1A    | 3721 | 1/1   | 0.97 | 0.10 | -    | 50,50,50,50                 | 0     |
| 56  | MG   | 1a    | 1684 | 1/1   | 0.89 | 0.14 | -    | 54,54,54,54                 | 0     |
| 56  | MG   | 2A    | 3203 | 1/1   | 0.93 | 0.14 | -    | 40,40,40,40                 | 0     |
| 56  | MG   | 2a    | 1781 | 1/1   | 0.89 | 0.17 | -    | 66,66,66,66                 | 0     |
| 56  | MG   | 1A    | 3252 | 1/1   | 0.96 | 0.17 | -    | 41,41,41,41                 | 0     |
| 56  | MG   | 1A    | 3876 | 1/1   | 0.93 | 0.13 | -    | 55,55,55,55                 | 0     |
| 56  | MG   | 1A    | 3834 | 1/1   | 0.96 | 0.37 | -    | 46,46,46,46                 | 0     |
| 56  | MG   | 2B    | 3007 | 1/1   | 0.95 | 0.13 | -    | 46,46,46,46                 | 0     |
| 56  | MG   | 1A    | 3718 | 1/1   | 0.84 | 0.16 | -    | 69,69,69,69                 | 0     |
| 56  | MG   | 1A    | 3433 | 1/1   | 0.98 | 0.18 | -    | 42,42,42,42                 | 0     |
| 56  | MG   | 2A    | 3589 | 1/1   | 0.96 | 0.08 | -    | 41,41,41,41                 | 0     |
| 56  | MG   | 2A    | 3456 | 1/1   | 0.95 | 0.16 | -    | 39,39,39,39                 | 0     |
| 56  | MG   | 1a    | 1706 | 1/1   | 0.91 | 0.17 | -    | 66,66,66,66                 | 0     |
| 56  | MG   | 2A    | 3388 | 1/1   | 0.89 | 0.11 | -    | 52,52,52,52                 | 0     |
| 56  | MG   | 2A    | 3371 | 1/1   | 0.84 | 0.10 | -    | 49,49,49,49                 | 0     |
| 56  | MG   | 2a    | 1640 | 1/1   | 0.96 | 0.11 | -    | 56,56,56,56                 | 0     |
| 56  | MG   | 1A    | 3312 | 1/1   | 0.97 | 0.22 | -    | 41,41,41,41                 | 0     |
| 56  | MG   | 2A    | 3257 | 1/1   | 0.97 | 0.13 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | 1A    | 3237 | 1/1   | 0.88 | 0.16 | -    | 44,44,44,44                 | 0     |
| 56  | MG   | 1O    | 203  | 1/1   | 0.86 | 0.11 | -    | 52,52,52,52                 | 0     |
| 56  | MG   | 1A    | 3857 | 1/1   | 0.94 | 0.11 | -    | 39,39,39,39                 | 0     |
| 56  | MG   | 2A    | 3026 | 1/1   | 0.87 | 0.09 | -    | 35,35,35,35                 | 0     |
| 56  | MG   | 1a    | 1607 | 1/1   | 0.87 | 0.21 | -    | 68,68,68,68                 | 0     |
| 56  | MG   | 2A    | 3004 | 1/1   | 0.96 | 0.14 | -    | 36,36,36,36                 | 0     |
| 56  | MG   | 2A    | 3226 | 1/1   | 0.90 | 0.32 | -    | 42,42,42,42                 | 0     |
| 56  | MG   | 1a    | 1620 | 1/1   | 0.88 | 0.13 | -    | 50,50,50,50                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56  | MG   | 1a    | 1778 | 1/1   | 0.94 | 0.15 | -    | 66,66,66,66                 | 0     |
| 56  | MG   | 2a    | 1638 | 1/1   | 0.96 | 0.10 | -    | 50,50,50,50                 | 0     |
| 56  | MG   | 1A    | 3367 | 1/1   | 0.82 | 0.20 | -    | 55,55,55,55                 | 0     |
| 56  | MG   | 2A    | 3180 | 1/1   | 0.96 | 0.19 | -    | 39,39,39,39                 | 0     |
| 56  | MG   | 2A    | 3615 | 1/1   | 0.89 | 0.13 | -    | 46,46,46,46                 | 0     |
| 56  | MG   | 1A    | 3132 | 1/1   | 0.92 | 0.22 | -    | 37,37,37,37                 | 0     |
| 56  | MG   | 1a    | 1622 | 1/1   | 0.97 | 0.13 | -    | 49,49,49,49                 | 0     |
| 56  | MG   | 1A    | 3068 | 1/1   | 0.95 | 0.18 | -    | 43,43,43,43                 | 0     |
| 56  | MG   | 1A    | 3932 | 1/1   | 0.68 | 0.22 | -    | 56,56,56,56                 | 0     |
| 56  | MG   | 1a    | 1704 | 1/1   | 0.89 | 0.22 | -    | 73,73,73,73                 | 0     |
| 56  | MG   | 2A    | 3145 | 1/1   | 0.95 | 0.10 | -    | 35,35,35,35                 | 0     |
| 56  | MG   | 2A    | 3610 | 1/1   | 0.90 | 0.20 | -    | 32,32,32,32                 | 0     |
| 56  | MG   | 1a    | 1735 | 1/1   | 0.92 | 0.16 | -    | 58,58,58,58                 | 0     |
| 56  | MG   | 2A    | 3076 | 1/1   | 0.94 | 0.21 | -    | 31,31,31,31                 | 0     |
| 56  | MG   | 1A    | 3416 | 1/1   | 0.95 | 0.14 | -    | 54,54,54,54                 | 0     |
| 56  | MG   | 2A    | 3387 | 1/1   | 0.96 | 0.28 | -    | 50,50,50,50                 | 0     |
| 56  | MG   | 2A    | 3013 | 1/1   | 0.95 | 0.12 | -    | 36,36,36,36                 | 0     |
| 56  | MG   | 2f    | 3002 | 1/1   | 0.89 | 0.21 | -    | 61,61,61,61                 | 0     |
| 56  | MG   | 2a    | 1737 | 1/1   | 0.95 | 0.22 | -    | 51,51,51,51                 | 0     |
| 56  | MG   | 2a    | 1609 | 1/1   | 0.94 | 0.08 | -    | 60,60,60,60                 | 0     |
| 56  | MG   | 1A    | 3395 | 1/1   | 0.98 | 0.20 | -    | 31,31,31,31                 | 0     |
| 56  | MG   | 1A    | 3747 | 1/1   | 0.85 | 0.18 | -    | 49,49,49,49                 | 0     |
| 56  | MG   | 2A    | 3023 | 1/1   | 0.94 | 0.61 | -    | 49,49,49,49                 | 0     |
| 56  | MG   | 1A    | 3789 | 1/1   | 0.96 | 0.09 | -    | 33,33,33,33                 | 0     |
| 56  | MG   | 2A    | 3649 | 1/1   | 0.98 | 0.18 | -    | 30,30,30,30                 | 0     |
| 56  | MG   | 2a    | 1768 | 1/1   | 0.96 | 0.13 | -    | 54,54,54,54                 | 0     |
| 56  | MG   | 1A    | 3760 | 1/1   | 0.90 | 0.12 | -    | 57,57,57,57                 | 0     |
| 56  | MG   | 2A    | 3284 | 1/1   | 0.95 | 0.17 | -    | 49,49,49,49                 | 0     |
| 56  | MG   | 1A    | 3414 | 1/1   | 0.76 | 0.13 | -    | 31,31,31,31                 | 0     |
| 56  | MG   | 2A    | 3250 | 1/1   | 0.88 | 0.12 | -    | 43,43,43,43                 | 0     |
| 56  | MG   | 2a    | 1668 | 1/1   | 0.90 | 0.12 | -    | 64,64,64,64                 | 0     |
| 56  | MG   | 1a    | 1754 | 1/1   | 0.96 | 0.10 | -    | 45,45,45,45                 | 0     |
| 56  | MG   | 1V    | 201  | 1/1   | 0.88 | 0.15 | -    | 52,52,52,52                 | 0     |
| 56  | MG   | 1B    | 3008 | 1/1   | 0.85 | 0.17 | -    | 57,57,57,57                 | 0     |
| 56  | MG   | 2A    | 3043 | 1/1   | 0.88 | 0.26 | -    | 39,39,39,39                 | 0     |
| 56  | MG   | 2A    | 3195 | 1/1   | 0.93 | 0.19 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | 1V    | 202  | 1/1   | 0.95 | 0.15 | -    | 59,59,59,59                 | 0     |
| 56  | MG   | 2A    | 3263 | 1/1   | 0.94 | 0.17 | -    | 45,45,45,45                 | 0     |
| 56  | MG   | 1a    | 1756 | 1/1   | 0.84 | 0.06 | -    | 65,65,65,65                 | 0     |
| 56  | MG   | 2A    | 3509 | 1/1   | 0.89 | 0.21 | -    | 50,50,50,50                 | 0     |
| 56  | MG   | 2a    | 1657 | 1/1   | 0.85 | 0.14 | -    | 54,54,54,54                 | 0     |
| 56  | MG   | 1A    | 3108 | 1/1   | 0.92 | 0.33 | -    | 39,39,39,39                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56  | MG   | 1A    | 3559 | 1/1   | 0.95 | 0.07 | -    | 41,41,41,41                 | 0     |
| 56  | MG   | 1A    | 3705 | 1/1   | 0.88 | 0.10 | -    | 52,52,52,52                 | 0     |
| 56  | MG   | 2a    | 1750 | 1/1   | 0.96 | 0.17 | -    | 72,72,72,72                 | 0     |
| 56  | MG   | 1A    | 3015 | 1/1   | 0.82 | 0.20 | -    | 43,43,43,43                 | 0     |
| 56  | MG   | 2A    | 3112 | 1/1   | 0.90 | 0.31 | -    | 49,49,49,49                 | 0     |
| 56  | MG   | 2A    | 3581 | 1/1   | 0.97 | 0.14 | -    | 66,66,66,66                 | 0     |
| 56  | MG   | 1A    | 3521 | 1/1   | 0.95 | 0.11 | -    | 35,35,35,35                 | 0     |
| 56  | MG   | 1A    | 3297 | 1/1   | 0.96 | 0.16 | -    | 19,19,19,19                 | 0     |
| 56  | MG   | 1A    | 3242 | 1/1   | 0.81 | 0.19 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | 1B    | 3004 | 1/1   | 0.94 | 0.22 | -    | 68,68,68,68                 | 0     |
| 56  | MG   | 2a    | 1710 | 1/1   | 0.97 | 0.09 | -    | 61,61,61,61                 | 0     |
| 56  | MG   | 1A    | 3887 | 1/1   | 0.97 | 0.08 | -    | 49,49,49,49                 | 0     |
| 56  | MG   | 1A    | 3512 | 1/1   | 0.89 | 0.20 | -    | 53,53,53,53                 | 0     |
| 56  | MG   | 1A    | 3692 | 1/1   | 0.93 | 0.21 | -    | 44,44,44,44                 | 0     |
| 56  | MG   | 1A    | 3466 | 1/1   | 0.95 | 0.11 | -    | 50,50,50,50                 | 0     |
| 56  | MG   | 1a    | 1762 | 1/1   | 0.98 | 0.14 | -    | 42,42,42,42                 | 0     |
| 56  | MG   | 1A    | 3710 | 1/1   | 0.94 | 0.10 | -    | 43,43,43,43                 | 0     |
| 56  | MG   | 1A    | 3281 | 1/1   | 0.93 | 0.14 | -    | 48,48,48,48                 | 0     |
| 56  | MG   | 1A    | 3722 | 1/1   | 0.77 | 0.48 | -    | 48,48,48,48                 | 0     |
| 56  | MG   | 1a    | 1723 | 1/1   | 0.94 | 0.12 | -    | 62,62,62,62                 | 0     |
| 56  | MG   | 1A    | 3323 | 1/1   | 0.94 | 0.26 | -    | 50,50,50,50                 | 0     |
| 56  | MG   | 13    | 101  | 1/1   | 0.96 | 0.11 | -    | 50,50,50,50                 | 0     |
| 56  | MG   | 1A    | 3350 | 1/1   | 0.95 | 0.15 | -    | 44,44,44,44                 | 0     |
| 56  | MG   | 2A    | 3512 | 1/1   | 0.84 | 0.12 | -    | 52,52,52,52                 | 0     |
| 56  | MG   | 1N    | 3007 | 1/1   | 0.96 | 0.19 | -    | 25,25,25,25                 | 0     |
| 56  | MG   | 1A    | 3491 | 1/1   | 0.96 | 0.09 | -    | 53,53,53,53                 | 0     |
| 56  | MG   | 1O    | 206  | 1/1   | 0.90 | 0.12 | -    | 62,62,62,62                 | 0     |
| 56  | MG   | 2A    | 3120 | 1/1   | 0.94 | 0.10 | -    | 53,53,53,53                 | 0     |
| 56  | MG   | 2A    | 3563 | 1/1   | 0.96 | 0.09 | -    | 36,36,36,36                 | 0     |
| 56  | MG   | 1A    | 3817 | 1/1   | 0.91 | 0.11 | -    | 45,45,45,45                 | 0     |
| 56  | MG   | 1A    | 3497 | 1/1   | 0.92 | 0.07 | -    | 29,29,29,29                 | 0     |
| 56  | MG   | 1A    | 3732 | 1/1   | 0.85 | 0.08 | -    | 60,60,60,60                 | 0     |
| 56  | MG   | 1A    | 3373 | 1/1   | 0.97 | 0.20 | -    | 53,53,53,53                 | 0     |
| 56  | MG   | 1B    | 3022 | 1/1   | 0.96 | 0.09 | -    | 53,53,53,53                 | 0     |
| 56  | MG   | 1A    | 3247 | 1/1   | 0.96 | 0.24 | -    | 27,27,27,27                 | 0     |
| 56  | MG   | 1A    | 3253 | 1/1   | 0.71 | 0.13 | -    | 51,51,51,51                 | 0     |
| 56  | MG   | 2a    | 1780 | 1/1   | 0.93 | 0.17 | -    | 64,64,64,64                 | 0     |
| 56  | MG   | 2A    | 3474 | 1/1   | 0.84 | 0.10 | -    | 44,44,44,44                 | 0     |
| 56  | MG   | 2A    | 3206 | 1/1   | 0.94 | 0.23 | -    | 38,38,38,38                 | 0     |
| 56  | MG   | 1a    | 1786 | 1/1   | 0.97 | 0.11 | -    | 56,56,56,56                 | 0     |
| 56  | MG   | 1A    | 3506 | 1/1   | 0.96 | 0.14 | -    | 62,62,62,62                 | 0     |
| 56  | MG   | 1a    | 1829 | 1/1   | 0.87 | 0.19 | -    | 57,57,57,57                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56  | MG   | 2A    | 3197 | 1/1   | 0.75 | 0.49 | -    | 50,50,50,50                 | 0     |
| 56  | MG   | 2A    | 3338 | 1/1   | 0.96 | 0.10 | -    | 42,42,42,42                 | 0     |
| 56  | MG   | 2A    | 3060 | 1/1   | 0.92 | 0.12 | -    | 42,42,42,42                 | 0     |
| 56  | MG   | 1A    | 3678 | 1/1   | 0.97 | 0.15 | -    | 36,36,36,36                 | 0     |
| 56  | MG   | 2A    | 3348 | 1/1   | 0.95 | 0.17 | -    | 55,55,55,55                 | 0     |
| 56  | MG   | 1a    | 1725 | 1/1   | 0.91 | 0.15 | -    | 54,54,54,54                 | 0     |
| 56  | MG   | 1A    | 3065 | 1/1   | 0.96 | 0.17 | -    | 14,14,14,14                 | 0     |
| 56  | MG   | 1a    | 1632 | 1/1   | 0.93 | 0.14 | -    | 54,54,54,54                 | 0     |
| 56  | MG   | 1A    | 3599 | 1/1   | 0.97 | 0.21 | -    | 28,28,28,28                 | 0     |
| 56  | MG   | 1A    | 3049 | 1/1   | 0.87 | 0.14 | -    | 60,60,60,60                 | 0     |
| 56  | MG   | 1A    | 3835 | 1/1   | 0.97 | 0.33 | -    | 30,30,30,30                 | 0     |
| 56  | MG   | 1A    | 3021 | 1/1   | 0.88 | 0.20 | -    | 50,50,50,50                 | 0     |
| 56  | MG   | 2a    | 1621 | 1/1   | 0.60 | 0.13 | -    | 74,74,74,74                 | 0     |
| 56  | MG   | 2A    | 3055 | 1/1   | 0.89 | 0.18 | -    | 54,54,54,54                 | 0     |
| 56  | MG   | 2A    | 3199 | 1/1   | 0.96 | 0.23 | -    | 43,43,43,43                 | 0     |
| 56  | MG   | 1A    | 3686 | 1/1   | 0.89 | 0.10 | -    | 29,29,29,29                 | 0     |
| 56  | MG   | 1A    | 3087 | 1/1   | 0.94 | 0.14 | -    | 20,20,20,20                 | 0     |
| 56  | MG   | 2A    | 3296 | 1/1   | 0.90 | 0.18 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | 2w    | 3002 | 1/1   | 0.91 | 0.11 | -    | 63,63,63,63                 | 0     |
| 56  | MG   | 1A    | 3050 | 1/1   | 0.94 | 0.21 | -    | 46,46,46,46                 | 0     |
| 56  | MG   | 1A    | 3476 | 1/1   | 0.93 | 0.07 | -    | 31,31,31,31                 | 0     |
| 56  | MG   | 1A    | 3340 | 1/1   | 0.92 | 0.15 | -    | 51,51,51,51                 | 0     |
| 56  | MG   | 2A    | 3233 | 1/1   | 0.83 | 0.22 | -    | 44,44,44,44                 | 0     |
| 56  | MG   | 2A    | 3153 | 1/1   | 0.98 | 0.14 | -    | 42,42,42,42                 | 0     |
| 56  | MG   | 1A    | 3822 | 1/1   | 0.95 | 0.08 | -    | 52,52,52,52                 | 0     |
| 56  | MG   | 2A    | 3429 | 1/1   | 0.92 | 0.11 | -    | 29,29,29,29                 | 0     |
| 56  | MG   | 1A    | 3520 | 1/1   | 0.97 | 0.11 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | 1A    | 3533 | 1/1   | 0.98 | 0.08 | -    | 28,28,28,28                 | 0     |
| 56  | MG   | 2A    | 3355 | 1/1   | 0.93 | 0.19 | -    | 49,49,49,49                 | 0     |
| 56  | MG   | 1A    | 3548 | 1/1   | 0.90 | 0.22 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | 1A    | 3062 | 1/1   | 0.91 | 0.18 | -    | 50,50,50,50                 | 0     |
| 56  | MG   | 2A    | 3191 | 1/1   | 0.89 | 0.23 | -    | 58,58,58,58                 | 0     |
| 56  | MG   | 1A    | 3869 | 1/1   | 0.93 | 0.13 | -    | 52,52,52,52                 | 0     |
| 56  | MG   | 1A    | 3882 | 1/1   | 0.92 | 0.13 | -    | 52,52,52,52                 | 0     |
| 56  | MG   | 1A    | 3744 | 1/1   | 0.96 | 0.15 | -    | 50,50,50,50                 | 0     |
| 56  | MG   | 2A    | 3632 | 1/1   | 0.82 | 0.21 | -    | 58,58,58,58                 | 0     |
| 56  | MG   | 1A    | 3481 | 1/1   | 0.91 | 0.17 | -    | 26,26,26,26                 | 0     |
| 56  | MG   | 2A    | 3359 | 1/1   | 0.93 | 0.11 | -    | 44,44,44,44                 | 0     |
| 56  | MG   | 2a    | 1613 | 1/1   | 0.81 | 0.18 | -    | 58,58,58,58                 | 0     |
| 56  | MG   | 1A    | 3327 | 1/1   | 0.90 | 0.17 | -    | 44,44,44,44                 | 0     |
| 56  | MG   | 2A    | 3435 | 1/1   | 0.95 | 0.14 | -    | 43,43,43,43                 | 0     |
| 56  | MG   | 2A    | 3575 | 1/1   | 0.85 | 0.08 | -    | 57,57,57,57                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56  | MG   | 2A    | 3279 | 1/1   | 0.97 | 0.13 | -    | 43,43,43,43                 | 0     |
| 56  | MG   | 1W    | 3004 | 1/1   | 0.92 | 0.16 | -    | 33,33,33,33                 | 0     |
| 56  | MG   | 1a    | 1789 | 1/1   | 0.88 | 0.16 | -    | 45,45,45,45                 | 0     |
| 56  | MG   | 2A    | 3113 | 1/1   | 0.90 | 0.22 | -    | 51,51,51,51                 | 0     |
| 56  | MG   | 2A    | 3450 | 1/1   | 0.97 | 0.12 | -    | 24,24,24,24                 | 0     |
| 56  | MG   | 1A    | 3449 | 1/1   | 0.95 | 0.21 | -    | 37,37,37,37                 | 0     |
| 56  | MG   | 2A    | 3608 | 1/1   | 0.94 | 0.14 | -    | 27,27,27,27                 | 0     |
| 56  | MG   | 2A    | 3674 | 1/1   | 0.92 | 0.16 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | 1A    | 3622 | 1/1   | 0.96 | 0.12 | -    | 52,52,52,52                 | 0     |
| 56  | MG   | 1A    | 3257 | 1/1   | 0.69 | 0.26 | -    | 65,65,65,65                 | 0     |
| 56  | MG   | 1A    | 3720 | 1/1   | 0.59 | 0.26 | -    | 71,71,71,71                 | 0     |
| 56  | MG   | 1A    | 3095 | 1/1   | 0.86 | 0.22 | -    | 54,54,54,54                 | 0     |
| 56  | MG   | 2A    | 3315 | 1/1   | 0.92 | 0.18 | -    | 40,40,40,40                 | 0     |
| 56  | MG   | 2a    | 1644 | 1/1   | 0.97 | 0.10 | -    | 66,66,66,66                 | 0     |
| 56  | MG   | 1A    | 3606 | 1/1   | 0.99 | 0.17 | -    | 19,19,19,19                 | 0     |
| 56  | MG   | 2A    | 3417 | 1/1   | 0.98 | 0.12 | -    | 43,43,43,43                 | 0     |
| 56  | MG   | 1A    | 3573 | 1/1   | 0.98 | 0.14 | -    | 34,34,34,34                 | 0     |
| 56  | MG   | 1f    | 3002 | 1/1   | 0.96 | 0.15 | -    | 54,54,54,54                 | 0     |
| 56  | MG   | 1a    | 1767 | 1/1   | 0.99 | 0.24 | -    | 67,67,67,67                 | 0     |
| 56  | MG   | 2A    | 3616 | 1/1   | 0.89 | 0.17 | -    | 55,55,55,55                 | 0     |
| 56  | MG   | 2A    | 3245 | 1/1   | 0.90 | 0.15 | -    | 42,42,42,42                 | 0     |
| 56  | MG   | 2A    | 3045 | 1/1   | 0.99 | 0.17 | -    | 36,36,36,36                 | 0     |
| 56  | MG   | 1A    | 3381 | 1/1   | 0.95 | 0.23 | -    | 57,57,57,57                 | 0     |
| 56  | MG   | 2A    | 3424 | 1/1   | 0.86 | 0.22 | -    | 43,43,43,43                 | 0     |
| 56  | MG   | 2A    | 3494 | 1/1   | 0.94 | 0.14 | -    | 45,45,45,45                 | 0     |
| 56  | MG   | 1A    | 3653 | 1/1   | 0.96 | 0.13 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | 1A    | 3826 | 1/1   | 0.89 | 0.20 | -    | 37,37,37,37                 | 0     |
| 56  | MG   | 1A    | 3035 | 1/1   | 0.97 | 0.33 | -    | 32,32,32,32                 | 0     |
| 56  | MG   | 1x    | 3002 | 1/1   | 0.96 | 0.15 | -    | 56,56,56,56                 | 0     |
| 56  | MG   | 1A    | 3392 | 1/1   | 0.94 | 0.19 | -    | 39,39,39,39                 | 0     |

## 6.5 Other polymers ⓘ

There are no such residues in this entry.