



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2016 – 04:41 PM EDT

PDB ID : 5F8K  
Title : Crystal structure of the Bac7(1-16) antimicrobial peptide bound to the *Thermus thermophilus* 70S ribosome  
Authors : Seefeldt, A.C.; Graf, M.; Perebaskine, N.; Nguyen, F.; Arenz, S.; Mardirossian, M.; Scocchi, M.; Wilson, D.N.; Innis, C.A.  
Deposited on : 2015-12-09  
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](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-20027107  |
| Percentile statistics          | : | 20151230.v01 (using entries in the PDB archive December 30th 2015) |
| Refmac                         | : | 5.8.0122   |
| CCP4                           | : | 6.5.0  |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)  |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)  |
| Validation Pipeline (wwPDB-VP) | : | rb-20027107  |

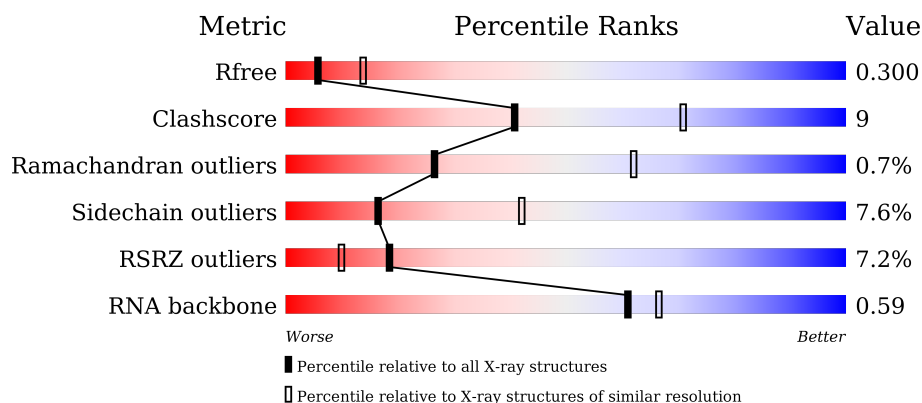
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 Å.

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




























| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 91344                       | 2393 (2.80-2.80)                                      |
| Clashscore            | 102246                      | 2827 (2.80-2.80)                                      |
| Ramachandran outliers | 100387                      | 2782 (2.80-2.80)                                      |
| Sidechain outliers    | 100360                      | 2784 (2.80-2.80)                                      |
| RSRZ outliers         | 91569                       | 2404 (2.80-2.80)                                      |
| RNA backbone          | 2183                        | 1091 (3.20-2.40)                                      |

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>8%</div> <div>63% 29% 6% ..</div> </div> |
| 1   | 2A    | 2915   | <div> <div>9%</div> <div>62% 30% 6% ..</div> </div> |
| 2   | 1B    | 120    | <div> <div>2%</div> <div>79% 16% 5%</div> </div>    |
| 2   | 2B    | 120    | <div> <div>9%</div> <div>64% 33% ..</div> </div>    |

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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 3   | 1D    | 275    |    |
| 3   | 2D    | 275    |    |
| 4   | 1E    | 204    |    |
| 4   | 2E    | 204    |    |
| 5   | 1F    | 203    |    |
| 5   | 2F    | 203    |    |
| 6   | 1G    | 181    |    |
| 6   | 2G    | 181    |    |
| 7   | 1H    | 174    |    |
| 7   | 2H    | 174    |    |
| 8   | 1I    | 147    |    |
| 8   | 2I    | 147    |   |
| 9   | 1N    | 140    |  |
| 9   | 2N    | 140    |  |
| 10  | 1O    | 122    |  |
| 10  | 2O    | 122    |  |
| 11  | 1P    | 149    |  |
| 11  | 2P    | 149    |  |
| 12  | 1Q    | 141    |  |
| 12  | 2Q    | 141    |  |
| 13  | 1R    | 118    |  |
| 13  | 2R    | 118    |  |
| 14  | 1S    | 110    |  |
| 14  | 2S    | 110    |  |
| 15  | 1T    | 131    |  |

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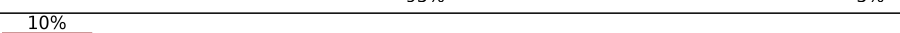
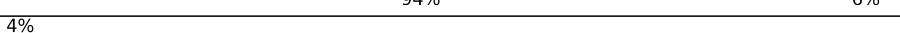
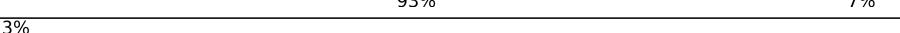
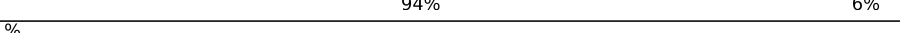
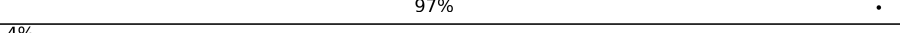


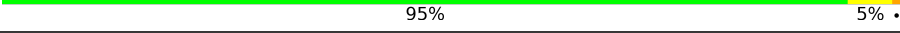
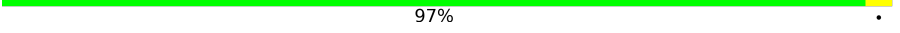
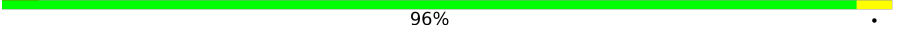
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| Mol | Chain | Length | Quality of chain  |
|-----|-------|--------|---|
| 15  | 2T    | 131    | <div> <div>3%</div> <div>76%</div> <div>21%</div> <div>.</div> </div>   |
| 16  | 1U    | 116    | <div> <div>80%</div> <div>19%</div> <div>.</div> </div>                 |
| 16  | 2U    | 116    | <div> <div>4%</div> <div>80%</div> <div>19%</div> <div>.</div> </div>   |
| 17  | 1V    | 101    | <div> <div>%</div> <div>79%</div> <div>18%</div> <div>.</div> </div>    |
| 17  | 2V    | 101    | <div> <div>5%</div> <div>75%</div> <div>23%</div> <div>..</div> </div>  |
| 18  | 1W    | 112    | <div> <div>86%</div> <div>12%</div> <div>.</div> </div>                 |
| 18  | 2W    | 112    | <div> <div>2%</div> <div>82%</div> <div>15%</div> <div>.</div> </div>   |
| 19  | 1X    | 95     | <div> <div>76%</div> <div>23%</div> <div>.</div> </div>                 |
| 19  | 2X    | 95     | <div> <div>%</div> <div>74%</div> <div>25%</div> <div>.</div> </div>    |
| 20  | 1Y    | 107    | <div> <div>70%</div> <div>29%</div> <div>.</div> </div>                 |
| 20  | 2Y    | 107    | <div> <div>5%</div> <div>79%</div> <div>21%</div> <div>.</div> </div>   |
| 21  | 1Z    | 203    | <div> <div>7%</div> <div>69%</div> <div>29%</div> <div>.</div> </div>   |
| 21  | 2Z    | 203    | <div> <div>12%</div> <div>63%</div> <div>33%</div> <div>..</div> </div> |
| 22  | 10    | 77     | <div> <div>%</div> <div>78%</div> <div>18%</div> <div>.</div> </div>    |
| 22  | 20    | 77     | <div> <div>4%</div> <div>81%</div> <div>18%</div> <div>.</div> </div>   |
| 23  | 11    | 97     | <div> <div>8%</div> <div>78%</div> <div>21%</div> <div>.</div> </div>   |
| 23  | 21    | 97     | <div> <div>5%</div> <div>65%</div> <div>30%</div> <div>5%</div> </div>  |
| 24  | 12    | 70     | <div> <div>80%</div> <div>17%</div> <div>.</div> </div>                 |
| 24  | 22    | 70     | <div> <div>%</div> <div>77%</div> <div>21%</div> <div>.</div> </div>    |
| 25  | 13    | 59     | <div> <div>75%</div> <div>25%</div> </div>                              |
| 25  | 23    | 59     | <div> <div>8%</div> <div>59%</div> <div>37%</div> <div>.</div> </div>   |
| 26  | 14    | 69     | <div> <div>16%</div> <div>58%</div> <div>38%</div> <div>..</div> </div> |
| 26  | 24    | 69     | <div> <div>45%</div> <div>52%</div> <div>45%</div> <div>.</div> </div>  |
| 27  | 15    | 59     | <div> <div>76%</div> <div>22%</div> <div>.</div> </div>                 |
| 27  | 25    | 59     | <div> <div>3%</div> <div>81%</div> <div>17%</div> <div>.</div> </div>   |

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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 28  | 16    | 53     |    |
| 28  | 26    | 53     |    |
| 29  | 17    | 48     |    |
| 29  | 27    | 48     |    |
| 30  | 18    | 64     |    |
| 30  | 28    | 64     |    |
| 31  | 19    | 37     |    |
| 31  | 29    | 37     |    |
| 32  | 1a    | 1520   |    |
| 32  | 2a    | 1520   |    |
| 33  | 1b    | 231    |    |
| 33  | 2b    | 231    |    |
| 34  | 1c    | 206    |  |
| 34  | 2c    | 206    |  |
| 35  | 1d    | 208    |  |
| 35  | 2d    | 208    |  |
| 36  | 1e    | 148    |  |
| 36  | 2e    | 148    |  |
| 37  | 1f    | 100    |  |
| 37  | 2f    | 100    |  |
| 38  | 1g    | 155    |  |
| 38  | 2g    | 155    |  |
| 39  | 1h    | 137    |  |
| 39  | 2h    | 137    |  |
| 40  | 1i    | 127    |  |

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| Mol | Chain | Length | Quality of chain  |
|-----|-------|--------|---|
| 40  | 2i    | 127    | <div> <div>26%</div> <div>87%</div> <div>12%</div> </div> |
| 41  | 1j    | 97     | <div> <div>16%</div> <div>90%</div> <div>10%</div> </div> |
| 41  | 2j    | 97     | <div> <div>25%</div> <div>91%</div> <div>8%</div> </div>  |
| 42  | 1k    | 114    | <div> <div>7%</div> <div>96%</div> <div></div> </div>     |
| 42  | 2k    | 114    | <div> <div>11%</div> <div>96%</div> <div></div> </div>    |
| 43  | 1l    | 122    | <div> <div>7%</div> <div>97%</div> <div></div> </div>     |
| 43  | 2l    | 122    | <div> <div>3%</div> <div>95%</div> <div>5%</div> </div>   |
| 44  | 1m    | 116    | <div> <div>12%</div> <div>92%</div> <div>8%</div> </div>  |
| 44  | 2m    | 116    | <div> <div>11%</div> <div>90%</div> <div>9%</div> </div>  |
| 45  | 1n    | 60     | <div> <div>7%</div> <div>90%</div> <div>10%</div> </div>  |
| 45  | 2n    | 60     | <div> <div>20%</div> <div>95%</div> <div>5%</div> </div>  |
| 46  | 1o    | 88     | <div> <div>%</div> <div>95%</div> <div>5%</div> </div>    |
| 46  | 2o    | 88     | <div> <div>%</div> <div>92%</div> <div>7%</div> </div>    |
| 47  | 1p    | 82     | <div> <div>7%</div> <div>87%</div> <div>13%</div> </div>  |
| 47  | 2p    | 82     | <div> <div>9%</div> <div>85%</div> <div>15%</div> </div>  |
| 48  | 1q    | 99     | <div> <div>%</div> <div>97%</div> <div></div> </div>      |
| 48  | 2q    | 99     | <div> <div>%</div> <div>96%</div> <div></div> </div>      |
| 49  | 1r    | 68     | <div> <div>12%</div> <div>96%</div> <div></div> </div>    |
| 49  | 2r    | 68     | <div> <div>16%</div> <div>94%</div> <div>6%</div> </div>  |
| 50  | 1s    | 83     | <div> <div>2%</div> <div>90%</div> <div>10%</div> </div>  |
| 50  | 2s    | 83     | <div> <div>18%</div> <div>94%</div> <div>6%</div> </div>  |
| 51  | 1t    | 98     | <div> <div>2%</div> <div>90%</div> <div>6%</div> </div>   |
| 51  | 2t    | 98     | <div> <div>4%</div> <div>92%</div> <div>7%</div> </div>   |
| 52  | 1u    | 23     | <div> <div></div> <div>96%</div> <div></div> </div>       |
| 52  | 2u    | 23     | <div> <div>35%</div> <div>100%</div> <div></div> </div>   |

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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 53  | 1v    | 3      |  100%        |
| 53  | 2v    | 3      |  100%        |
| 54  | 1x    | 76     |  3% 74% 26%  |
| 54  | 2x    | 76     |  21% 83% 17% |
| 55  | 1y    | 16     |  75% 19% 6%  |
| 55  | 2y    | 16     |  81% 13% 6%  |

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   | 15    | 105  | -         | -        | -       | X                |
| 56  | MG   | 18    | 101  | -         | -        | -       | X                |
| 56  | MG   | 19    | 101  | -         | -        | -       | X                |
| 56  | MG   | 1A    | 8008 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 8020 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 8021 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 8022 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 8024 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 8025 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 8026 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 8030 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 8032 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 8041 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 8045 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 8070 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 8080 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 8091 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 8098 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 8107 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 8108 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 8110 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 8111 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 8117 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 8126 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 8131 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 8147 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 8156 | -         | -        | -       | X                |

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| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 56  | MG   | 1A    | 8161 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 8167 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 8173 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 8178 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 8207 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 8208 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 8210 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 8212 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 8215 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 8217 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 8223 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 8256 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 8258 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 8266 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 8268 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 8275 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 8276 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 8291 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 8347 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 8363 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 8467 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 8478 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 8484 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 8489 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 8494 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 8532 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 8556 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 8565 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 8589 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 8597 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 8647 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 8657 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 8658 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 8683 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 8726 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 8741 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 8743 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 8753 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 8759 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 8798 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 8806 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 8832 | -         | -        | -       | X                |

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| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 56  | MG   | 1A    | 8855 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 8911 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 8917 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 8920 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 8922 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 8927 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 8928 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 8933 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 8936 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 8943 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 8949 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 8952 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 8955 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 8965 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 8969 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 8970 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 8972 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 8973 | -         | -        | -       | X                |
| 56  | MG   | 1B    | 3005 | -         | -        | -       | X                |
| 56  | MG   | 1D    | 307  | -         | -        | -       | X                |
| 56  | MG   | 1D    | 314  | -         | -        | -       | X                |
| 56  | MG   | 1E    | 305  | -         | -        | -       | X                |
| 56  | MG   | 1F    | 301  | -         | -        | -       | X                |
| 56  | MG   | 1F    | 302  | -         | -        | -       | X                |
| 56  | MG   | 1F    | 303  | -         | -        | -       | X                |
| 56  | MG   | 1a    | 1613 | -         | -        | -       | X                |
| 56  | MG   | 1a    | 1625 | -         | -        | -       | X                |
| 56  | MG   | 1a    | 1649 | -         | -        | -       | X                |
| 56  | MG   | 1a    | 1653 | -         | -        | -       | X                |
| 56  | MG   | 1a    | 1668 | -         | -        | -       | X                |
| 56  | MG   | 1a    | 1669 | -         | -        | -       | X                |
| 56  | MG   | 1a    | 1682 | -         | -        | -       | X                |
| 56  | MG   | 1a    | 1740 | -         | -        | -       | X                |
| 56  | MG   | 1a    | 1751 | -         | -        | -       | X                |
| 56  | MG   | 1a    | 1833 | -         | -        | -       | X                |
| 56  | MG   | 1a    | 1836 | -         | -        | -       | X                |
| 56  | MG   | 1o    | 101  | -         | -        | -       | X                |
| 56  | MG   | 20    | 105  | -         | -        | -       | X                |
| 56  | MG   | 25    | 103  | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3016 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3024 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3028 | -         | -        | -       | X                |

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| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 56  | MG   | 2A    | 3029 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3061 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3070 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3080 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3084 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3086 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3090 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3092 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3106 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3108 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3113 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3131 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3138 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3142 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3150 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3151 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3169 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3177 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3187 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3196 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3199 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3203 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3211 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3219 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3227 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3244 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3261 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3269 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3291 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3330 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3348 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3350 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3364 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3391 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3405 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3482 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3487 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3523 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3527 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3530 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3558 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3561 | -         | -        | -       | X                |

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| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 56  | MG   | 2A    | 3563 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3572 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3575 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3585 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3593 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3611 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3629 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3641 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3654 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3656 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3657 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3667 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3702 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3727 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3740 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3744 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3748 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3757 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3774 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3804 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3831 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3833 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3854 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3891 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3917 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3921 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3924 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3926 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3934 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3938 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3939 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3944 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3946 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3947 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3948 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3949 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3951 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3954 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3955 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3956 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3957 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3959 | -         | -        | -       | X                |

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| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 56  | MG   | 2A    | 3961 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3964 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3971 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3976 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3977 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3981 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3984 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3987 | -         | -        | -       | X                |
| 56  | MG   | 2B    | 3008 | -         | -        | -       | X                |
| 56  | MG   | 2B    | 3014 | -         | -        | -       | X                |
| 56  | MG   | 2B    | 3020 | -         | -        | -       | X                |
| 56  | MG   | 2F    | 302  | -         | -        | -       | X                |
| 56  | MG   | 2F    | 307  | -         | -        | -       | X                |
| 56  | MG   | 2F    | 308  | -         | -        | -       | X                |
| 56  | MG   | 2N    | 201  | -         | -        | -       | X                |
| 56  | MG   | 2R    | 201  | -         | -        | -       | X                |
| 56  | MG   | 2U    | 204  | -         | -        | -       | X                |
| 56  | MG   | 2a    | 1635 | -         | -        | -       | X                |
| 56  | MG   | 2a    | 1657 | -         | -        | -       | X                |
| 56  | MG   | 2a    | 1660 | -         | -        | -       | X                |
| 56  | MG   | 2a    | 1661 | -         | -        | -       | X                |
| 56  | MG   | 2a    | 1667 | -         | -        | -       | X                |
| 56  | MG   | 2a    | 1712 | -         | -        | -       | X                |
| 56  | MG   | 2a    | 1718 | -         | -        | -       | X                |
| 56  | MG   | 2a    | 1725 | -         | -        | -       | X                |
| 56  | MG   | 2a    | 1728 | -         | -        | -       | X                |
| 56  | MG   | 2a    | 1729 | -         | -        | -       | X                |
| 56  | MG   | 2a    | 1765 | -         | -        | -       | X                |
| 56  | MG   | 2a    | 1767 | -         | -        | -       | X                |
| 56  | MG   | 2a    | 1780 | -         | -        | -       | X                |
| 56  | MG   | 2a    | 1799 | -         | -        | -       | X                |
| 56  | MG   | 2a    | 1810 | -         | -        | -       | X                |
| 56  | MG   | 2x    | 104  | -         | -        | -       | X                |



## 2 Entry composition [i](#)

There are 60 unique types of molecules in this entry. The entry contains 296108 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

| Mol | Chain | Residues | Atoms |       |       |       |      | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|---------|-------|
| 1   | 1A    | 2872     | Total | C     | N     | O     | P    | 0       | 0       | 0     |
|     |       |          | 61872 | 27540 | 11574 | 19886 | 2872 |         |         |       |
| 1   | 2A    | 2867     | Total | C     | N     | O     | P    | 0       | 0       | 0     |
|     |       |          | 61761 | 27491 | 11552 | 19852 | 2866 |         |         |       |

- 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     |
|     |       |          | 2575  | 1145 | 476 | 834 | 120 |         |         |       |
| 2   | 2B    | 120      | Total | C    | N   | O   | P   | 0       | 0       | 0     |
|     |       |          | 2571  | 1146 | 476 | 831 | 118 |         |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 3   | 1D    | 275      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2131  | 1346 | 422 | 360 | 3 |         |         |       |
| 3   | 2D    | 275      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2136  | 1349 | 423 | 361 | 3 |         |         |       |

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

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

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

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

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 6   | 1G    | 181      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1426  | 916 | 253 | 253 | 4 |         |         |       |
| 6   | 2G    | 181      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1424  | 912 | 259 | 249 | 4 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 7   | 1H    | 174      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1330  | 845 | 248 | 236 | 1 |         |         |       |
| 7   | 2H    | 173      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1324  | 842 | 247 | 234 | 1 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 8   | 1I    | 147      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1094  | 699 | 191 | 203 | 1 |         |         |       |
| 8   | 2I    | 146      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1076  | 687 | 186 | 202 | 1 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 9   | 1N    | 140      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1121  | 722 | 208 | 187 | 4 |         |         |       |
| 9   | 2N    | 140      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1117  | 719 | 207 | 187 | 4 |         |         |       |

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

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

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

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

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

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

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

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

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

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

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 14  | 1S    | 110      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 877   | 553 | 175 | 149 |         |         |       |
| 14  | 2S    | 110      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 870   | 549 | 173 | 148 |         |         |       |

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

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

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

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

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 17  | 1V    | 101      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 775   | 498 | 141 | 135 | 1 |         |         |       |
| 17  | 2V    | 101      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 771   | 495 | 140 | 135 | 1 |         |         |       |

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

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

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

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

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 20  | 1Y    | 107      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 810   | 520 | 153 | 131 | 6 |         |         |       |
| 20  | 2Y    | 107      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 810   | 519 | 153 | 132 | 6 |         |         |       |

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

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

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 22  | 10    | 77       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 608   | 375 | 129 | 103 | 1 |         |         |       |
| 22  | 20    | 77       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 608   | 375 | 129 | 103 | 1 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 23  | 11    | 97       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 754   | 475 | 148 | 130 | 1 |         |         |       |
| 23  | 21    | 97       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 759   | 478 | 149 | 131 | 1 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 24  | 12    | 70       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 588   | 365 | 118 | 103 | 2 |         |         |       |
| 24  | 22    | 70       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 592   | 368 | 119 | 103 | 2 |         |         |       |

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

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

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

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 26  | 14    | 69       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 546   | 346 | 96 | 99 | 5 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 26  | 24    | 69       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 536   | 342 | 98 | 91 | 5 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 27  | 15    | 59       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 459   | 288 | 90 | 76 | 5 |         |         |       |
| 27  | 25    | 59       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 455   | 285 | 89 | 76 | 5 |         |         |       |

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

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

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

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

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

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

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

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

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

| Mol | Chain | Residues | Atoms |       |      |       |      | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|---------|-------|
| 32  | 1a    | 1500     | Total | C     | N    | O     | P    | 0       | 0       | 0     |
|     |       |          | 32246 | 14358 | 5975 | 10413 | 1500 |         |         |       |
| 32  | 2a    | 1504     | Total | C     | N    | O     | P    | 0       | 0       | 0     |
|     |       |          | 32331 | 14396 | 5990 | 10441 | 1504 |         |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 33  | 1b    | 231      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1842  | 1175 | 330 | 332 | 5 |         |         |       |
| 33  | 2b    | 231      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1825  | 1167 | 326 | 327 | 5 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 34  | 1c    | 206      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1558  | 979 | 305 | 273 | 1 |         |         |       |
| 34  | 2c    | 206      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1542  | 968 | 300 | 273 | 1 |         |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 35  | 1d    | 208      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1665  | 1043 | 329 | 286 | 7 |         |         |       |
| 35  | 2d    | 208      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1668  | 1047 | 330 | 284 | 7 |         |         |       |

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

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

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 37  | 1f    | 100      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 814   | 516 | 144 | 151 | 3 |         |         |       |
| 37  | 2f    | 100      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 816   | 516 | 146 | 151 | 3 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 38  | 1g    | 155      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1235  | 769 | 244 | 216 | 6 |         |         |       |
| 38  | 2g    | 155      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1229  | 766 | 241 | 216 | 6 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 39  | 1h    | 137      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1098  | 694 | 210 | 192 | 2 |         |         |       |
| 39  | 2h    | 137      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1088  | 689 | 206 | 191 | 2 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 40  | 1i    | 127      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 986   | 625 | 193 | 168 |         |         |       |
| 40  | 2i    | 126      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 966   | 613 | 186 | 167 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 41  | 1j    | 97       | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 719   | 446 | 142 | 131 |         |         |       |
| 41  | 2j    | 96       | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 710   | 442 | 137 | 131 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 42  | 1k    | 114      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 834   | 520 | 156 | 155 | 3 |         |         |       |

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

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

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

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 44  | 1m    | 116      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 914   | 564 | 189 | 159 | 2 |         |         |       |
| 44  | 2m    | 114      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 895   | 550 | 186 | 157 | 2 |         |         |       |

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

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

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

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

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

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

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

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

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

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

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 50  | 1s    | 83       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 648   | 415 | 120 | 111 | 2 |         |         |       |
| 50  | 2s    | 83       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 645   | 410 | 118 | 115 | 2 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 51  | 1t    | 96       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 732   | 449 | 157 | 124 | 2 |         |         |       |
| 51  | 2t    | 98       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 733   | 451 | 154 | 126 | 2 |         |         |       |

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

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

- Molecule 53 is a RNA chain called mRNA.

| Mol | Chain | Residues | Atoms |    |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---|---------|---------|-------|
| 53  | 1v    | 3        | Total | C  | N  | O  | P | 0       | 0       | 0     |
|     |       |          | 65    | 29 | 12 | 21 | 3 |         |         |       |
| 53  | 2v    | 3        | Total | C  | N  | O  | P | 0       | 0       | 0     |
|     |       |          | 65    | 29 | 12 | 21 | 3 |         |         |       |

- Molecule 54 is a RNA chain called tRNAiMet.

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

- Molecule 55 is a protein called Cathelicidin-3.

| Mol | Chain | Residues | Atoms |    |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---------|---------|-------|
| 55  | 1y    | 16       | Total | C  | N  | O  | 0       | 0       | 0     |
|     |       |          | 147   | 90 | 40 | 17 |         |         |       |
| 55  | 2y    | 16       | Total | C  | N  | O  | 0       | 0       | 0     |
|     |       |          | 147   | 90 | 40 | 17 |         |         |       |

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

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 56  | 2E    | 6        | Total | Mg | 0       | 0       |
|     |       |          | 6     | 6  |         |         |
| 56  | 17    | 2        | Total | Mg | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 56  | 2d    | 4        | Total | Mg | 0       | 0       |
|     |       |          | 4     | 4  |         |         |
| 56  | 1T    | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 56  | 1N    | 4        | Total | Mg | 0       | 0       |
|     |       |          | 4     | 4  |         |         |
| 56  | 20    | 5        | Total | Mg | 0       | 0       |
|     |       |          | 5     | 5  |         |         |
| 56  | 18    | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 56  | 1o    | 2        | Total | Mg | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 56  | 2W    | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

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| Mol | Chain | Residues | Atoms        |           | ZeroOcc | AltConf |
|-----|-------|----------|--------------|-----------|---------|---------|
| 56  | 13    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 56  | 1f    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 56  | 2h    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 56  | 1P    | 4        | Total<br>4   | Mg<br>4   | 0       | 0       |
| 56  | 2B    | 25       | Total<br>25  | Mg<br>25  | 0       | 0       |
| 56  | 1q    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 56  | 2a    | 221      | Total<br>221 | Mg<br>221 | 0       | 0       |
| 56  | 1E    | 7        | Total<br>7   | Mg<br>7   | 0       | 0       |
| 56  | 1b    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 56  | 2l    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 56  | 2F    | 9        | Total<br>9   | Mg<br>9   | 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    | 3        | Total<br>3   | Mg<br>3   | 0       | 0       |
| 56  | 1A    | 973      | Total<br>973 | Mg<br>973 | 0       | 0       |
| 56  | 1t    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 56  | 1n    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 56  | 2P    | 3        | Total<br>3   | Mg<br>3   | 0       | 0       |
| 56  | 1X    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 56  | 2i    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 56  | 1S    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |

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| Mol | Chain | Residues | Atoms        |           | ZeroOcc | AltConf |
|-----|-------|----------|--------------|-----------|---------|---------|
| 56  | 25    | 3        | Total<br>3   | Mg<br>3   | 0       | 0       |
| 56  | 2b    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 56  | 1D    | 14       | Total<br>14  | Mg<br>14  | 0       | 0       |
| 56  | 2N    | 3        | Total<br>3   | Mg<br>3   | 0       | 0       |
| 56  | 1e    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 56  | 2G    | 3        | Total<br>3   | Mg<br>3   | 0       | 0       |
| 56  | 29    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 56  | 2f    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 56  | 1V    | 3        | Total<br>3   | Mg<br>3   | 0       | 0       |
| 56  | 2X    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 56  | 1a    | 240      | Total<br>240 | Mg<br>240 | 0       | 0       |
| 56  | 2Q    | 4        | Total<br>4   | Mg<br>4   | 0       | 0       |
| 56  | 15    | 7        | Total<br>7   | Mg<br>7   | 0       | 0       |
| 56  | 1x    | 13       | Total<br>13  | Mg<br>13  | 0       | 0       |
| 56  | 2j    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 56  | 1R    | 4        | Total<br>4   | Mg<br>4   | 0       | 0       |
| 56  | 2t    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 56  | 2v    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 56  | 2U    | 7        | Total<br>7   | Mg<br>7   | 0       | 0       |
| 56  | 1G    | 3        | Total<br>3   | Mg<br>3   | 0       | 0       |
| 56  | 11    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |

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| Mol | Chain | Residues | Atoms       |          | ZeroOcc | AltConf |
|-----|-------|----------|-------------|----------|---------|---------|
| 56  | 1d    | 5        | Total<br>5  | Mg<br>5  | 0       | 0       |
| 56  | 2n    | 1        | Total<br>1  | Mg<br>1  | 0       | 0       |
| 56  | 1H    | 2        | Total<br>2  | Mg<br>2  | 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  | 2Y    | 2        | Total<br>2  | Mg<br>2  | 0       | 0       |
| 56  | 23    | 2        | Total<br>2  | Mg<br>2  | 0       | 0       |
| 56  | 2x    | 12       | Total<br>12 | Mg<br>12 | 0       | 0       |
| 56  | 2R    | 2        | Total<br>2  | Mg<br>2  | 0       | 0       |
| 56  | 2D    | 17       | Total<br>17 | Mg<br>17 | 0       | 0       |
| 56  | 1U    | 3        | Total<br>3  | Mg<br>3  | 0       | 0       |
| 56  | 27    | 2        | Total<br>2  | Mg<br>2  | 0       | 0       |
| 56  | 19    | 3        | Total<br>3  | Mg<br>3  | 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    | 10       | Total<br>10 | Mg<br>10 | 0       | 0       |
| 56  | 2H    | 2        | Total<br>2  | Mg<br>2  | 0       | 0       |
| 56  | 10    | 8        | Total<br>8  | Mg<br>8  | 0       | 0       |
| 56  | 1g    | 1        | Total<br>1  | Mg<br>1  | 0       | 0       |
| 56  | 2o    | 1        | Total<br>1  | Mg<br>1  | 0       | 0       |
| 56  | 1Q    | 6        | Total<br>6  | Mg<br>6  | 0       | 0       |

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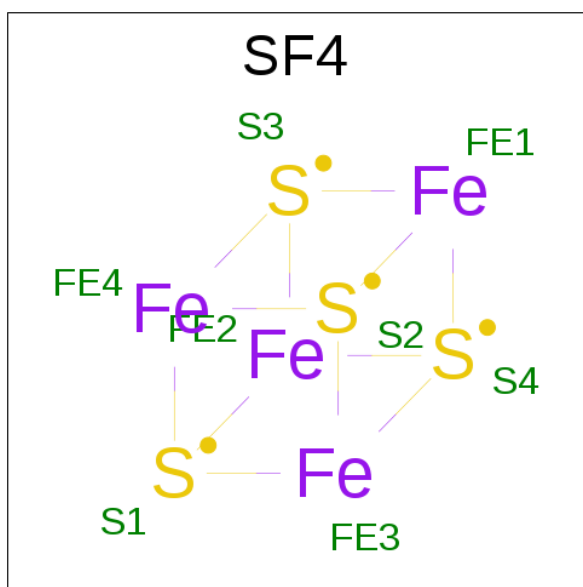
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| Mol | Chain | Residues | Atoms        |           | ZeroOcc | AltConf |
|-----|-------|----------|--------------|-----------|---------|---------|
| 56  | 2A    | 986      | Total<br>986 | Mg<br>986 | 0       | 0       |
| 56  | 1h    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 56  | 1B    | 27       | Total<br>27  | Mg<br>27  | 0       | 0       |
| 56  | 2S    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |

- Molecule 57 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms      |         | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 57  | 1Y    | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 57  | 14    | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 57  | 1n    | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 57  | 15    | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 57  | 29    | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 57  | 19    | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 57  | 26    | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 57  | 25    | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 57  | 24    | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 57  | 2n    | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 57  | 2Y    | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 57  | 16    | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |

- Molecule 58 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



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

- Molecule 59 is POTASSIUM ION (three-letter code: K) (formula: K).

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

- Molecule 60 is water.

| Mol | Chain | Residues | Atoms |      | ZeroOcc | AltConf |
|-----|-------|----------|-------|------|---------|---------|
| 60  | 1A    | 1795     | Total | O    | 0       | 0       |
|     |       |          | 1795  | 1795 |         |         |
| 60  | 1B    | 49       | Total | O    | 0       | 0       |
|     |       |          | 49    | 49   |         |         |
| 60  | 1D    | 23       | Total | O    | 0       | 0       |
|     |       |          | 23    | 23   |         |         |
| 60  | 1E    | 16       | Total | O    | 0       | 0       |
|     |       |          | 16    | 16   |         |         |
| 60  | 1F    | 9        | Total | O    | 0       | 0       |
|     |       |          | 9     | 9    |         |         |

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| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 60  | 1G    | 2        | Total | O   | 0       | 0       |
|     |       |          | 2     | 2   |         |         |
| 60  | 1H    | 4        | Total | O   | 0       | 0       |
|     |       |          | 4     | 4   |         |         |
| 60  | 1N    | 8        | Total | O   | 0       | 0       |
|     |       |          | 8     | 8   |         |         |
| 60  | 1P    | 14       | Total | O   | 0       | 0       |
|     |       |          | 14    | 14  |         |         |
| 60  | 1Q    | 6        | Total | O   | 0       | 0       |
|     |       |          | 6     | 6   |         |         |
| 60  | 1R    | 6        | Total | O   | 0       | 0       |
|     |       |          | 6     | 6   |         |         |
| 60  | 1T    | 5        | Total | O   | 0       | 0       |
|     |       |          | 5     | 5   |         |         |
| 60  | 1U    | 3        | Total | O   | 0       | 0       |
|     |       |          | 3     | 3   |         |         |
| 60  | 1V    | 6        | Total | O   | 0       | 0       |
|     |       |          | 6     | 6   |         |         |
| 60  | 1W    | 1        | Total | O   | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 60  | 1X    | 6        | Total | O   | 0       | 0       |
|     |       |          | 6     | 6   |         |         |
| 60  | 1Y    | 4        | Total | O   | 0       | 0       |
|     |       |          | 4     | 4   |         |         |
| 60  | 10    | 5        | Total | O   | 0       | 0       |
|     |       |          | 5     | 5   |         |         |
| 60  | 11    | 5        | Total | O   | 0       | 0       |
|     |       |          | 5     | 5   |         |         |
| 60  | 13    | 1        | Total | O   | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 60  | 15    | 3        | Total | O   | 0       | 0       |
|     |       |          | 3     | 3   |         |         |
| 60  | 16    | 1        | Total | O   | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 60  | 17    | 2        | Total | O   | 0       | 0       |
|     |       |          | 2     | 2   |         |         |
| 60  | 18    | 8        | Total | O   | 0       | 0       |
|     |       |          | 8     | 8   |         |         |
| 60  | 19    | 2        | Total | O   | 0       | 0       |
|     |       |          | 2     | 2   |         |         |
| 60  | 1a    | 408      | Total | O   | 0       | 0       |
|     |       |          | 408   | 408 |         |         |

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| Mol | Chain | Residues | Atoms         |           | ZeroOcc | AltConf |
|-----|-------|----------|---------------|-----------|---------|---------|
| 60  | 1d    | 8        | Total<br>8    | O<br>8    | 0       | 0       |
| 60  | 1e    | 3        | Total<br>3    | O<br>3    | 0       | 0       |
| 60  | 1f    | 1        | Total<br>1    | O<br>1    | 0       | 0       |
| 60  | 1h    | 1        | Total<br>1    | O<br>1    | 0       | 0       |
| 60  | 1j    | 1        | Total<br>1    | O<br>1    | 0       | 0       |
| 60  | 1l    | 4        | Total<br>4    | O<br>4    | 0       | 0       |
| 60  | 1m    | 1        | Total<br>1    | O<br>1    | 0       | 0       |
| 60  | 1o    | 2        | Total<br>2    | O<br>2    | 0       | 0       |
| 60  | 1p    | 1        | Total<br>1    | O<br>1    | 0       | 0       |
| 60  | 1t    | 2        | Total<br>2    | O<br>2    | 0       | 0       |
| 60  | 1v    | 2        | Total<br>2    | O<br>2    | 0       | 0       |
| 60  | 1x    | 5        | Total<br>5    | O<br>5    | 0       | 0       |
| 60  | 1y    | 2        | Total<br>2    | O<br>2    | 0       | 0       |
| 60  | 2A    | 1787     | Total<br>1787 | O<br>1787 | 0       | 0       |
| 60  | 2B    | 46       | Total<br>46   | O<br>46   | 0       | 0       |
| 60  | 2D    | 20       | Total<br>20   | O<br>20   | 0       | 0       |
| 60  | 2E    | 15       | Total<br>15   | O<br>15   | 0       | 0       |
| 60  | 2F    | 11       | Total<br>11   | O<br>11   | 0       | 0       |
| 60  | 2G    | 2        | Total<br>2    | O<br>2    | 0       | 0       |
| 60  | 2H    | 4        | Total<br>4    | O<br>4    | 0       | 0       |
| 60  | 2N    | 8        | Total<br>8    | O<br>8    | 0       | 0       |

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| Mol | Chain | Residues | Atoms        |          | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 60  | 2P    | 17       | Total<br>17  | O<br>17  | 0       | 0       |
| 60  | 2Q    | 4        | Total<br>4   | O<br>4   | 0       | 0       |
| 60  | 2R    | 6        | Total<br>6   | O<br>6   | 0       | 0       |
| 60  | 2T    | 4        | Total<br>4   | O<br>4   | 0       | 0       |
| 60  | 2U    | 5        | Total<br>5   | O<br>5   | 0       | 0       |
| 60  | 2V    | 3        | Total<br>3   | O<br>3   | 0       | 0       |
| 60  | 2W    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 60  | 2X    | 5        | Total<br>5   | O<br>5   | 0       | 0       |
| 60  | 2Y    | 8        | Total<br>8   | O<br>8   | 0       | 0       |
| 60  | 20    | 9        | Total<br>9   | O<br>9   | 0       | 0       |
| 60  | 21    | 2        | Total<br>2   | O<br>2   | 0       | 0       |
| 60  | 23    | 2        | Total<br>2   | O<br>2   | 0       | 0       |
| 60  | 25    | 2        | Total<br>2   | O<br>2   | 0       | 0       |
| 60  | 26    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 60  | 27    | 2        | Total<br>2   | O<br>2   | 0       | 0       |
| 60  | 28    | 9        | Total<br>9   | O<br>9   | 0       | 0       |
| 60  | 29    | 4        | Total<br>4   | O<br>4   | 0       | 0       |
| 60  | 2a    | 408      | Total<br>408 | O<br>408 | 0       | 0       |
| 60  | 2d    | 7        | Total<br>7   | O<br>7   | 0       | 0       |
| 60  | 2e    | 4        | Total<br>4   | O<br>4   | 0       | 0       |
| 60  | 2f    | 1        | Total<br>1   | O<br>1   | 0       | 0       |

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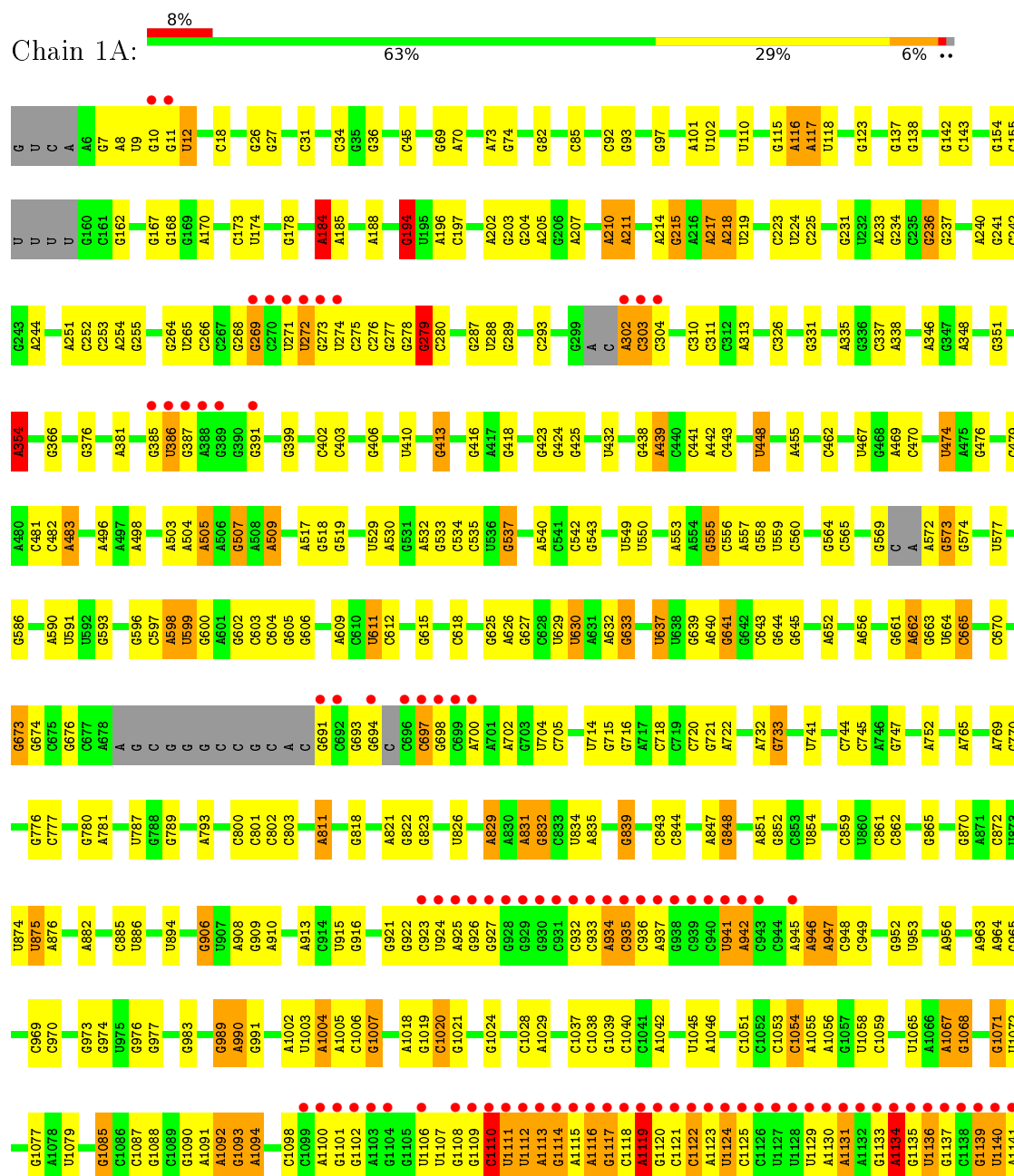
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| Mol | Chain | Residues | Atoms |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---------|---------|
| 60  | 2h    | 1        | Total | O | 0       | 0       |
|     |       |          | 1     | 1 |         |         |
| 60  | 2j    | 2        | Total | O | 0       | 0       |
|     |       |          | 2     | 2 |         |         |
| 60  | 2l    | 7        | Total | O | 0       | 0       |
|     |       |          | 7     | 7 |         |         |
| 60  | 2m    | 1        | Total | O | 0       | 0       |
|     |       |          | 1     | 1 |         |         |
| 60  | 2n    | 1        | Total | O | 0       | 0       |
|     |       |          | 1     | 1 |         |         |
| 60  | 2t    | 1        | Total | O | 0       | 0       |
|     |       |          | 1     | 1 |         |         |
| 60  | 2v    | 3        | Total | O | 0       | 0       |
|     |       |          | 3     | 3 |         |         |
| 60  | 2x    | 4        | Total | O | 0       | 0       |
|     |       |          | 4     | 4 |         |         |
| 60  | 2y    | 4        | Total | O | 0       | 0       |
|     |       |          | 4     | 4 |         |         |

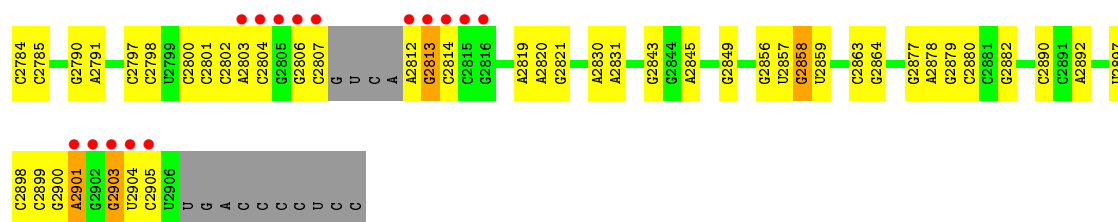
### 3 Residue-property plots

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.

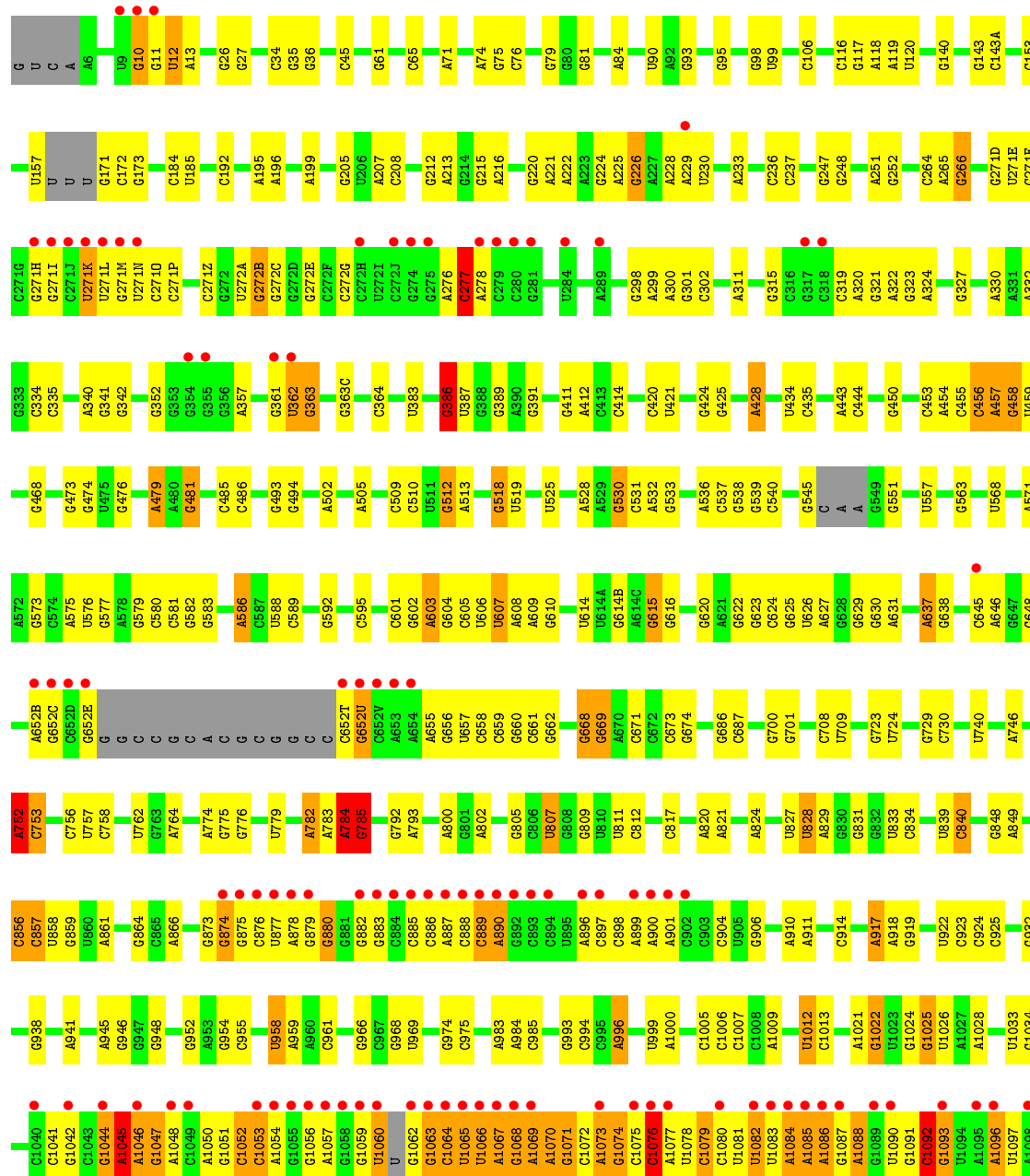
#### • Molecule 1: 23S ribosomal RNA





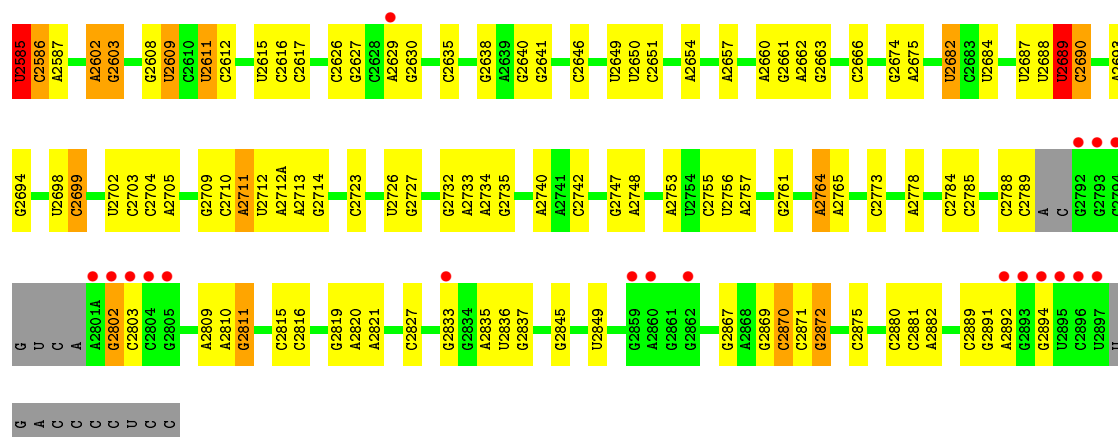


● Molecule 1: 23S ribosomal RNA

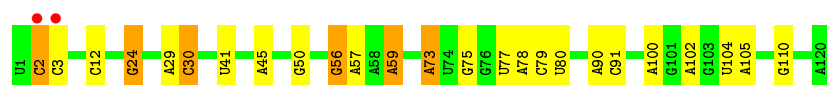
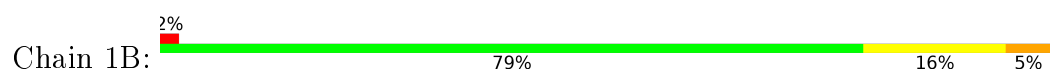


|       |       |       |       |       |       |        |        |        |       |        |        |
|-------|-------|-------|-------|-------|-------|--------|--------|--------|-------|--------|--------|
| U2473 | G2383 | G2297 | C2174 | A2114 | A1789 | U1839  | A1528A | C1430  | G1296 | G1186  | G1099  |
| C2474 | G2384 | A2298 | C2175 | G2115 | C1790 | C1640  | A1528A | U1431  | C1297 | G1187  | C1100  |
| A2475 | G2385 | G2302 | A2176 | G2116 | A1791 | A1641  | G1529  | G1441  | U1300 | U1188  | U1101  |
| C2476 | G2386 | G2302 | C2177 | A2117 | G1792 | G1642  | C2021  | G1442  | A1301 | U1189  | A1102  |
| C2483 | U2387 | A2305 | C2178 | U2118 | G1793 | C1648  | G1903  | A1445  | A1302 | G1200  | A1103  |
| G2489 | U2390 | G2308 | U2180 | A2119 | C1794 | C1795  | G1904  | U1446  | A1308 | C1201  | C1104  |
| G2490 | G2391 | A2309 | G2181 | G2121 | C1796 | C1657  | C1905  | U1448  | U1312 | C1202  | U1105  |
| U2491 | A2392 | G2310 | G2182 | U2122 | U1797 | C1658  | G1906  | A1449  | U1313 | G1106  | G1107  |
| G2495 | C2395 | U2312 | C2185 | G2123 | U1798 | G1667  | A1913  | A1450  | U1314 | U1108  | U1108  |
| C2496 | G2396 | C2313 | C2186 | G2124 | G1799 | G1667  | C1914  | C1450A | C1314 | A1204  | C1109  |
| A2497 | U2406 | C2314 | G2187 | A2125 | C1800 | G1674  | U1915  | U1451  | U1315 | U1205  | G1110  |
| C2498 | G2410 | G2315 | C2188 | G2126 | G1801 | U1688  | U1916  | A1460  | U1316 | A1210  | G1111  |
| C2499 | G2411 | C2316 | C2189 | G2127 | A1802 | U1688  | A1919  | U1461  | U1317 | U1211  | G1112  |
| G2502 | G2412 | U2317 | U2189 | C2128 | A1803 | G1681  | A1919  | G1465  | A1317 | U1212  | G1113  |
| A2503 | G2413 | U2318 | G2190 | U2129 | C1804 | G1682  | C1924  | U1466  | A1317 | U1114  | G1114  |
| U2504 | A2411 | G2319 | G2191 | G2130 | U1805 | C1683  | G1924  | G1467  | C1327 | G1115  | G1115  |
| U2505 | G2414 | G2320 | A2198 | U2132 | G1813 | C1684  | A1927  | C1468  | C1351 | G1116  | G1117  |
| U2506 | G2417 | G2321 | G2206 | U2133 | G1814 | C1686  | A1928  | C1469  | U1352 | G1118  | G1118  |
| U2511 | G2422 | G2322 | C2207 | A2134 | U1815 | U1688  | A1929  | G1470  | A1359 | G1125  | G1125  |
| G2518 | A2425 | G2323 | A2208 | C2136 | G1816 | U1688  | G1930  | A1471  | A1360 | A1220  | A1129  |
| U2519 | G2427 | C2324 | U2218 | G2137 | A1829 | G1696  | G1935  | A1472  | A1360 | C1221  | U1130  |
| C2520 | G2428 | G2325 | G2224 | C2138 | C1830 | A1700  | A1936  | G1482  | G1364 | G1221A | U1131  |
| G2525 | A2430 | G2326 | C2225 | C2140 | U1833 | G1719  | A1937  | G1483  | A1365 | G1229  | G1132  |
| G2526 | U2431 | A2330 | G2226 | G2141 | U1834 | U1720  | A1938  | G1484  | A1366 | G1230  | U1133  |
| C2529 | A2432 | G2331 | G2227 | C2142 | G1835 | G1721  | U1946  | G1485  | A1367 | G1231  | G1136  |
| U2537 | A2433 | G2332 | G2228 | U2144 | C1836 | A1722  | C1947  | G1486  | C1370 | G1235  | G1139  |
| C2538 | A2434 | G2333 | G2229 | C2145 | G1839 | U1739  | U1947  | G1490  | G1371 | G1243  | C1140  |
| U2542 | A2435 | G2334 | G2230 | G2146 | U1842 | G1740  | U1948  | G1491  | A1372 | G1244  | U1141  |
| G2543 | A2436 | A2335 | G2231 | U2147 | C1843 | A1741  | U1949  | G1492  | A1379 | U1142  | U1142  |
| U2547 | U2438 | G2336 | G2232 | G2148 | U1844 | G1742  | A1950  | G1493  | G1380 | A1142A | A1142A |
| C2552 | A2439 | C2342 | G2233 | U2150 | A1847 | G1747A | A1951  | G1494  | A1384 | G1248  | C1153  |
| G2553 | C2440 | G2347 | A2268 | G2151 | A1848 | G1756  | G1952  | U1503  | G1385 | A1253  | G1154  |
| U2554 | G2444 | U2348 | A2269 | G2152 | G1857 | G1756  | A1953  | C1504  | C1387 | A1254  | A1155  |
| A2561 | G2445 | G2357 | A2273 | C2153 | U1858 | G1760  | U1954  | C1505  | G1388 | U1255  | U1159  |
| C2565 | G2446 | G2358 | A2274 | G2154 | A1859 | G1761  | G1955  | C1506  | C1399 | G1256  | G1160  |
| U2566 | G2447 | C2359 | C2275 | G2155 | U1864 | G1763  | G1956  | A1507  | U1405 | G1264  | U1165  |
| U2567 | A2448 | A2361 | G2279 | A2158 | G1865 | G1764  | G1957  | A1509  | U1406 | A1265  | U1166  |
| C2568 | A2451 | G2364 | G2282 | G2160 | C1866 | A1773  | U1958  | A1509A | A1412 | G1266  | U1167  |
| G2573 | G2461 | G2370 | C2285 | C2161 | A1876 | U1775  | G1959  | C1510  | G1413 | U1267  | G1168  |
| U2574 | U2462 | G2371 | A2286 | G2162 | A1877 | C1774  | G1960  | C1511  | A1413 | A1268  | G1169  |
| G2575 | C2463 | C2374 | A2287 | C2163 | G1878 | U1775  | A1608  | U1514  | G1416 | G1270  | G1170  |
| C2576 | G2464 | G2375 | U2291 | C2164 | A1884 | U1778  | A1609  | G1515  | C1417 | G1271  | G      |
| G2577 | A2469 | A2376 | C2292 | G2165 | A1885 | U1779  | G1622  | C1516  | A1418 | A1272  | A      |
| A2578 | G2470 | G2377 | C2293 | C2166 | A1889 | G1781  | G1633  | G1517  | A1419 | U1273  | U      |
| C2582 | C2471 | C2378 | C2294 | U2167 | A1890 | C1782  | A1634  | U1518  | U1420 | A1278  | G      |
|       | G2472 | C2380 | U2296 | A2169 | G1893 | A1783  | G1635  | G1519  | G1422 | A1286  | A      |
|       |       |       |       | G2170 | C1894 | A1784  | G1636  | G1525  | G1422 | A1287  | C1178  |
|       |       |       |       | A2171 | C1895 | A1786  | A1637  | G1526  | C1428 | U1288  | C1179  |
|       |       |       |       | A2172 | G2112 |        |        |        |       |        | C1180  |
|       |       |       |       | A2173 | U2113 |        |        |        |       |        | C1181  |

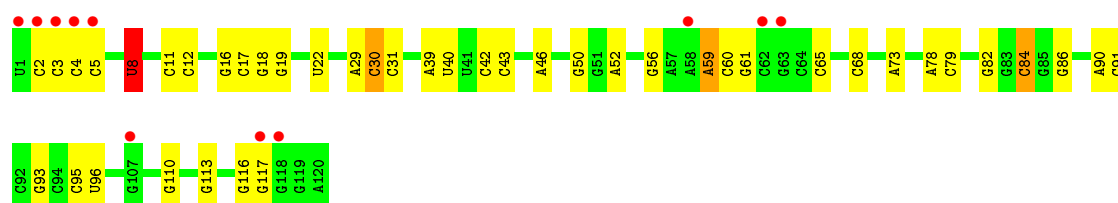




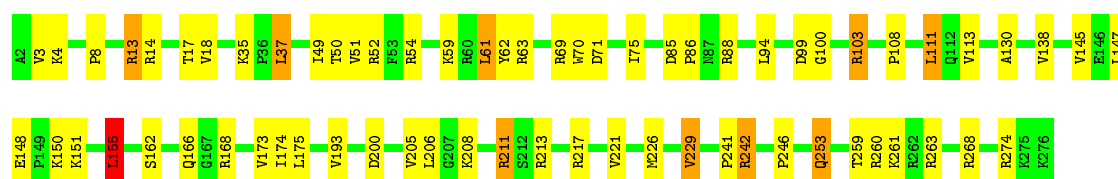
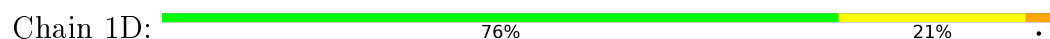
• Molecule 2: 5S ribosomal RNA



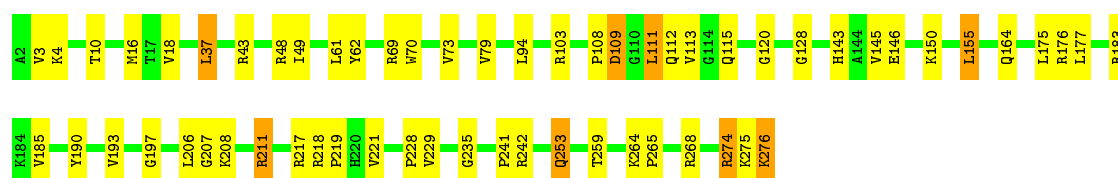
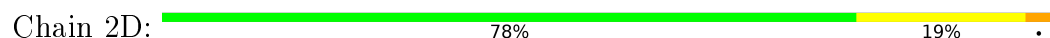
• Molecule 2: 5S ribosomal RNA



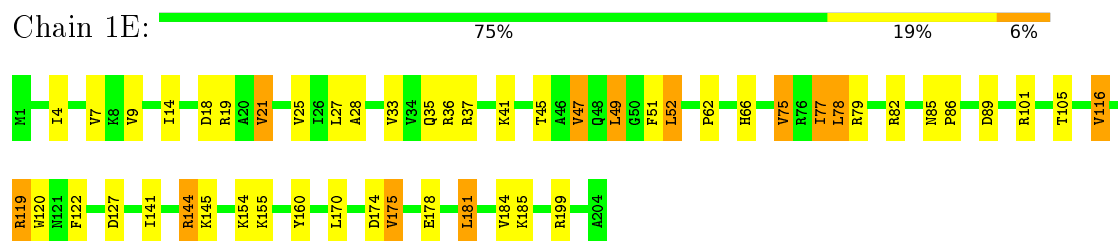
• Molecule 3: 50S ribosomal protein L2



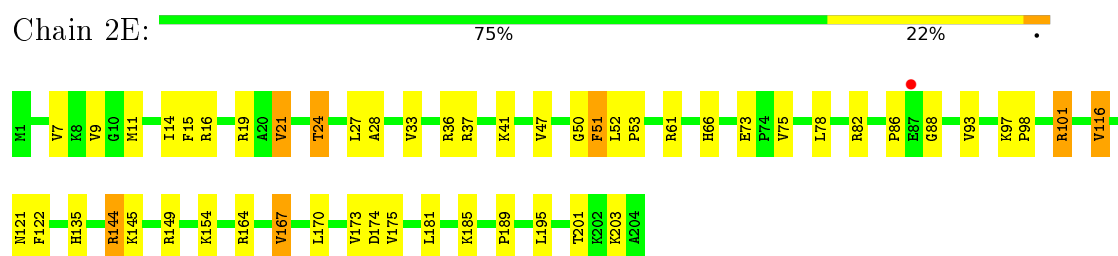
• Molecule 3: 50S ribosomal protein L2



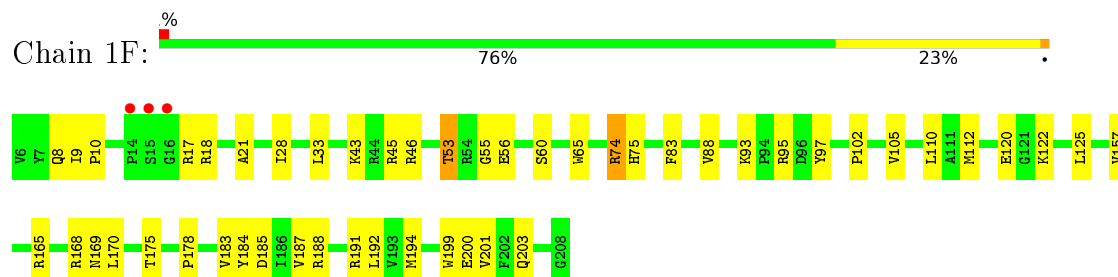
- Molecule 4: 50S ribosomal protein L3



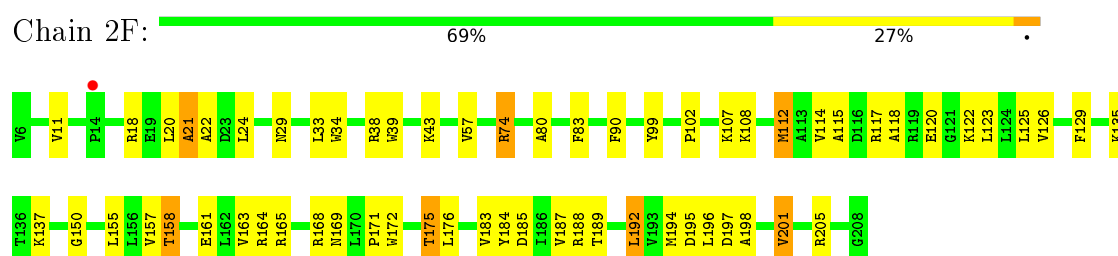
- Molecule 4: 50S ribosomal protein L3



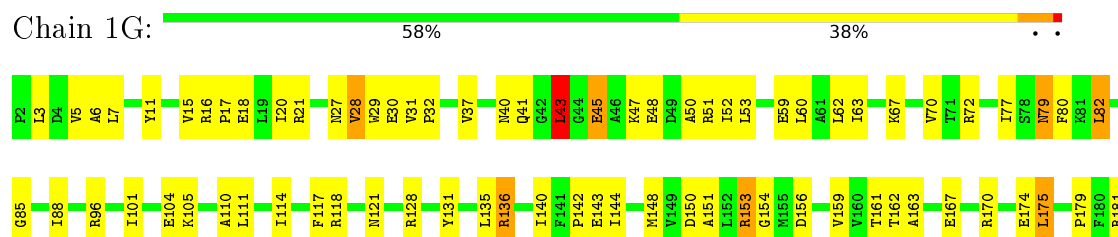
- Molecule 5: 50S ribosomal protein L4



- Molecule 5: 50S ribosomal protein L4

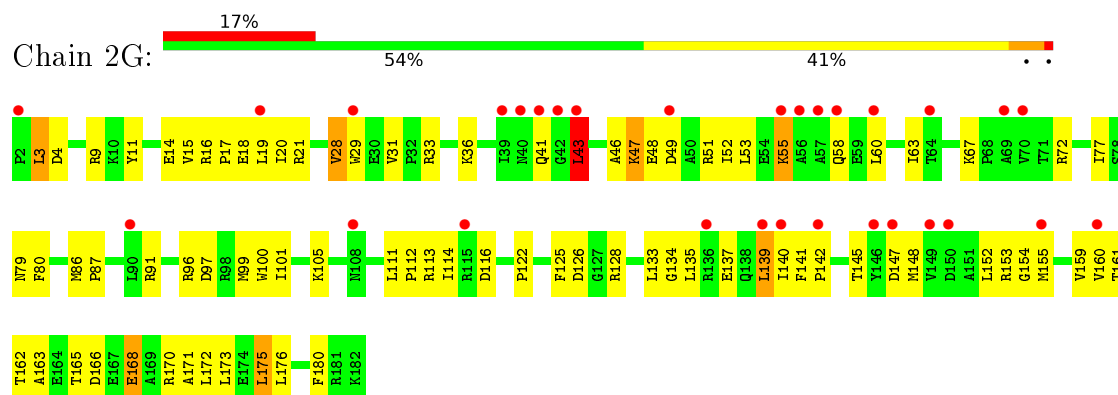


- Molecule 6: 50S ribosomal protein L5

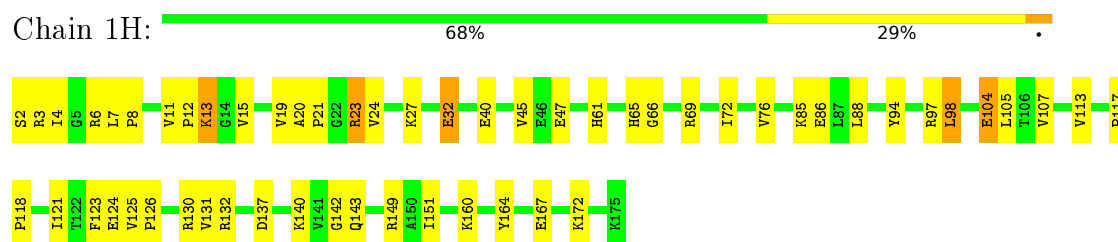


K182

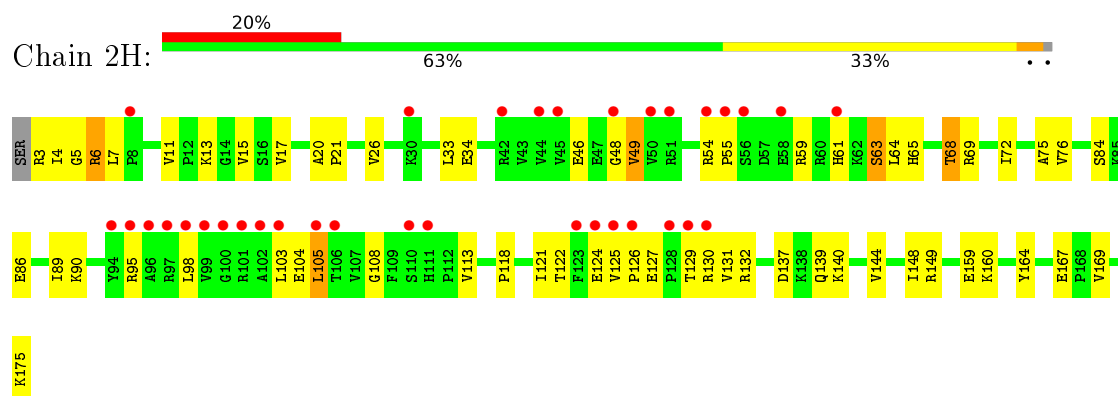
- Molecule 6: 50S ribosomal protein L5



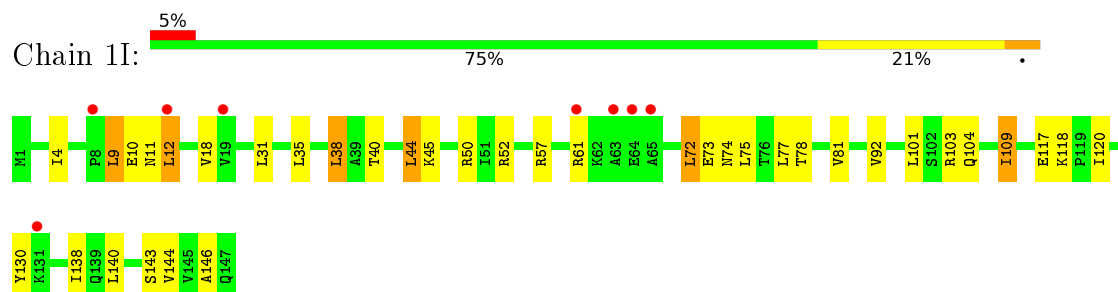
- Molecule 7: 50S ribosomal protein L6



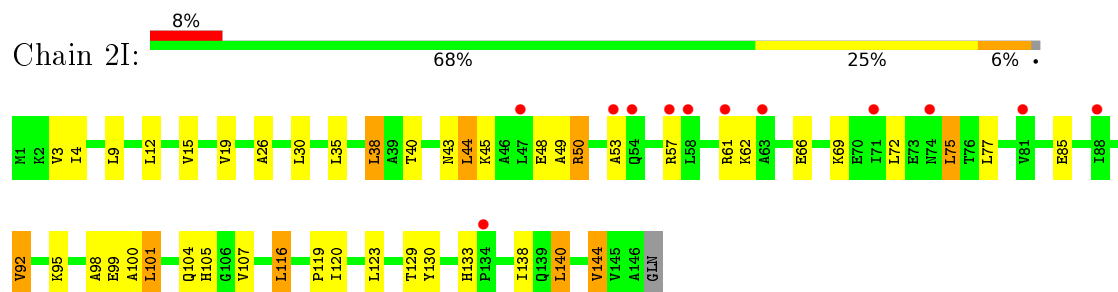
- Molecule 7: 50S ribosomal protein L6



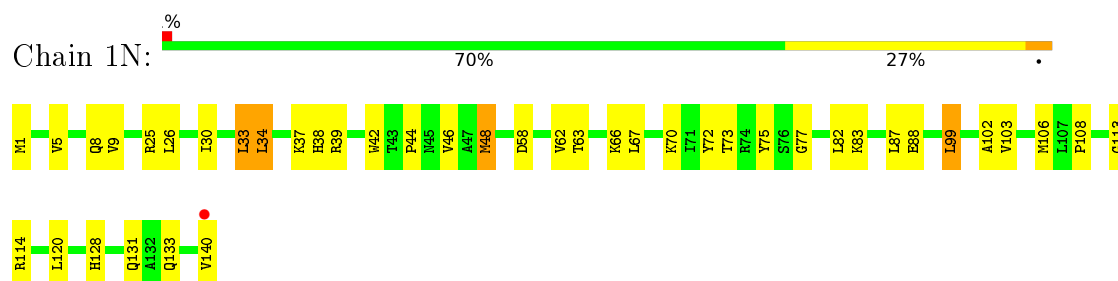
- Molecule 8: 50S ribosomal protein L9



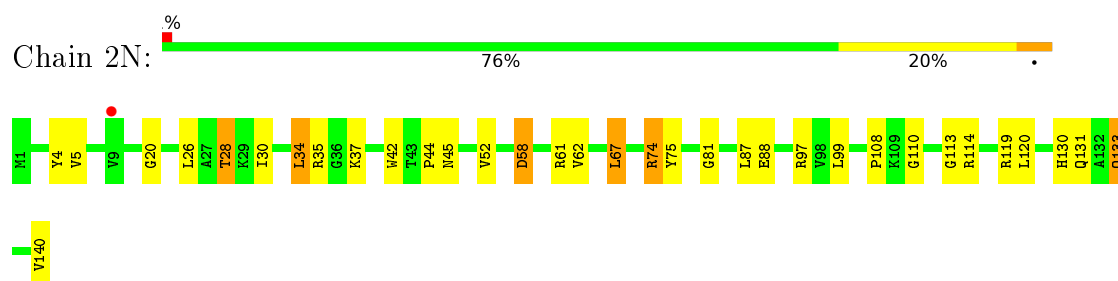
- Molecule 8: 50S ribosomal protein L9



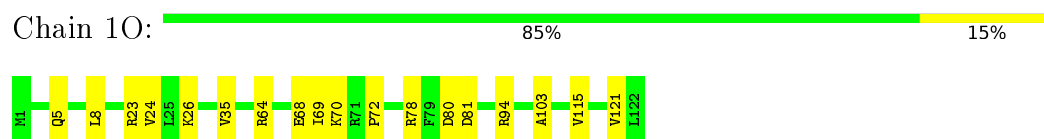
- Molecule 9: 50S ribosomal protein L13



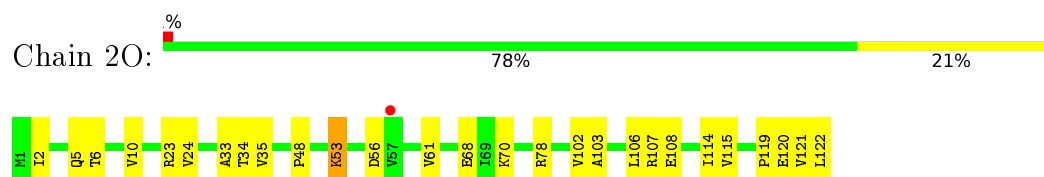
- Molecule 9: 50S ribosomal protein L13



- Molecule 10: 50S ribosomal protein L14

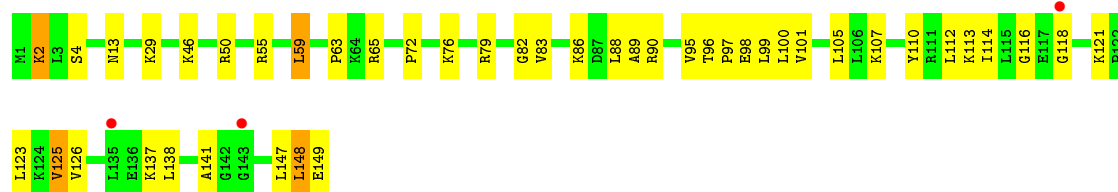


- Molecule 10: 50S ribosomal protein L14

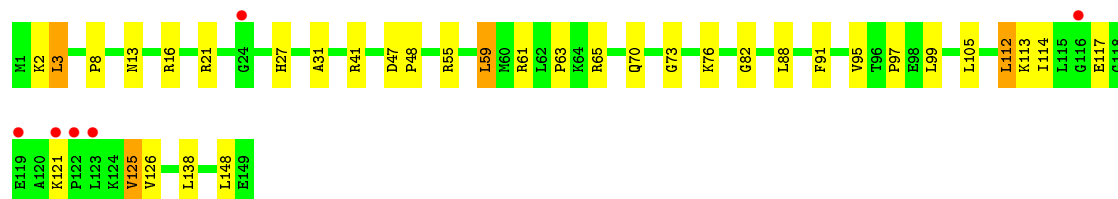
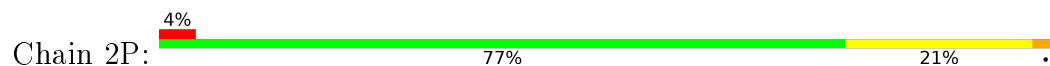


- Molecule 11: 50S ribosomal protein L15

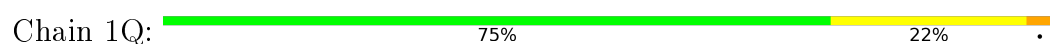




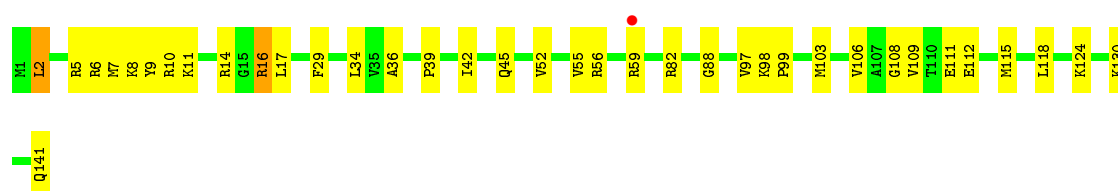
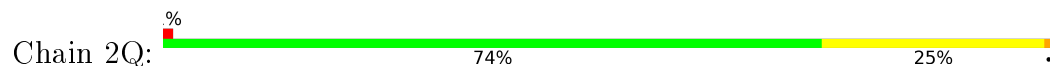
- Molecule 11: 50S ribosomal protein L15



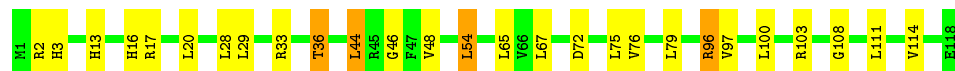
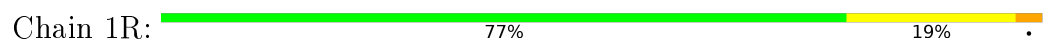
- Molecule 12: 50S ribosomal protein L16



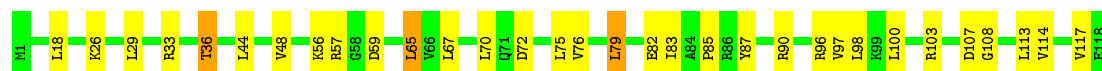
- Molecule 12: 50S ribosomal protein L16




- Molecule 13: 50S ribosomal protein L17



- Molecule 13: 50S ribosomal protein L17




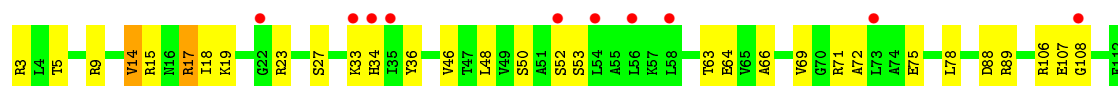
- Molecule 14: 50S ribosomal protein L18

Chain 1S:  77% 20% ..




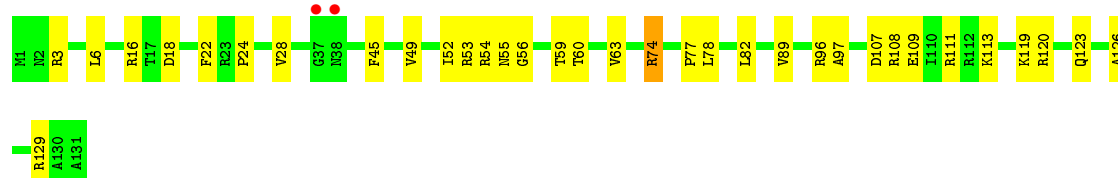
- Molecule 14: 50S ribosomal protein L18

Chain 2S:  9% 72% 26% .




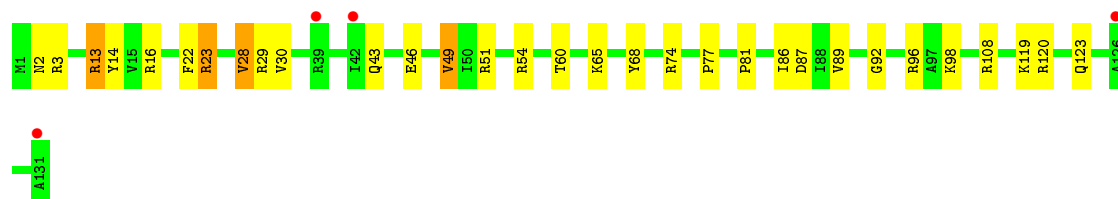
- Molecule 15: 50S ribosomal protein L19

Chain 1T:  2% 74% 25% .




- Molecule 15: 50S ribosomal protein L19

Chain 2T:  3% 76% 21% .




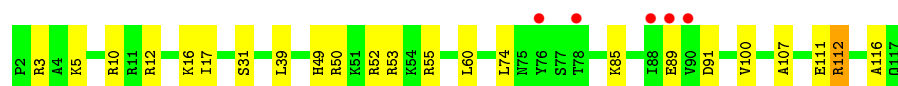
- Molecule 16: 50S ribosomal protein L20

Chain 1U:  80% 19% .




- Molecule 16: 50S ribosomal protein L20

Chain 2U:  4% 80% 19% .

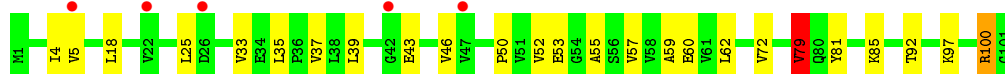
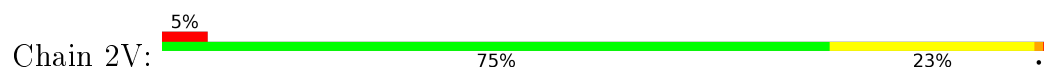


- Molecule 17: 50S ribosomal protein L21

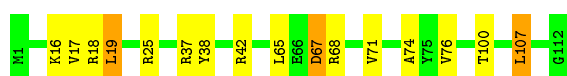
Chain 1V:  79% 18% .



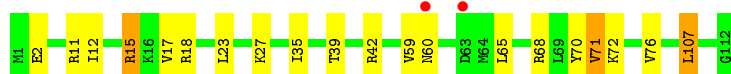
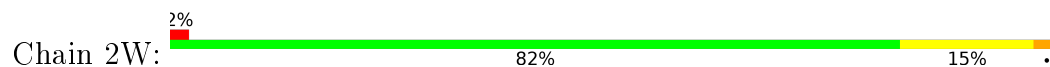
- Molecule 17: 50S ribosomal protein L21



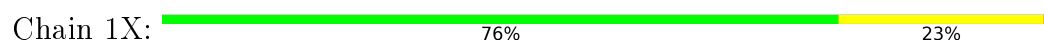
- Molecule 18: 50S ribosomal protein L22



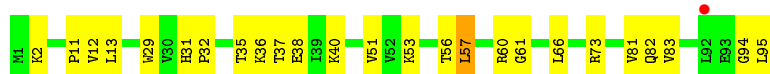
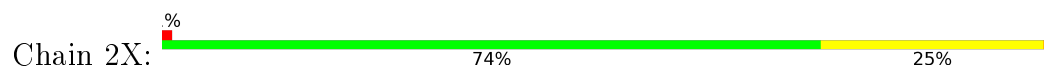
- Molecule 18: 50S ribosomal protein L22



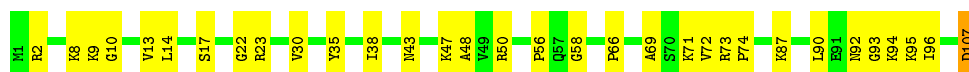
- Molecule 19: 50S ribosomal protein L23



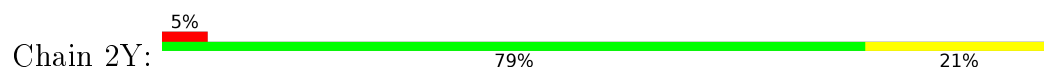
- Molecule 19: 50S ribosomal protein L23

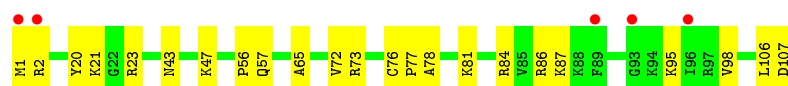


- Molecule 20: 50S ribosomal protein L24

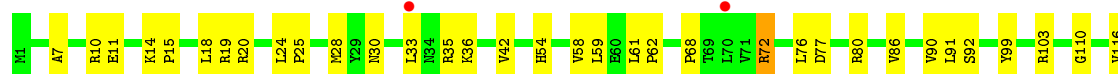


- Molecule 20: 50S ribosomal protein L24

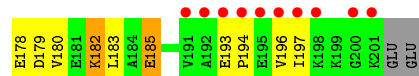
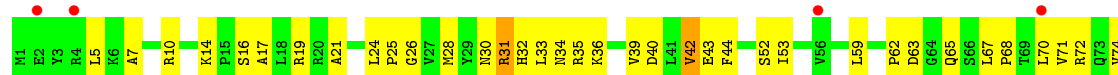




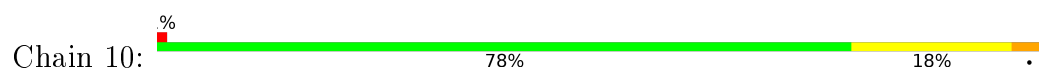
- Molecule 21: 50S ribosomal protein L25



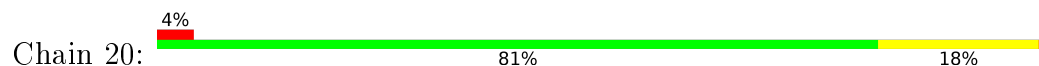
- Molecule 21: 50S ribosomal protein L25



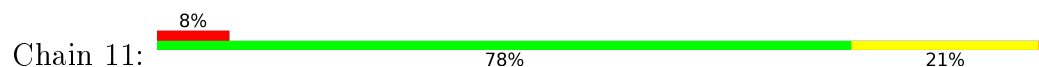
- Molecule 22: 50S ribosomal protein L27



- Molecule 22: 50S ribosomal protein L27

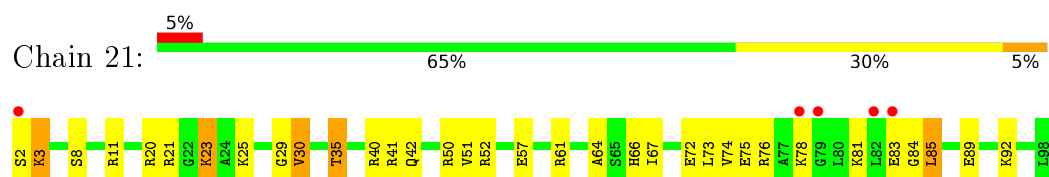


- Molecule 23: 50S ribosomal protein L28

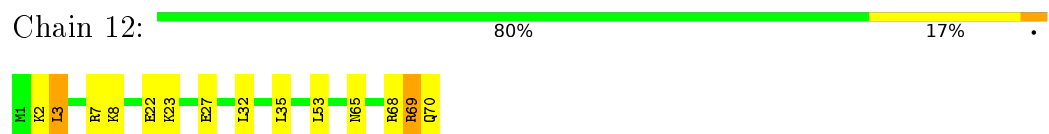


- Molecule 23: 50S ribosomal protein L28

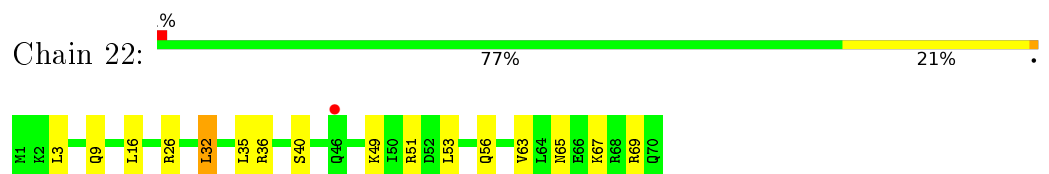




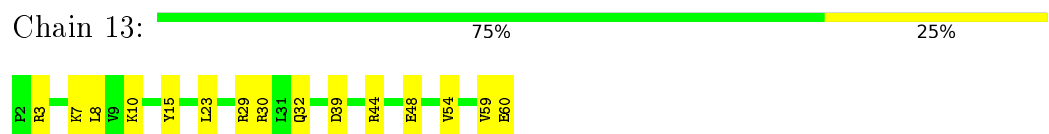
- Molecule 24: 50S ribosomal protein L29



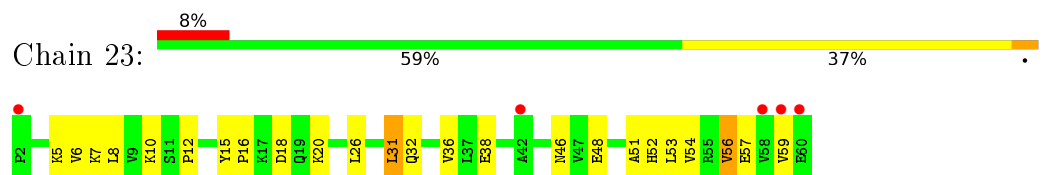
- Molecule 24: 50S ribosomal protein L29



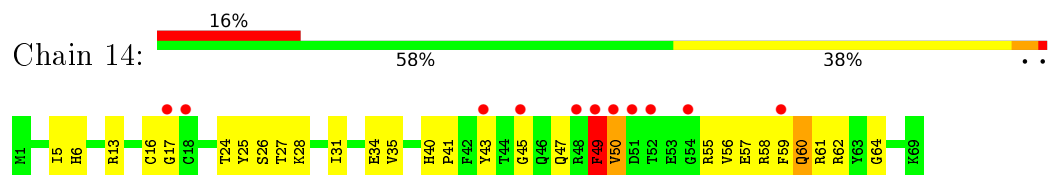
- Molecule 25: 50S ribosomal protein L30



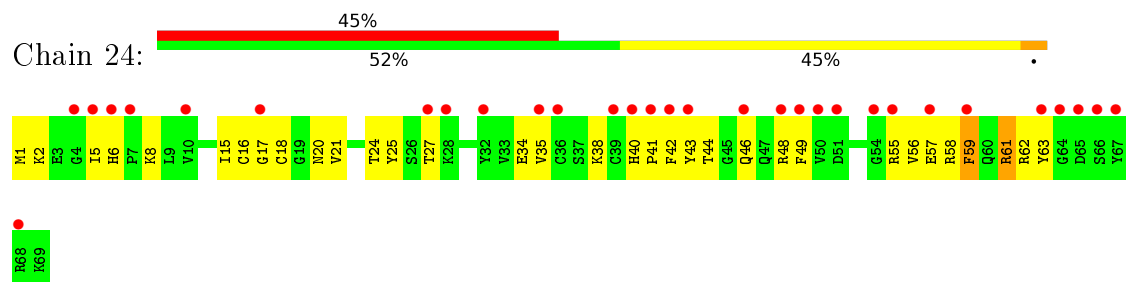
- Molecule 25: 50S ribosomal protein L30




- Molecule 26: 50S ribosomal protein L31



- Molecule 26: 50S ribosomal protein L31




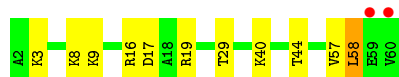
- Molecule 27: 50S ribosomal protein L32

Chain 15:  76% 22% .



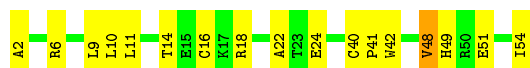
- Molecule 27: 50S ribosomal protein L32

Chain 25:  3% 81% 17% .



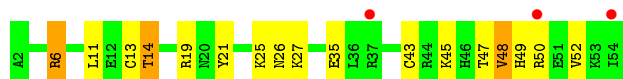
- Molecule 28: 50S ribosomal protein L33

Chain 16:  68% 30% .




- Molecule 28: 50S ribosomal protein L33

Chain 26:  6% 68% 26% 6% .




- Molecule 29: 50S ribosomal protein L34

Chain 17:  77% 21% .



- Molecule 29: 50S ribosomal protein L34

Chain 27:  2% 83% 17% .



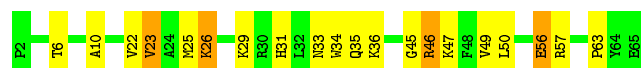
- Molecule 30: 50S ribosomal protein L35

Chain 18:  61% 38% .



- Molecule 30: 50S ribosomal protein L35

Chain 28:  69% 25% 6%



- Molecule 31: 50S ribosomal protein L36

Chain 19:  73% 27%




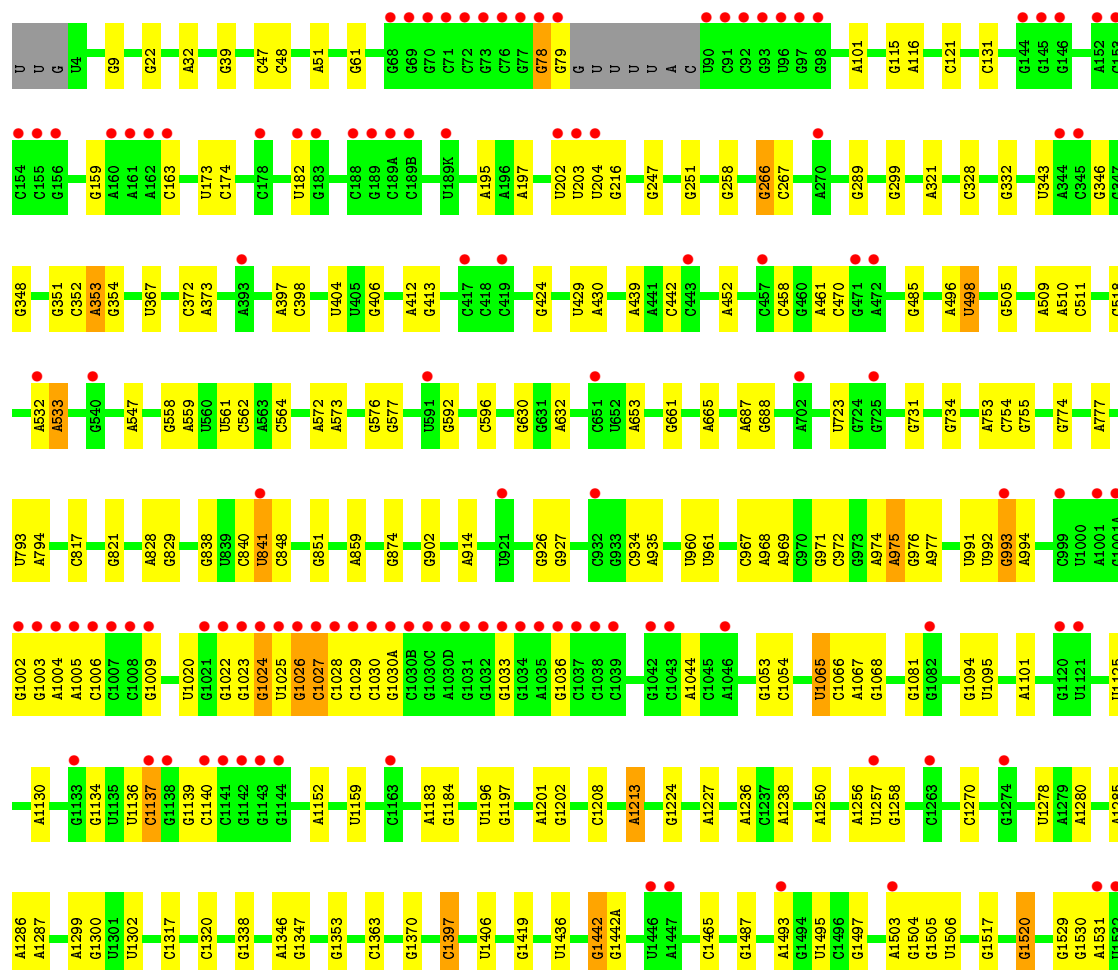
- Molecule 31: 50S ribosomal protein L36

Chain 29:  73% 27%



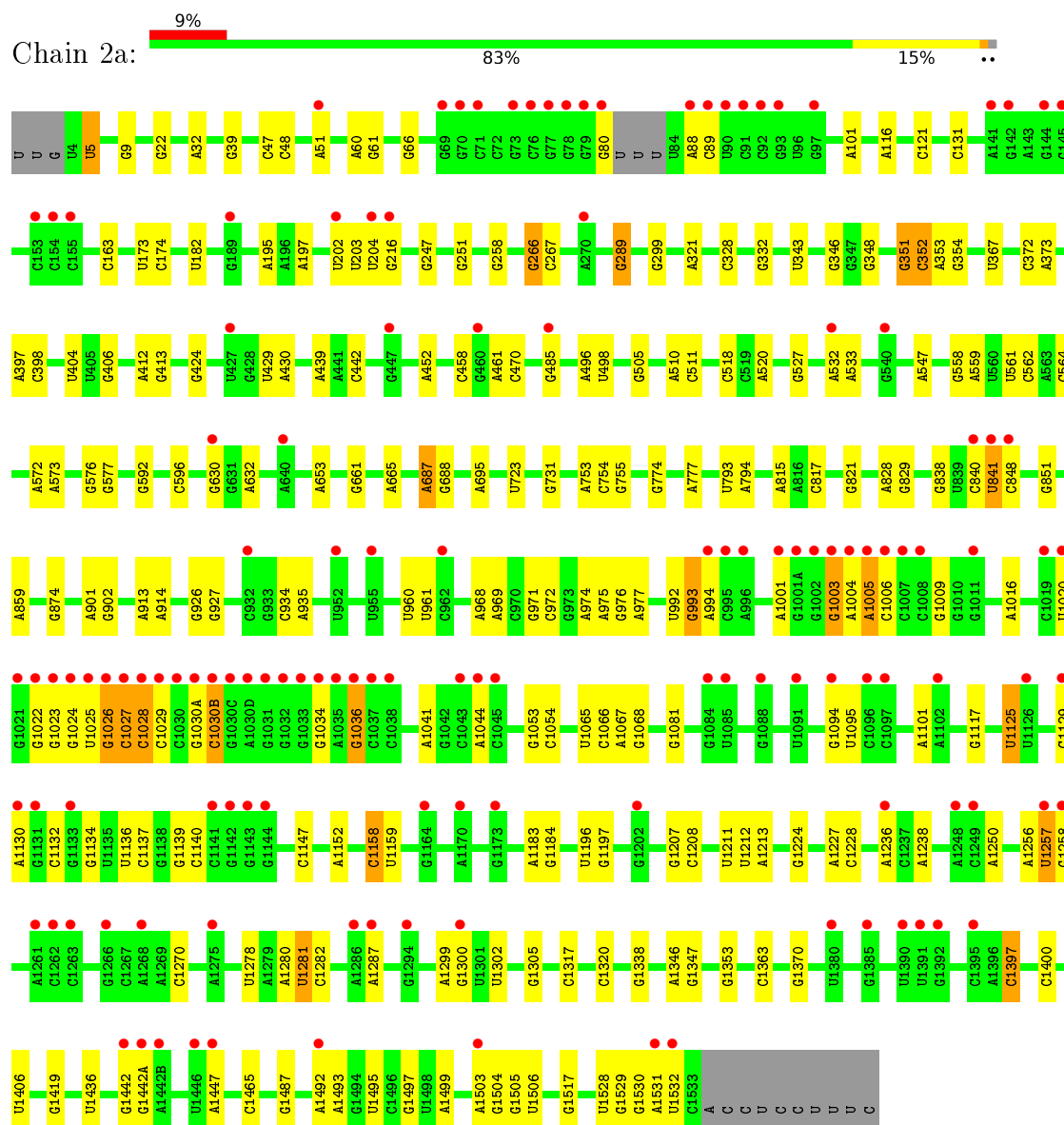
- Molecule 32: 16S ribosomal RNA

Chain 1a:  8% 84% 14% ..

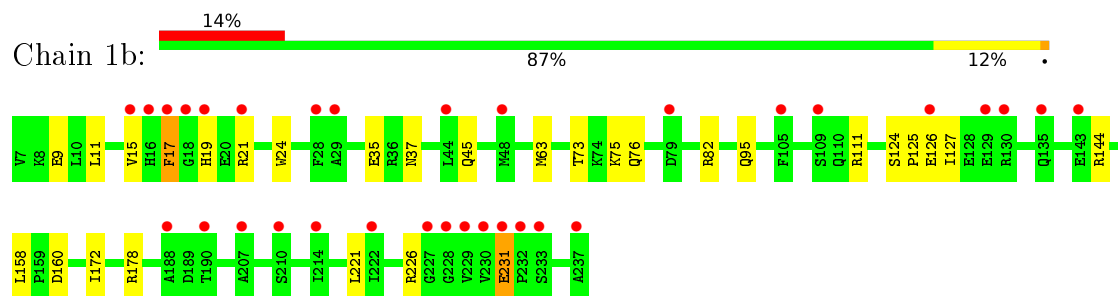




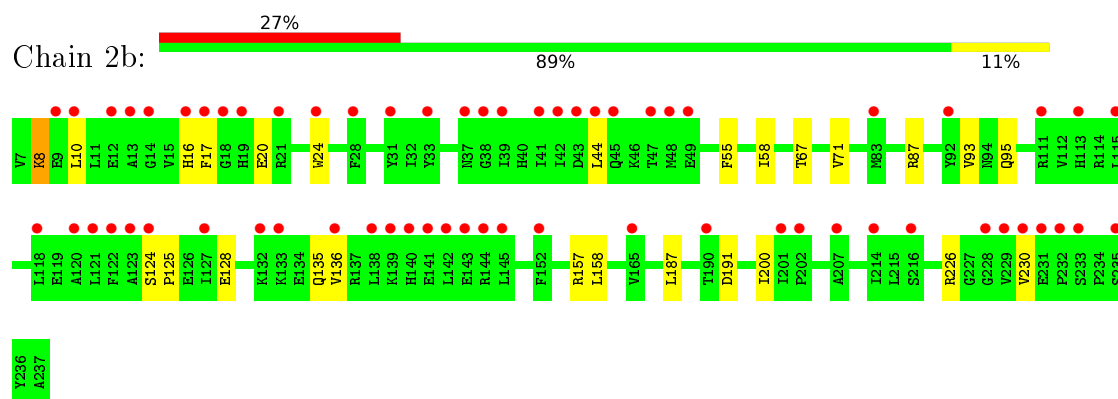
• Molecule 32: 16S ribosomal RNA



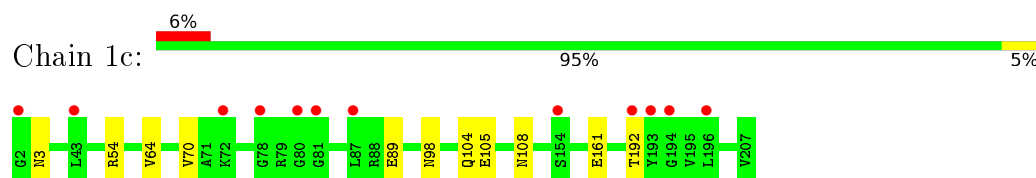
• Molecule 33: 30S ribosomal protein S2



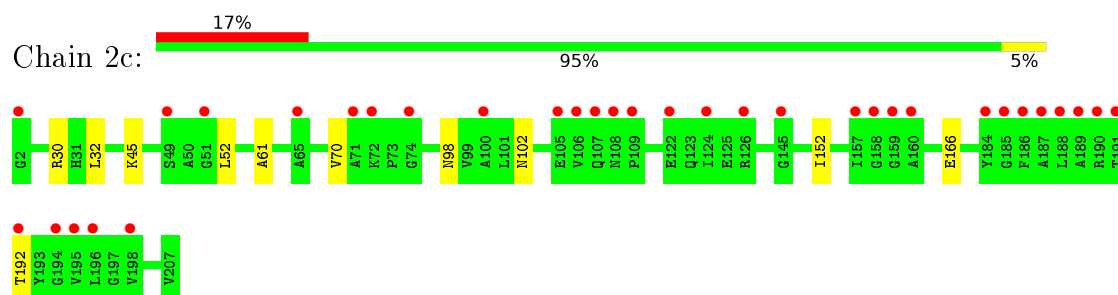
• Molecule 33: 30S ribosomal protein S2



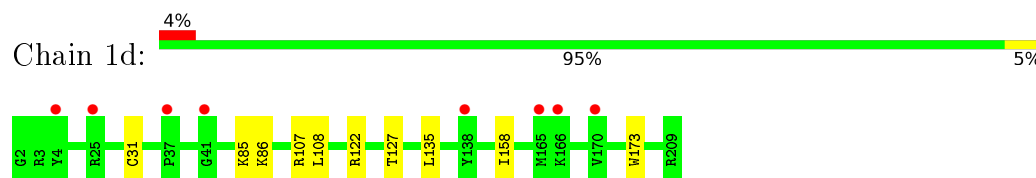
- Molecule 34: 30S ribosomal protein S3



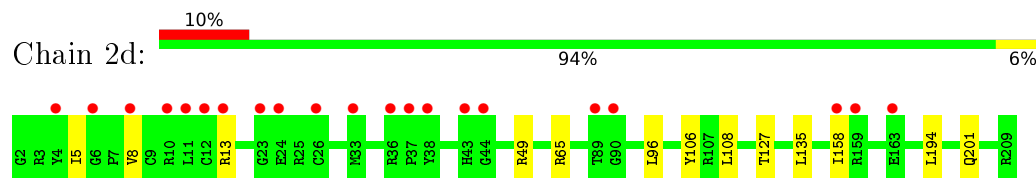
- Molecule 34: 30S ribosomal protein S3



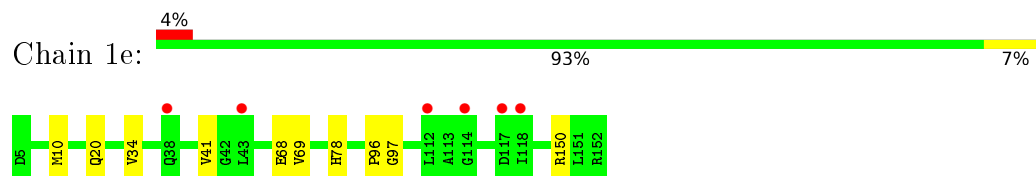
- Molecule 35: 30S ribosomal protein S4



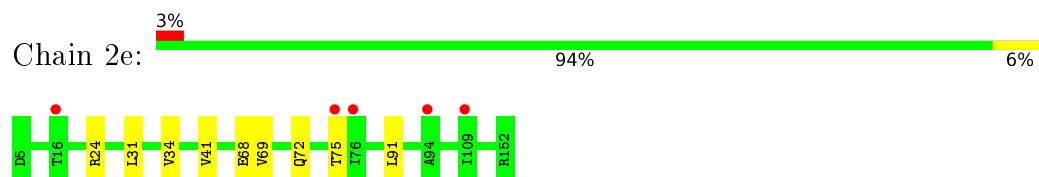
- Molecule 35: 30S ribosomal protein S4



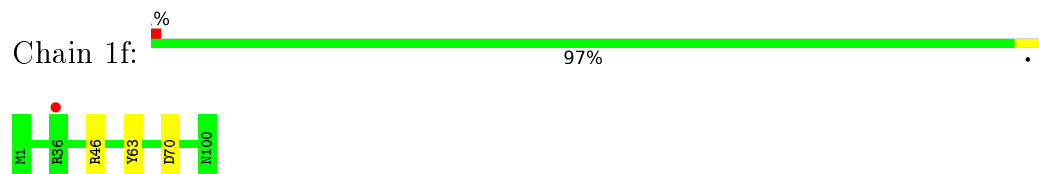
- Molecule 36: 30S ribosomal protein S5



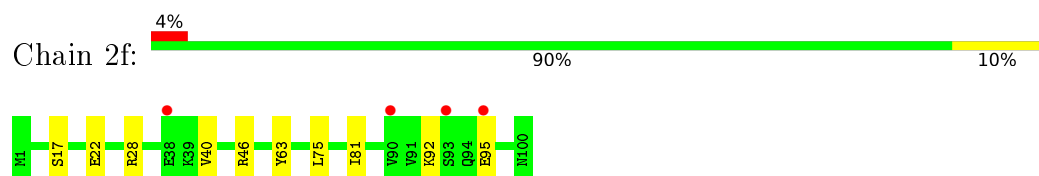
- Molecule 36: 30S ribosomal protein S5



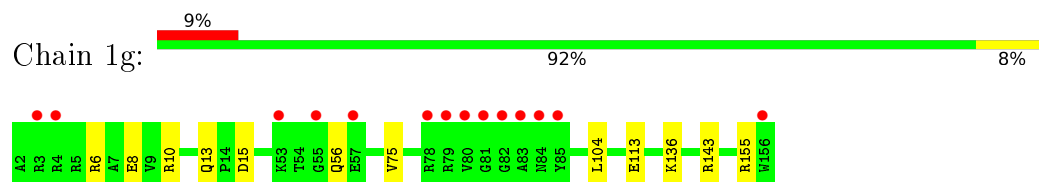
- Molecule 37: 30S ribosomal protein S6



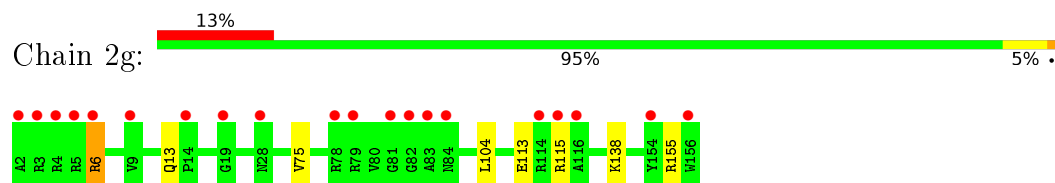
- Molecule 37: 30S ribosomal protein S6



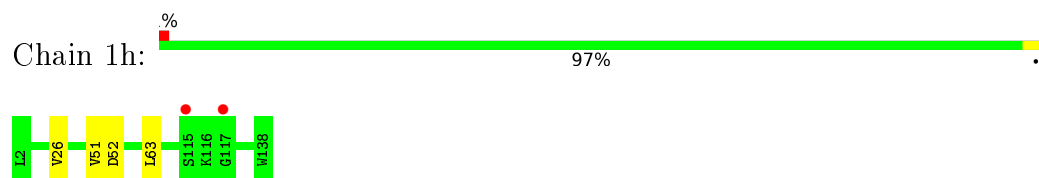
- Molecule 38: 30S ribosomal protein S7



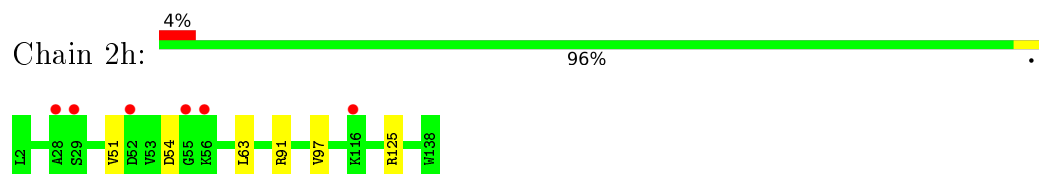
- Molecule 38: 30S ribosomal protein S7



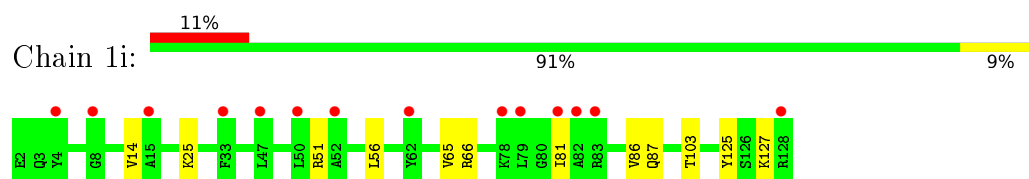
- Molecule 39: 30S ribosomal protein S8



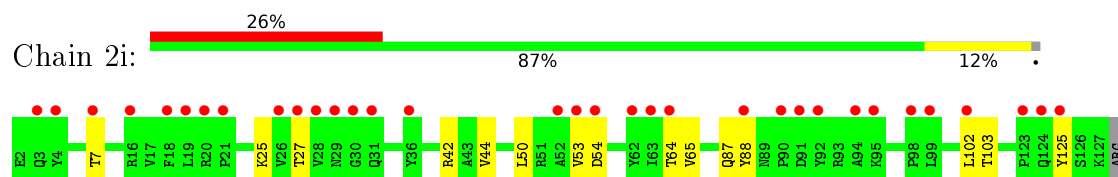
- Molecule 39: 30S ribosomal protein S8



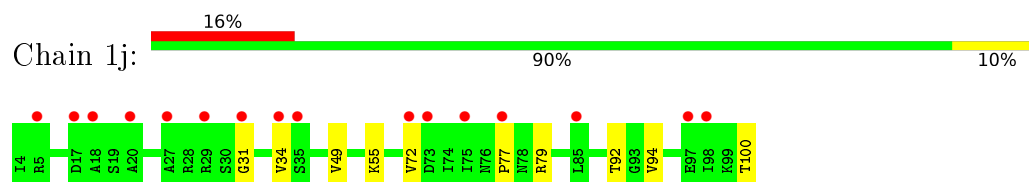
- Molecule 40: 30S ribosomal protein S9



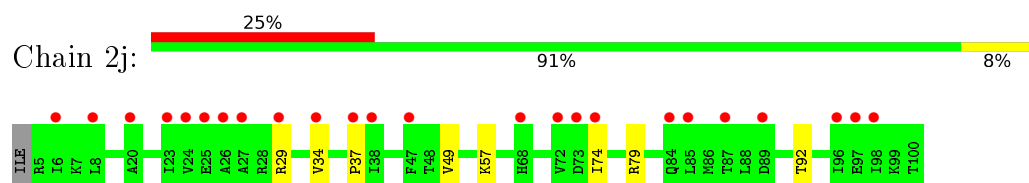
- Molecule 40: 30S ribosomal protein S9



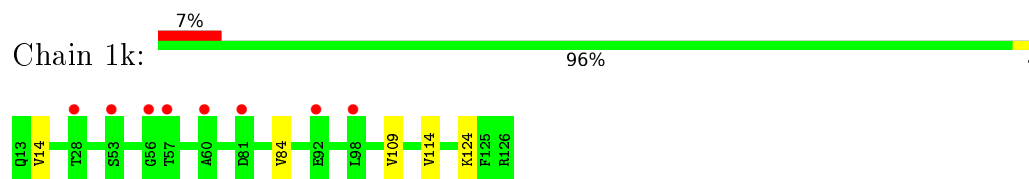
- Molecule 41: 30S ribosomal protein S10



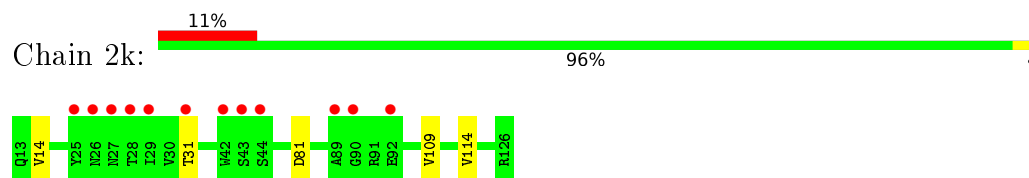
- Molecule 41: 30S ribosomal protein S10



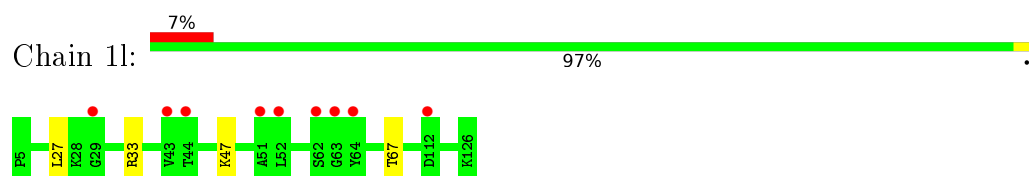
- Molecule 42: 30S ribosomal protein S11



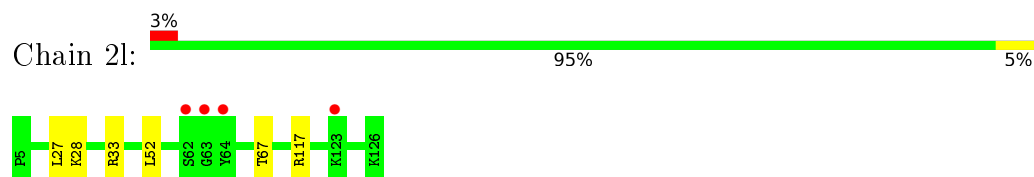
- Molecule 42: 30S ribosomal protein S11



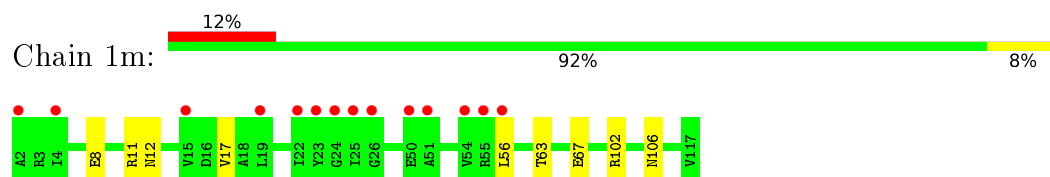
- Molecule 43: 30S ribosomal protein S12



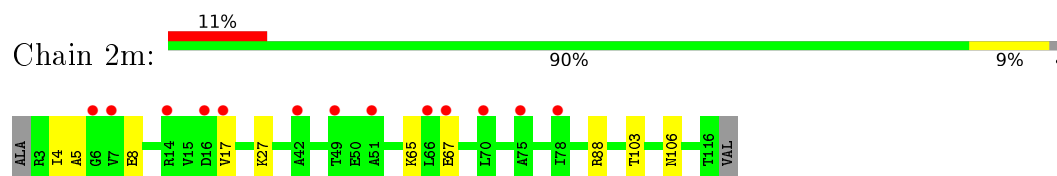
- Molecule 43: 30S ribosomal protein S12



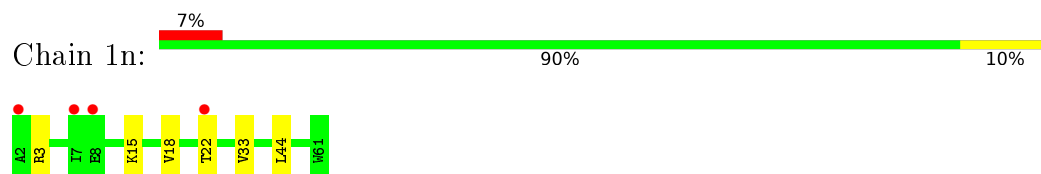
- Molecule 44: 30S ribosomal protein S13



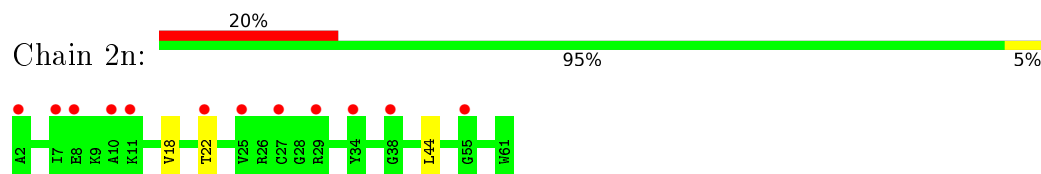
- Molecule 44: 30S ribosomal protein S13



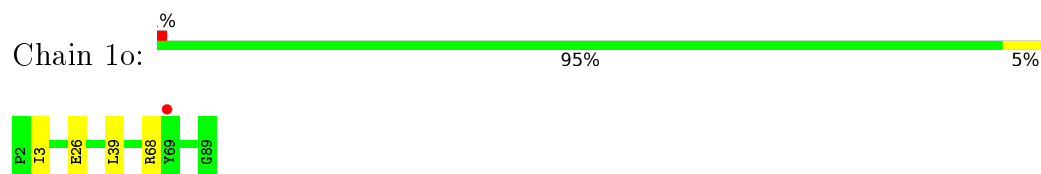
- Molecule 45: 30S ribosomal protein S14 type Z



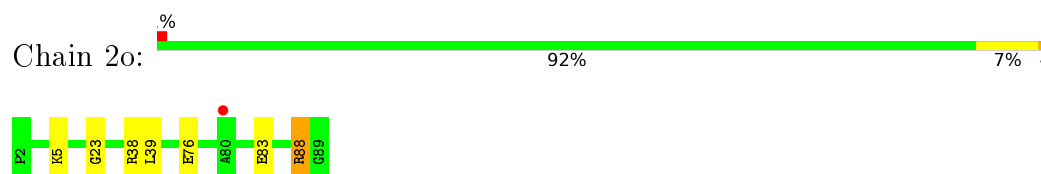
- Molecule 45: 30S ribosomal protein S14 type Z



- Molecule 46: 30S ribosomal protein S15

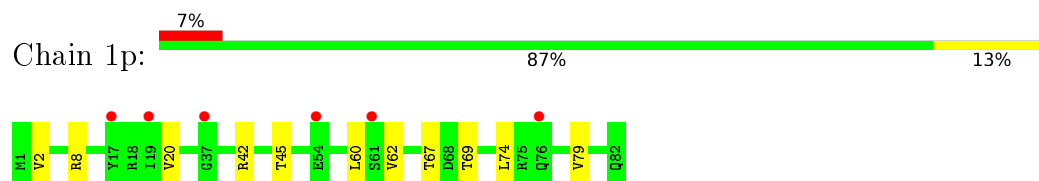


- Molecule 46: 30S ribosomal protein S15

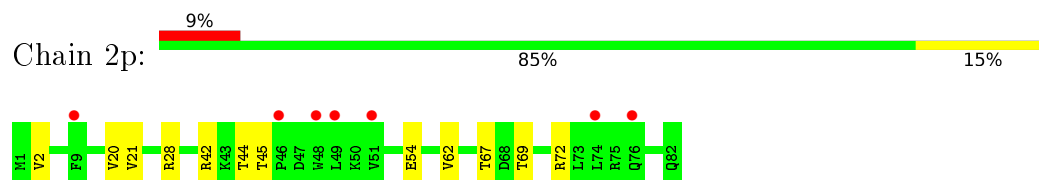




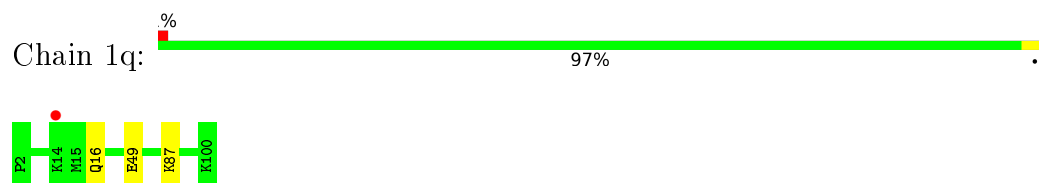
- Molecule 47: 30S ribosomal protein S16



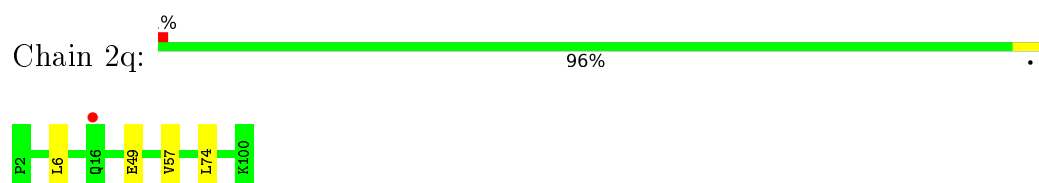
- Molecule 47: 30S ribosomal protein S16



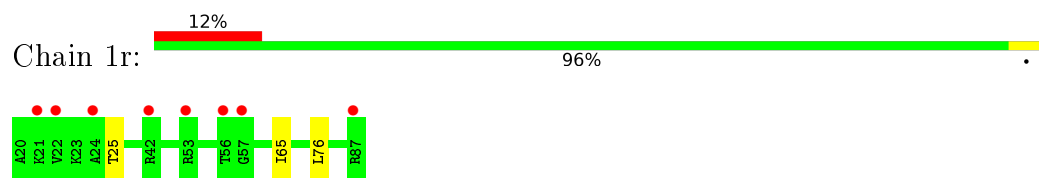
- Molecule 48: 30S ribosomal protein S17



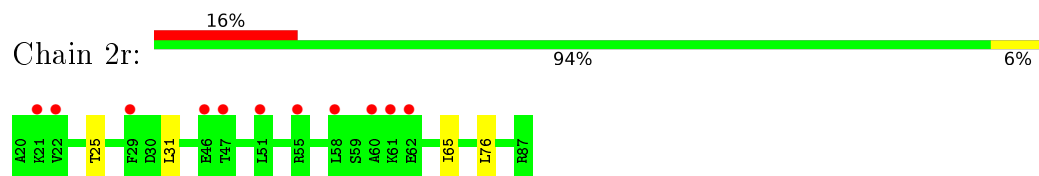
- Molecule 48: 30S ribosomal protein S17



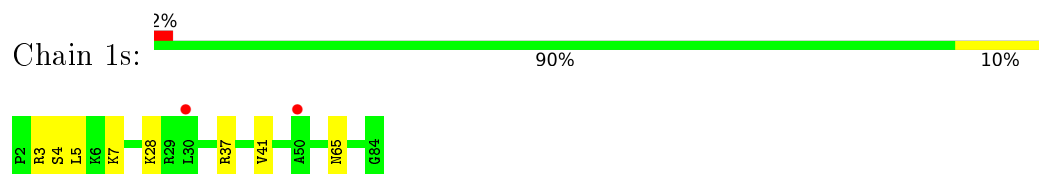
- Molecule 49: 30S ribosomal protein S18



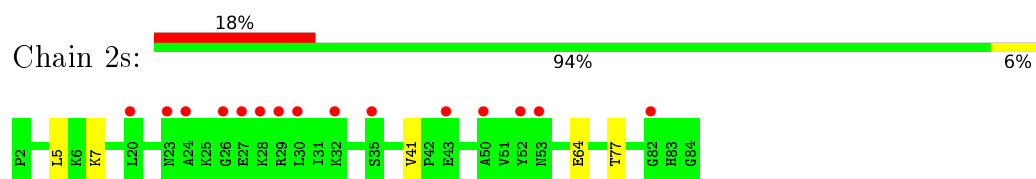
- Molecule 49: 30S ribosomal protein S18



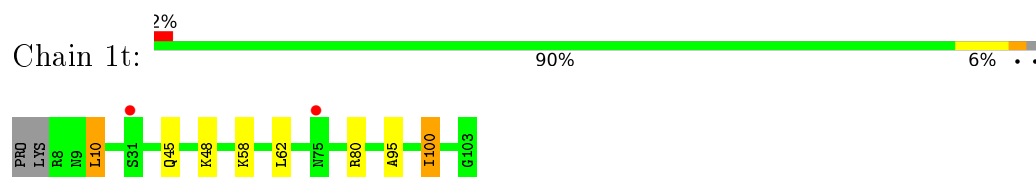
- Molecule 50: 30S ribosomal protein S19



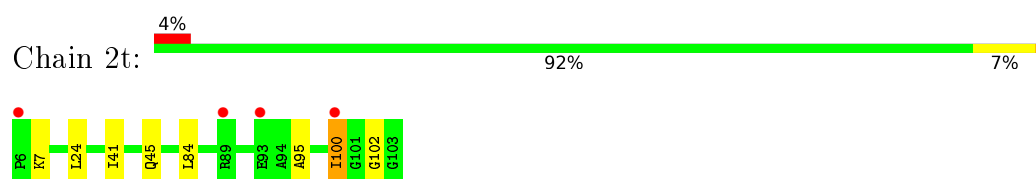
- Molecule 50: 30S ribosomal protein S19



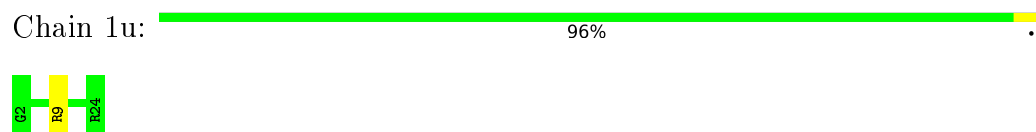
- Molecule 51: 30S ribosomal protein S20



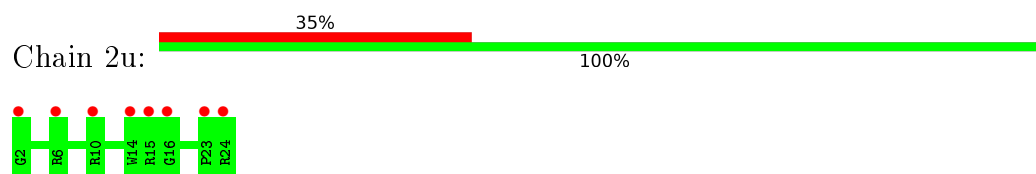
- Molecule 51: 30S ribosomal protein S20



- Molecule 52: 30S ribosomal protein Thx



- Molecule 52: 30S ribosomal protein Thx



- Molecule 53: mRNA



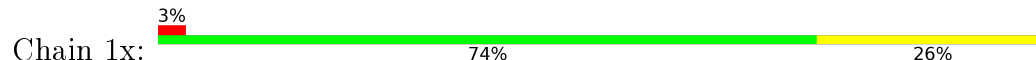
There are no outlier residues recorded for this chain.

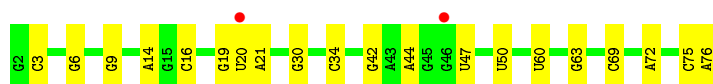
- Molecule 53: mRNA



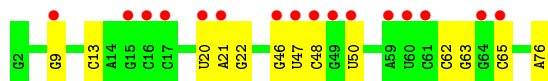
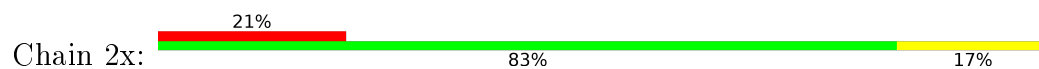
There are no outlier residues recorded for this chain.

- Molecule 54: tRNA<sup>i</sup>Met

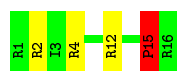
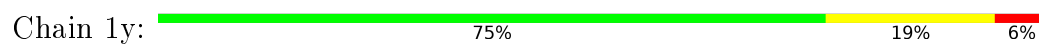




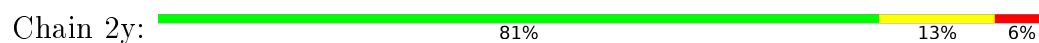
- Molecule 54: tRNAiMet



- Molecule 55: Cathelicidin-3



- Molecule 55: Cathelicidin-3



## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 21 21 21  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 209.96Å 450.13Å 622.82Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)  | 48.62 – 2.80<br>48.98 – 2.80                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.5 (48.62-2.80)<br>99.6 (48.98-2.80)                      | Depositor<br>EDS |
| $R_{merge}$   | 0.51  | Depositor        |
| $R_{sym}$   | (Not available)   | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.14 (at 2.81Å)   | Xtriage          |
| Refinement program  | PHENIX  | Depositor        |
| R, $R_{free}$   | 0.249 , 0.292<br>0.260 , 0.300                              | Depositor<br>DCC |
| $R_{free}$ test set   | 70217 reflections (5.19%)                                   | DCC              |
| Wilson B-factor (Å <sup>2</sup> )                                       | 42.0  | Xtriage          |
| Anisotropy  | 0.182   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.28 , 18.2   | EDS              |
| Estimated twinning fraction   | No twinning to report.                                      | Xtriage          |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.38$ , $\langle L^2 \rangle = 0.20$ | Xtriage          |
| Outliers  | 0 of 1422885 reflections                                    | Xtriage          |
| $F_o, F_c$ correlation  | 0.84  | EDS              |
| Total number of atoms   | 296108  | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 44.0  | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.60% 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, OMC, ZN, M2G, OMG, OMU, MA6, SF4, 0TD, MG, 2MA, 2MG, 5MC, UR3, 4OC, 4SU, 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    | 0.54         | 0/69034       | 1.07        | 167/107758 (0.2%) |
| 1   | 2A    | 0.44         | 0/68906       | 0.97        | 77/107556 (0.1%)  |
| 2   | 1B    | 0.46         | 0/2879        | 1.03        | 11/4490 (0.2%)    |
| 2   | 2B    | 0.41         | 0/2874        | 0.97        | 2/4482 (0.0%)     |
| 3   | 1D    | 0.39         | 0/2181        | 0.64        | 1/2940 (0.0%)     |
| 3   | 2D    | 0.34         | 0/2186        | 0.61        | 0/2944            |
| 4   | 1E    | 0.38         | 0/1592        | 0.61        | 0/2149            |
| 4   | 2E    | 0.34         | 0/1592        | 0.62        | 0/2149            |
| 5   | 1F    | 0.36         | 0/1619        | 0.60        | 0/2193            |
| 5   | 2F    | 0.32         | 0/1615        | 0.56        | 0/2188            |
| 6   | 1G    | 0.33         | 0/1451        | 0.61        | 0/1961            |
| 6   | 2G    | 0.31         | 0/1449        | 0.60        | 0/1957            |
| 7   | 1H    | 0.34         | 0/1356        | 0.55        | 0/1834            |
| 7   | 2H    | 0.31         | 0/1350        | 0.54        | 0/1826            |
| 8   | 1I    | 0.31         | 0/1109        | 0.62        | 0/1512            |
| 8   | 2I    | 0.29         | 0/1091        | 0.58        | 0/1490            |
| 9   | 1N    | 0.36         | 0/1148        | 0.60        | 0/1547            |
| 9   | 2N    | 0.30         | 0/1144        | 0.55        | 0/1543            |
| 10  | 1O    | 0.41         | 0/943         | 0.61        | 0/1269            |
| 10  | 2O    | 0.35         | 0/943         | 0.58        | 0/1269            |
| 11  | 1P    | 0.35         | 0/1152        | 0.62        | 0/1533            |
| 11  | 2P    | 0.31         | 0/1152        | 0.57        | 0/1533            |
| 12  | 1Q    | 0.44         | 1/1143 (0.1%) | 0.64        | 2/1527 (0.1%)     |
| 12  | 2Q    | 0.32         | 0/1143        | 0.54        | 0/1527            |
| 13  | 1R    | 0.37         | 0/982         | 0.61        | 0/1312            |
| 13  | 2R    | 0.32         | 0/982         | 0.57        | 0/1312            |
| 14  | 1S    | 0.32         | 0/887         | 0.59        | 0/1180            |
| 14  | 2S    | 0.31         | 0/880         | 0.58        | 0/1172            |
| 15  | 1T    | 0.34         | 0/1105        | 0.60        | 0/1477            |
| 15  | 2T    | 0.32         | 0/1097        | 0.58        | 0/1468            |
| 16  | 1U    | 0.37         | 0/977         | 0.58        | 0/1301            |

| Mol | Chain | Bond lengths |                | Bond angles |                 |
|-----|-------|--------------|----------------|-------------|-----------------|
|     |       | RMSZ         | # Z  >5        | RMSZ        | # Z  >5         |
| 16  | 2U    | 0.31         | 0/977          | 0.53        | 0/1301          |
| 17  | 1V    | 0.37         | 0/786          | 0.60        | 0/1053          |
| 17  | 2V    | 0.32         | 0/782          | 0.60        | 0/1049          |
| 18  | 1W    | 0.39         | 0/897          | 0.60        | 0/1205          |
| 18  | 2W    | 0.32         | 0/897          | 0.55        | 0/1205          |
| 19  | 1X    | 0.39         | 0/764          | 0.60        | 0/1025          |
| 19  | 2X    | 0.34         | 0/764          | 0.63        | 1/1025 (0.1%)   |
| 20  | 1Y    | 0.38         | 0/823          | 0.62        | 0/1099          |
| 20  | 2Y    | 0.33         | 0/823          | 0.63        | 0/1100          |
| 21  | 1Z    | 0.33         | 0/1620         | 0.57        | 0/2200          |
| 21  | 2Z    | 0.32         | 0/1590         | 0.58        | 0/2162          |
| 22  | 10    | 0.36         | 0/616          | 0.61        | 0/821           |
| 22  | 20    | 0.33         | 0/616          | 0.58        | 0/821           |
| 23  | 11    | 0.36         | 0/761          | 0.57        | 0/1013          |
| 23  | 21    | 0.33         | 0/766          | 0.56        | 0/1018          |
| 24  | 12    | 0.35         | 0/590          | 0.63        | 1/781 (0.1%)    |
| 24  | 22    | 0.31         | 0/594          | 0.53        | 0/785           |
| 25  | 13    | 0.35         | 0/474          | 0.57        | 0/635           |
| 25  | 23    | 0.30         | 0/469          | 0.53        | 0/630           |
| 26  | 14    | 0.35         | 0/559          | 0.68        | 0/754           |
| 26  | 24    | 0.37         | 0/549          | 0.67        | 0/741           |
| 27  | 15    | 0.39         | 0/473          | 0.63        | 0/639           |
| 27  | 25    | 0.31         | 0/469          | 0.61        | 1/635 (0.2%)    |
| 28  | 16    | 0.36         | 0/460          | 0.59        | 0/613           |
| 28  | 26    | 0.34         | 0/456          | 0.57        | 0/608           |
| 29  | 17    | 0.41         | 0/426          | 0.65        | 0/561           |
| 29  | 27    | 0.36         | 0/426          | 0.55        | 0/561           |
| 30  | 18    | 0.38         | 0/525          | 0.61        | 0/691           |
| 30  | 28    | 0.34         | 0/525          | 0.57        | 0/691           |
| 31  | 19    | 0.36         | 0/310          | 0.61        | 0/407           |
| 31  | 29    | 0.31         | 0/310          | 0.58        | 0/407           |
| 32  | 1a    | 0.41         | 0/35795        | 0.99        | 69/55864 (0.1%) |
| 32  | 2a    | 0.40         | 1/35890 (0.0%) | 1.00        | 91/56012 (0.2%) |
| 33  | 1b    | 0.34         | 0/1876         | 0.63        | 0/2533          |
| 33  | 2b    | 0.33         | 0/1860         | 0.59        | 0/2518          |
| 34  | 1c    | 0.31         | 0/1582         | 0.57        | 0/2137          |
| 34  | 2c    | 0.31         | 0/1566         | 0.58        | 0/2119          |
| 35  | 1d    | 0.32         | 0/1695         | 0.60        | 0/2274          |
| 35  | 2d    | 0.29         | 0/1698         | 0.55        | 0/2277          |
| 36  | 1e    | 0.32         | 0/1149         | 0.58        | 0/1548          |
| 36  | 2e    | 0.32         | 0/1149         | 0.58        | 0/1548          |
| 37  | 1f    | 0.32         | 0/827          | 0.57        | 0/1120          |
| 37  | 2f    | 0.31         | 0/829          | 0.57        | 0/1123          |

| Mol | Chain | Bond lengths |                 | Bond angles |                   |
|-----|-------|--------------|-----------------|-------------|-------------------|
|     |       | RMSZ         | # Z  >5         | RMSZ        | # Z  >5           |
| 38  | 1g    | 0.32         | 0/1254          | 0.55        | 0/1683            |
| 38  | 2g    | 0.29         | 0/1248          | 0.52        | 0/1676            |
| 39  | 1h    | 0.30         | 0/1118          | 0.58        | 0/1506            |
| 39  | 2h    | 0.30         | 0/1108          | 0.56        | 0/1494            |
| 40  | 1i    | 0.30         | 0/1005          | 0.58        | 0/1351            |
| 40  | 2i    | 0.32         | 0/985           | 0.57        | 0/1329            |
| 41  | 1j    | 0.32         | 0/732           | 0.58        | 0/993             |
| 41  | 2j    | 0.32         | 0/723           | 0.60        | 0/984             |
| 42  | 1k    | 0.33         | 0/849           | 0.59        | 0/1150            |
| 42  | 2k    | 0.36         | 0/848           | 0.61        | 0/1149            |
| 43  | 1l    | 0.31         | 0/937           | 0.56        | 0/1260            |
| 43  | 2l    | 0.31         | 0/937           | 0.61        | 0/1260            |
| 44  | 1m    | 0.29         | 0/924           | 0.60        | 0/1242            |
| 44  | 2m    | 0.31         | 0/905           | 0.58        | 0/1217            |
| 45  | 1n    | 0.31         | 0/501           | 0.55        | 0/664             |
| 45  | 2n    | 0.33         | 0/501           | 0.55        | 0/664             |
| 46  | 1o    | 0.31         | 0/739           | 0.58        | 0/985             |
| 46  | 2o    | 0.29         | 0/739           | 0.52        | 0/985             |
| 47  | 1p    | 0.30         | 0/697           | 0.56        | 0/939             |
| 47  | 2p    | 0.31         | 0/693           | 0.55        | 0/935             |
| 48  | 1q    | 0.32         | 0/836           | 0.60        | 0/1117            |
| 48  | 2q    | 0.31         | 0/836           | 0.56        | 0/1117            |
| 49  | 1r    | 0.30         | 0/560           | 0.56        | 0/746             |
| 49  | 2r    | 0.31         | 0/560           | 0.56        | 0/746             |
| 50  | 1s    | 0.30         | 0/663           | 0.61        | 0/895             |
| 50  | 2s    | 0.29         | 0/660           | 0.60        | 0/893             |
| 51  | 1t    | 0.31         | 0/734           | 0.57        | 0/969             |
| 51  | 2t    | 0.29         | 0/736           | 0.54        | 0/976             |
| 52  | 1u    | 0.28         | 0/203           | 0.57        | 0/266             |
| 52  | 2u    | 0.30         | 0/203           | 0.57        | 0/266             |
| 53  | 1v    | 0.45         | 0/72            | 0.91        | 0/110             |
| 53  | 2v    | 0.48         | 0/72            | 1.04        | 0/110             |
| 54  | 1x    | 0.42         | 0/1725          | 0.94        | 0/2689            |
| 54  | 2x    | 0.40         | 0/1725          | 0.96        | 3/2689 (0.1%)     |
| 55  | 1y    | 0.37         | 0/152           | 0.83        | 1/203 (0.5%)      |
| 55  | 2y    | 0.33         | 0/152           | 0.87        | 1/203 (0.5%)      |
| All | All   | 0.43         | 2/312307 (0.0%) | 0.92        | 428/467169 (0.1%) |

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  | 24    | 0                   | 1                   |
| 33  | 1b    | 0                   | 1                   |
| 55  | 1y    | 0                   | 1                   |
| 55  | 2y    | 0                   | 1                   |
| All | All   | 0                   | 4                   |

All (2) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 12  | 1Q    | 41   | TRP  | NE1-CE2 | 6.34 | 1.45        | 1.37     |
| 32  | 2a    | 1034 | G    | N9-C4   | 5.00 | 1.42        | 1.38     |

All (428) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms     | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|--------|-------------|----------|
| 32  | 2a    | 1208 | C    | O5'-P-OP1 | -31.64 | 72.74       | 110.70   |
| 32  | 1a    | 1520 | G    | O5'-P-OP1 | -30.14 | 74.54       | 110.70   |
| 32  | 2a    | 1208 | C    | OP1-P-OP2 | -27.27 | 78.69       | 119.60   |
| 32  | 1a    | 1520 | G    | OP1-P-OP2 | -26.36 | 80.06       | 119.60   |
| 32  | 1a    | 1520 | G    | O5'-P-OP2 | 19.44  | 134.03      | 110.70   |
| 32  | 2a    | 1208 | C    | O5'-P-OP2 | 17.89  | 132.16      | 110.70   |
| 32  | 2a    | 1207 | 2MG  | OP1-P-O3' | 13.62  | 135.16      | 105.20   |
| 32  | 2a    | 1207 | 2MG  | OP2-P-O3' | -12.53 | 77.64       | 105.20   |
| 1   | 1A    | 720  | C    | C2-N3-C4  | -12.23 | 113.79      | 119.90   |
| 1   | 1A    | 787  | U    | O5'-P-OP2 | -11.63 | 95.24       | 105.70   |
| 1   | 1A    | 834  | U    | O5'-P-OP1 | -11.59 | 95.27       | 105.70   |
| 32  | 1a    | 558  | G    | O5'-P-OP1 | -11.56 | 95.29       | 105.70   |
| 1   | 2A    | 1639 | U    | O5'-P-OP2 | -10.79 | 95.99       | 105.70   |
| 32  | 1a    | 1495 | U    | N1-C2-O2  | 10.76  | 130.33      | 122.80   |
| 1   | 1A    | 1686 | U    | O5'-P-OP2 | -10.56 | 96.19       | 105.70   |
| 32  | 2a    | 351  | G    | OP1-P-O3' | -10.39 | 82.33       | 105.20   |
| 32  | 2a    | 404  | U    | N1-C2-O2  | 10.16  | 129.91      | 122.80   |
| 1   | 1A    | 2694 | U    | O5'-P-OP2 | -10.05 | 96.65       | 105.70   |
| 1   | 2A    | 2711 | A    | O5'-P-OP1 | -9.70  | 96.97       | 105.70   |
| 2   | 1B    | 75   | G    | C6-N1-C2  | -9.56  | 119.36      | 125.10   |
| 1   | 1A    | 1045 | U    | O5'-P-OP2 | -9.54  | 97.12       | 105.70   |
| 1   | 1A    | 2227 | G    | C4-N9-C1' | -9.53  | 114.12      | 126.50   |
| 1   | 2A    | 673  | C    | C2-N3-C4  | -9.51  | 115.15      | 119.90   |
| 1   | 2A    | 2682 | U    | O5'-P-OP2 | -9.46  | 97.18       | 105.70   |
| 1   | 1A    | 2188 | G    | N3-C4-N9  | -9.08  | 120.55      | 126.00   |
| 32  | 2a    | 1495 | U    | N1-C2-O2  | 8.97   | 129.08      | 122.80   |
| 1   | 1A    | 2083 | G    | O5'-P-OP2 | -8.90  | 97.69       | 105.70   |
| 32  | 2a    | 352  | C    | OP1-P-OP2 | 8.89   | 132.94      | 119.60   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | 2A    | 948  | G    | O5'-P-OP1  | -8.85 | 97.73       | 105.70   |
| 1   | 1A    | 854  | U    | C2-N3-C4   | -8.73 | 121.76      | 127.00   |
| 32  | 1a    | 343  | U    | C2-N1-C1'  | -8.67 | 107.30      | 117.70   |
| 32  | 2a    | 351  | G    | OP2-P-O3'  | -8.63 | 86.20       | 105.20   |
| 1   | 1A    | 2227 | G    | C8-N9-C1'  | 8.63  | 138.22      | 127.00   |
| 1   | 1A    | 2442 | A    | O5'-P-OP2  | -8.53 | 98.03       | 105.70   |
| 1   | 1A    | 932  | C    | C6-N1-C2   | -8.49 | 116.90      | 120.30   |
| 32  | 2a    | 299  | G    | C5-C6-O6   | -8.40 | 123.56      | 128.60   |
| 32  | 2a    | 558  | G    | O5'-P-OP1  | -8.39 | 98.14       | 105.70   |
| 32  | 1a    | 404  | U    | N1-C2-O2   | 8.39  | 128.67      | 122.80   |
| 32  | 1a    | 841  | U    | C5-C6-N1   | 8.28  | 126.84      | 122.70   |
| 1   | 1A    | 354  | A    | C2-N3-C4   | -8.24 | 106.48      | 110.60   |
| 32  | 1a    | 1137 | C    | C6-N1-C2   | -8.22 | 117.01      | 120.30   |
| 32  | 1a    | 1436 | U    | C2-N3-C4   | -8.19 | 122.08      | 127.00   |
| 32  | 1a    | 1465 | C    | C2-N3-C4   | -8.19 | 115.81      | 119.90   |
| 1   | 1A    | 82   | G    | N9-C4-C5   | -8.16 | 102.14      | 105.40   |
| 32  | 2a    | 1034 | G    | C5-C6-N1   | 8.03  | 115.51      | 111.50   |
| 32  | 2a    | 1034 | G    | N3-C4-C5   | -8.00 | 124.60      | 128.60   |
| 32  | 2a    | 343  | U    | C5-C4-O4   | 7.98  | 130.69      | 125.90   |
| 1   | 2A    | 785  | G    | O5'-P-OP2  | -7.92 | 98.57       | 105.70   |
| 1   | 1A    | 354  | A    | N1-C2-N3   | 7.90  | 133.25      | 129.30   |
| 1   | 1A    | 2058 | C    | O5'-P-OP1  | -7.89 | 98.60       | 105.70   |
| 32  | 2a    | 343  | U    | N3-C4-O4   | -7.86 | 113.90      | 119.40   |
| 32  | 2a    | 343  | U    | C2-N1-C1'  | -7.77 | 108.38      | 117.70   |
| 1   | 1A    | 952  | G    | C5-C6-O6   | 7.75  | 133.25      | 128.60   |
| 1   | 2A    | 807  | U    | C2-N3-C4   | -7.74 | 122.36      | 127.00   |
| 32  | 2a    | 1465 | C    | C2-N3-C4   | -7.54 | 116.13      | 119.90   |
| 32  | 2a    | 1034 | G    | C6-N1-C2   | -7.54 | 120.58      | 125.10   |
| 32  | 1a    | 1495 | U    | N3-C2-O2   | -7.53 | 116.93      | 122.20   |
| 32  | 1a    | 299  | G    | C5-C6-O6   | -7.46 | 124.12      | 128.60   |
| 55  | 2y    | 15   | PRO  | O-C-N      | -7.46 | 110.76      | 122.70   |
| 1   | 1A    | 1700 | G    | P-O3'-C3'  | 7.46  | 128.65      | 119.70   |
| 1   | 2A    | 906  | G    | C5-C6-O6   | 7.46  | 133.07      | 128.60   |
| 32  | 1a    | 1397 | C    | N1-C2-O2   | 7.45  | 123.37      | 118.90   |
| 32  | 2a    | 1027 | C    | C6-N1-C2   | -7.43 | 117.33      | 120.30   |
| 32  | 1a    | 1495 | U    | C2-N1-C1'  | 7.42  | 126.60      | 117.70   |
| 1   | 1A    | 1358 | U    | C5-C4-O4   | 7.41  | 130.35      | 125.90   |
| 1   | 1A    | 952  | G    | N3-C4-N9   | -7.39 | 121.57      | 126.00   |
| 1   | 1A    | 2858 | G    | O4'-C1'-N9 | 7.29  | 114.03      | 108.20   |
| 2   | 1B    | 102  | A    | C6-N1-C2   | -7.28 | 114.23      | 118.60   |
| 32  | 1a    | 343  | U    | O4'-C1'-N1 | 7.24  | 114.00      | 108.20   |
| 32  | 2a    | 1001 | A    | O4'-C1'-N9 | 7.18  | 113.94      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 32  | 2a    | 1034 | G    | N3-C4-N9   | 7.15  | 130.29      | 126.00   |
| 1   | 1A    | 2604 | G    | O5'-P-OP1  | -7.15 | 99.27       | 105.70   |
| 1   | 2A    | 740  | U    | O5'-P-OP2  | -7.12 | 99.29       | 105.70   |
| 1   | 1A    | 2227 | G    | N3-C4-N9   | -7.08 | 121.75      | 126.00   |
| 32  | 2a    | 1125 | U    | C2-N1-C1'  | 7.06  | 126.17      | 117.70   |
| 2   | 1B    | 59   | A    | C6-N1-C2   | -7.04 | 114.38      | 118.60   |
| 2   | 1B    | 24   | G    | N3-C4-C5   | -7.03 | 125.09      | 128.60   |
| 32  | 2a    | 1034 | G    | C2-N3-C4   | 6.99  | 115.39      | 111.90   |
| 1   | 1A    | 2188 | G    | C8-N9-C1'  | 6.96  | 136.05      | 127.00   |
| 1   | 1A    | 720  | C    | N3-C4-C5   | 6.94  | 124.68      | 121.90   |
| 1   | 1A    | 1378 | G    | O5'-P-OP1  | -6.93 | 99.47       | 105.70   |
| 1   | 1A    | 932  | C    | C5-C6-N1   | 6.91  | 124.46      | 121.00   |
| 32  | 2a    | 1436 | U    | C2-N3-C4   | -6.88 | 122.87      | 127.00   |
| 1   | 1A    | 2188 | G    | C6-C5-N7   | 6.87  | 134.52      | 130.40   |
| 1   | 1A    | 194  | G    | O5'-P-OP2  | -6.84 | 99.54       | 105.70   |
| 1   | 1A    | 2802 | C    | C2-N1-C1'  | -6.84 | 111.28      | 118.80   |
| 1   | 1A    | 2188 | G    | C4-N9-C1'  | -6.83 | 117.63      | 126.50   |
| 1   | 1A    | 2188 | G    | N9-C4-C5   | 6.81  | 108.12      | 105.40   |
| 1   | 1A    | 101  | A    | N1-C6-N6   | 6.79  | 122.67      | 118.60   |
| 32  | 2a    | 993  | G    | N3-C4-N9   | 6.79  | 130.07      | 126.00   |
| 19  | 2X    | 57   | LEU  | CA-CB-CG   | 6.78  | 130.88      | 115.30   |
| 32  | 1a    | 1397 | C    | C2-N1-C1'  | 6.77  | 126.24      | 118.80   |
| 1   | 2A    | 1092 | C    | N1-C2-O2   | 6.76  | 122.96      | 118.90   |
| 32  | 1a    | 1137 | C    | C5-C6-N1   | 6.75  | 124.38      | 121.00   |
| 32  | 2a    | 404  | U    | C2-N1-C1'  | 6.73  | 125.77      | 117.70   |
| 1   | 1A    | 848  | G    | O5'-P-OP2  | -6.72 | 99.65       | 105.70   |
| 32  | 2a    | 1003 | G    | C8-N9-C4   | -6.72 | 103.71      | 106.40   |
| 1   | 1A    | 2459 | G    | C6-N1-C2   | -6.71 | 121.07      | 125.10   |
| 1   | 2A    | 383  | U    | N1-C2-O2   | 6.69  | 127.48      | 122.80   |
| 1   | 1A    | 215  | G    | C2-N3-C4   | 6.68  | 115.24      | 111.90   |
| 1   | 2A    | 1416 | G    | O4'-C1'-N9 | 6.67  | 113.54      | 108.20   |
| 32  | 2a    | 299  | G    | N1-C6-O6   | 6.66  | 123.90      | 119.90   |
| 32  | 2a    | 993  | G    | N3-C4-C5   | -6.64 | 125.28      | 128.60   |
| 1   | 1A    | 952  | G    | N9-C4-C5   | 6.62  | 108.05      | 105.40   |
| 32  | 1a    | 343  | U    | C6-N1-C1'  | 6.62  | 130.47      | 121.20   |
| 1   | 1A    | 537  | G    | O4'-C1'-N9 | 6.62  | 113.50      | 108.20   |
| 1   | 1A    | 418  | G    | C6-N1-C2   | -6.62 | 121.13      | 125.10   |
| 32  | 2a    | 993  | G    | C4-N9-C1'  | 6.59  | 135.07      | 126.50   |
| 1   | 2A    | 2130 | U    | C5-C6-N1   | 6.54  | 125.97      | 122.70   |
| 1   | 1A    | 1140 | U    | O4'-C1'-N1 | 6.52  | 113.41      | 108.20   |
| 32  | 1a    | 1436 | U    | C5-C4-O4   | -6.49 | 122.01      | 125.90   |
| 32  | 2a    | 1397 | C    | C2-N1-C1'  | 6.49  | 125.94      | 118.80   |

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| Mol | Chain | Res     | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|---------|------|------------|-------|-------------|----------|
| 1   | 1A    | 2188    | G    | C5-C6-O6   | 6.48  | 132.49      | 128.60   |
| 32  | 2a    | 1030(B) | C    | C2-N1-C1'  | 6.47  | 125.92      | 118.80   |
| 32  | 2a    | 404     | U    | N3-C2-O2   | -6.47 | 117.67      | 122.20   |
| 32  | 2a    | 299     | G    | C4-C5-N7   | 6.46  | 113.38      | 110.80   |
| 55  | 1y    | 15      | PRO  | O-C-N      | -6.45 | 112.38      | 122.70   |
| 1   | 2A    | 807     | U    | C5-C4-O4   | -6.41 | 122.05      | 125.90   |
| 32  | 1a    | 78      | G    | C8-N9-C1'  | 6.40  | 135.32      | 127.00   |
| 1   | 1A    | 215     | G    | N1-C2-N2   | 6.38  | 121.94      | 116.20   |
| 1   | 1A    | 720     | C    | N1-C2-N3   | 6.36  | 123.65      | 119.20   |
| 1   | 1A    | 2227    | G    | N3-C4-C5   | 6.36  | 131.78      | 128.60   |
| 32  | 2a    | 1003    | G    | N3-C4-C5   | -6.36 | 125.42      | 128.60   |
| 1   | 2A    | 2102    | U    | N1-C2-O2   | 6.34  | 127.24      | 122.80   |
| 1   | 2A    | 1835    | G    | C4-N9-C1'  | 6.34  | 134.74      | 126.50   |
| 1   | 1A    | 1462    | G    | O4'-C1'-N9 | 6.33  | 113.26      | 108.20   |
| 1   | 1A    | 2180    | A    | O4'-C1'-N9 | 6.32  | 113.25      | 108.20   |
| 1   | 2A    | 2689    | U    | N3-C2-O2   | -6.30 | 117.79      | 122.20   |
| 32  | 2a    | 1003    | G    | C4-N9-C1'  | 6.29  | 134.68      | 126.50   |
| 1   | 2A    | 1076    | C    | O4'-C1'-N1 | 6.28  | 113.23      | 108.20   |
| 1   | 2A    | 2447    | G    | C6-N1-C2   | -6.28 | 121.33      | 125.10   |
| 1   | 1A    | 2136    | A    | N1-C6-N6   | -6.28 | 114.83      | 118.60   |
| 1   | 1A    | 2390    | A    | C4-C5-C6   | 6.28  | 120.14      | 117.00   |
| 1   | 1A    | 410     | U    | N1-C2-O2   | 6.28  | 127.19      | 122.80   |
| 1   | 1A    | 1134    | A    | O4'-C1'-N9 | 6.28  | 113.22      | 108.20   |
| 32  | 2a    | 299     | G    | C6-C5-N7   | -6.28 | 126.64      | 130.40   |
| 32  | 1a    | 343     | U    | C5-C4-O4   | 6.25  | 129.65      | 125.90   |
| 1   | 1A    | 2802    | C    | C6-N1-C1'  | 6.25  | 128.30      | 120.80   |
| 32  | 1a    | 533     | A    | N1-C6-N6   | 6.25  | 122.35      | 118.60   |
| 32  | 1a    | 1406    | U    | C2-N3-C4   | -6.23 | 123.26      | 127.00   |
| 2   | 2B    | 59      | A    | C6-N1-C2   | -6.22 | 114.87      | 118.60   |
| 32  | 2a    | 5       | U    | C2-N1-C1'  | 6.22  | 125.17      | 117.70   |
| 1   | 1A    | 1398    | U    | O5'-P-OP1  | -6.21 | 100.11      | 105.70   |
| 1   | 2A    | 1052    | C    | C2-N1-C1'  | 6.20  | 125.62      | 118.80   |
| 32  | 2a    | 346     | G    | C6-N1-C2   | -6.20 | 121.38      | 125.10   |
| 1   | 2A    | 2699    | C    | C6-N1-C2   | 6.19  | 122.78      | 120.30   |
| 1   | 1A    | 2903    | G    | N3-C4-N9   | -6.19 | 122.29      | 126.00   |
| 1   | 2A    | 1835    | G    | C8-N9-C1'  | -6.19 | 118.96      | 127.00   |
| 1   | 2A    | 2187    | G    | C6-C5-N7   | -6.18 | 126.69      | 130.40   |
| 32  | 2a    | 1030(B) | C    | N1-C2-O2   | 6.18  | 122.61      | 118.90   |
| 1   | 1A    | 1386    | U    | C2-N3-C4   | -6.16 | 123.30      | 127.00   |
| 32  | 1a    | 1465    | C    | N3-C4-C5   | 6.15  | 124.36      | 121.90   |
| 1   | 1A    | 82      | G    | C2-N3-C4   | -6.14 | 108.83      | 111.90   |
| 32  | 2a    | 1228    | C    | N1-C2-O2   | 6.14  | 122.59      | 118.90   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | 2A    | 1087 | G    | N3-C4-N9   | -6.10 | 122.34      | 126.00   |
| 1   | 1A    | 1110 | C    | C5-C6-N1   | 6.09  | 124.05      | 121.00   |
| 32  | 2a    | 1036 | G    | N7-C8-N9   | 6.08  | 116.14      | 113.10   |
| 2   | 1B    | 24   | G    | C6-N1-C2   | -6.07 | 121.46      | 125.10   |
| 1   | 2A    | 1053 | C    | P-O3'-C3'  | 6.07  | 126.98      | 119.70   |
| 32  | 2a    | 343  | U    | C6-N1-C1'  | 6.07  | 129.69      | 121.20   |
| 32  | 1a    | 1024 | G    | N3-C4-N9   | 6.06  | 129.64      | 126.00   |
| 1   | 1A    | 598  | A    | O5'-P-OP1  | -6.06 | 100.25      | 105.70   |
| 32  | 1a    | 78   | G    | C4-N9-C1'  | -6.06 | 118.63      | 126.50   |
| 32  | 2a    | 1028 | C    | C6-N1-C2   | -6.05 | 117.88      | 120.30   |
| 1   | 1A    | 2188 | G    | C4-C5-N7   | -6.03 | 108.39      | 110.80   |
| 1   | 1A    | 720  | C    | N1-C2-O2   | -6.02 | 115.29      | 118.90   |
| 32  | 1a    | 1024 | G    | C8-N9-C1'  | -6.02 | 119.17      | 127.00   |
| 32  | 1a    | 1024 | G    | C4-N9-C1'  | 6.02  | 134.32      | 126.50   |
| 1   | 1A    | 1418 | U    | C2-N1-C1'  | 6.01  | 124.91      | 117.70   |
| 32  | 1a    | 498  | U    | C5-C4-O4   | 6.00  | 129.50      | 125.90   |
| 32  | 1a    | 1495 | U    | C5-C6-N1   | 6.00  | 125.70      | 122.70   |
| 1   | 1A    | 2161 | C    | C5-C6-N1   | 5.99  | 124.00      | 121.00   |
| 1   | 2A    | 2103 | C    | C6-N1-C2   | -5.99 | 117.90      | 120.30   |
| 32  | 2a    | 5    | U    | N3-C2-O2   | -5.99 | 118.01      | 122.20   |
| 1   | 1A    | 2125 | C    | N1-C2-O2   | 5.98  | 122.48      | 118.90   |
| 1   | 1A    | 2227 | G    | C6-C5-N7   | 5.97  | 133.99      | 130.40   |
| 1   | 1A    | 1578 | C    | C6-N1-C2   | -5.96 | 117.92      | 120.30   |
| 32  | 2a    | 1005 | A    | C8-N9-C4   | -5.96 | 103.42      | 105.80   |
| 32  | 1a    | 299  | G    | C4-C5-N7   | 5.96  | 113.18      | 110.80   |
| 2   | 1B    | 75   | G    | C5-C6-O6   | -5.96 | 125.03      | 128.60   |
| 1   | 2A    | 1087 | G    | C8-N9-C1'  | 5.94  | 134.72      | 127.00   |
| 1   | 1A    | 215  | G    | C6-C5-N7   | 5.93  | 133.96      | 130.40   |
| 1   | 1A    | 637  | U    | O4'-C1'-N1 | 5.93  | 112.94      | 108.20   |
| 32  | 1a    | 1285 | A    | P-O3'-C3'  | 5.93  | 126.81      | 119.70   |
| 32  | 2a    | 1495 | U    | C2-N1-C1'  | 5.91  | 124.79      | 117.70   |
| 1   | 1A    | 952  | G    | C4-C5-N7   | -5.91 | 108.44      | 110.80   |
| 32  | 1a    | 1495 | U    | C2-N3-C4   | 5.90  | 130.54      | 127.00   |
| 32  | 2a    | 1495 | U    | N3-C2-O2   | -5.87 | 118.09      | 122.20   |
| 1   | 1A    | 952  | G    | C6-C5-N7   | 5.86  | 133.92      | 130.40   |
| 32  | 2a    | 346  | G    | C5-C6-N1   | 5.84  | 114.42      | 111.50   |
| 1   | 1A    | 1959 | A    | N1-C6-N6   | -5.84 | 115.09      | 118.60   |
| 1   | 2A    | 277  | C    | N1-C2-O2   | 5.84  | 122.40      | 118.90   |
| 2   | 1B    | 75   | G    | N3-C4-C5   | -5.84 | 125.68      | 128.60   |
| 1   | 1A    | 2136 | A    | C8-N9-C4   | -5.83 | 103.47      | 105.80   |
| 32  | 2a    | 1465 | C    | C5-C4-N4   | -5.82 | 116.12      | 120.20   |
| 1   | 2A    | 2430 | A    | O5'-P-OP2  | -5.82 | 100.46      | 105.70   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 32  | 2a    | 5    | U    | N1-C2-O2   | 5.82  | 126.88      | 122.80   |
| 32  | 1a    | 841  | U    | C6-N1-C2   | -5.82 | 117.51      | 121.00   |
| 1   | 2A    | 1992 | G    | P-O3'-C3'  | 5.82  | 126.68      | 119.70   |
| 32  | 2a    | 1228 | C    | N3-C2-O2   | -5.81 | 117.83      | 121.90   |
| 32  | 1a    | 1397 | C    | N3-C2-O2   | -5.80 | 117.84      | 121.90   |
| 32  | 2a    | 1026 | G    | N7-C8-N9   | 5.79  | 116.00      | 113.10   |
| 1   | 1A    | 217  | A    | C5-N7-C8   | -5.78 | 101.01      | 103.90   |
| 1   | 2A    | 752  | A    | P-O3'-C3'  | 5.78  | 126.63      | 119.70   |
| 32  | 1a    | 78   | G    | O4'-C1'-N9 | 5.77  | 112.81      | 108.20   |
| 32  | 2a    | 266  | G    | P-O3'-C3'  | 5.77  | 126.62      | 119.70   |
| 1   | 1A    | 1440 | U    | O5'-P-OP1  | -5.76 | 100.51      | 105.70   |
| 1   | 1A    | 2157 | A    | N1-C6-N6   | 5.76  | 122.06      | 118.60   |
| 32  | 2a    | 1024 | G    | C2-N3-C4   | 5.75  | 114.78      | 111.90   |
| 32  | 2a    | 754  | C    | C2-N1-C1'  | 5.75  | 125.12      | 118.80   |
| 32  | 1a    | 343  | U    | C5-C6-N1   | -5.75 | 119.83      | 122.70   |
| 32  | 2a    | 346  | G    | C5-C6-O6   | -5.74 | 125.16      | 128.60   |
| 1   | 2A    | 1313 | U    | C2-N1-C1'  | 5.73  | 124.58      | 117.70   |
| 32  | 1a    | 533  | A    | C5-C6-N6   | -5.71 | 119.13      | 123.70   |
| 1   | 2A    | 673  | C    | N3-C4-C5   | 5.71  | 124.18      | 121.90   |
| 1   | 2A    | 2144 | U    | O4'-C1'-N1 | 5.71  | 112.76      | 108.20   |
| 32  | 1a    | 343  | U    | N3-C4-O4   | -5.70 | 115.41      | 119.40   |
| 1   | 1A    | 529  | U    | C2-N1-C1'  | 5.70  | 124.54      | 117.70   |
| 32  | 1a    | 533  | A    | C6-C5-N7   | -5.69 | 128.32      | 132.30   |
| 1   | 2A    | 2451 | A    | C5-N7-C8   | -5.68 | 101.06      | 103.90   |
| 1   | 1A    | 989  | G    | N7-C8-N9   | 5.68  | 115.94      | 113.10   |
| 1   | 1A    | 2209 | G    | C5-C6-O6   | -5.67 | 125.20      | 128.60   |
| 1   | 2A    | 1052 | C    | N1-C2-O2   | 5.67  | 122.30      | 118.90   |
| 54  | 2x    | 22   | G    | C5-N7-C8   | -5.67 | 101.47      | 104.30   |
| 1   | 1A    | 780  | G    | C5-N7-C8   | 5.66  | 107.13      | 104.30   |
| 32  | 1a    | 1067 | A    | P-O3'-C3'  | 5.66  | 126.49      | 119.70   |
| 1   | 1A    | 215  | G    | N1-C2-N3   | -5.66 | 120.51      | 123.90   |
| 32  | 2a    | 1406 | U    | C2-N3-C4   | -5.66 | 123.61      | 127.00   |
| 32  | 2a    | 1067 | A    | P-O3'-C3'  | 5.64  | 126.47      | 119.70   |
| 1   | 1A    | 2123 | G    | O4'-C1'-N9 | 5.64  | 112.71      | 108.20   |
| 1   | 1A    | 1718 | U    | O5'-P-OP2  | -5.63 | 100.63      | 105.70   |
| 1   | 2A    | 383  | U    | N3-C2-O2   | -5.63 | 118.26      | 122.20   |
| 2   | 1B    | 75   | G    | C5-C6-N1   | 5.63  | 114.31      | 111.50   |
| 32  | 2a    | 1281 | U    | C2-N1-C1'  | 5.63  | 124.45      | 117.70   |
| 32  | 2a    | 993  | G    | C8-N9-C1'  | -5.62 | 119.69      | 127.00   |
| 1   | 1A    | 2275 | C    | N1-C2-O2   | -5.61 | 115.53      | 118.90   |
| 2   | 1B    | 24   | G    | N3-C4-N9   | 5.61  | 129.37      | 126.00   |
| 1   | 2A    | 1087 | G    | C4-N9-C1'  | -5.60 | 119.22      | 126.50   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 32  | 1a    | 1397 | C    | C6-N1-C2   | -5.58 | 118.07      | 120.30   |
| 32  | 2a    | 299  | G    | N9-C4-C5   | -5.58 | 103.17      | 105.40   |
| 1   | 1A    | 2136 | A    | N9-C4-C5   | 5.57  | 108.03      | 105.80   |
| 1   | 1A    | 2802 | C    | O4'-C1'-N1 | 5.57  | 112.66      | 108.20   |
| 1   | 2A    | 512  | G    | O4'-C1'-N9 | 5.57  | 112.66      | 108.20   |
| 32  | 2a    | 1034 | G    | C5-C6-O6   | -5.57 | 125.26      | 128.60   |
| 2   | 2B    | 8    | U    | C5-C6-N1   | 5.57  | 125.48      | 122.70   |
| 1   | 1A    | 1838 | G    | C2-N3-C4   | -5.56 | 109.12      | 111.90   |
| 1   | 2A    | 2102 | U    | N3-C2-O2   | -5.56 | 118.31      | 122.20   |
| 1   | 1A    | 1811 | A    | O5'-P-OP1  | -5.56 | 100.70      | 105.70   |
| 1   | 2A    | 673  | C    | C5-C4-N4   | -5.56 | 116.31      | 120.20   |
| 1   | 1A    | 2903 | G    | N9-C4-C5   | 5.55  | 107.62      | 105.40   |
| 2   | 1B    | 102  | A    | N1-C2-N3   | 5.55  | 132.07      | 129.30   |
| 1   | 1A    | 215  | G    | N9-C4-C5   | 5.55  | 107.62      | 105.40   |
| 1   | 2A    | 1092 | C    | C2-N1-C1'  | 5.54  | 124.89      | 118.80   |
| 32  | 1a    | 1065 | U    | P-O3'-C3'  | 5.54  | 126.34      | 119.70   |
| 1   | 1A    | 31   | C    | O5'-P-OP1  | -5.53 | 100.72      | 105.70   |
| 1   | 1A    | 2589 | A    | O5'-P-OP1  | -5.53 | 100.72      | 105.70   |
| 1   | 1A    | 2903 | G    | C6-C5-N7   | 5.53  | 133.72      | 130.40   |
| 1   | 1A    | 1054 | C    | C6-N1-C2   | -5.53 | 118.09      | 120.30   |
| 1   | 2A    | 226  | G    | C4-N9-C1'  | -5.52 | 119.32      | 126.50   |
| 32  | 1a    | 1465 | C    | C5-C4-N4   | -5.52 | 116.33      | 120.20   |
| 32  | 2a    | 1158 | C    | C6-N1-C2   | -5.52 | 118.09      | 120.30   |
| 32  | 2a    | 1005 | A    | N7-C8-N9   | 5.52  | 116.56      | 113.80   |
| 1   | 1A    | 215  | G    | O4'-C1'-N9 | 5.52  | 112.61      | 108.20   |
| 1   | 1A    | 2181 | G    | O4'-C1'-N9 | 5.51  | 112.61      | 108.20   |
| 32  | 2a    | 841  | U    | C5-C6-N1   | 5.51  | 125.45      | 122.70   |
| 32  | 1a    | 266  | G    | P-O3'-C3'  | 5.50  | 126.31      | 119.70   |
| 32  | 1a    | 993  | G    | C4-N9-C1'  | 5.50  | 133.65      | 126.50   |
| 32  | 1a    | 991  | U    | P-O3'-C3'  | 5.49  | 126.28      | 119.70   |
| 27  | 25    | 58   | LEU  | CA-CB-CG   | 5.49  | 127.92      | 115.30   |
| 32  | 2a    | 1026 | G    | C5-N7-C8   | -5.49 | 101.56      | 104.30   |
| 1   | 1A    | 1398 | U    | O5'-P-OP2  | 5.48  | 117.28      | 110.70   |
| 32  | 1a    | 1442 | G    | N3-C4-C5   | -5.47 | 125.86      | 128.60   |
| 1   | 2A    | 2870 | C    | C6-N1-C2   | -5.47 | 118.11      | 120.30   |
| 32  | 2a    | 299  | G    | N3-C4-N9   | 5.46  | 129.28      | 126.00   |
| 1   | 1A    | 952  | G    | C8-N9-C1'  | 5.46  | 134.10      | 127.00   |
| 1   | 1A    | 1222 | A    | O5'-P-OP1  | -5.46 | 100.78      | 105.70   |
| 1   | 1A    | 2167 | C    | C5-C6-N1   | 5.46  | 123.73      | 121.00   |
| 32  | 2a    | 289  | G    | O5'-P-OP2  | 5.45  | 117.24      | 110.70   |
| 32  | 2a    | 520  | A    | N9-C4-C5   | 5.45  | 107.98      | 105.80   |
| 32  | 2a    | 1436 | U    | C5-C4-O4   | -5.45 | 122.63      | 125.90   |

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| Mol | Chain | Res     | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|---------|------|------------|-------|-------------|----------|
| 1   | 1A    | 101     | A    | C4-C5-C6   | 5.44  | 119.72      | 117.00   |
| 1   | 1A    | 215     | G    | C8-N9-C1'  | 5.44  | 134.07      | 127.00   |
| 1   | 2A    | 1312    | U    | C5-C4-O4   | 5.44  | 129.16      | 125.90   |
| 54  | 2x    | 47      | U    | C5-C6-N1   | 5.44  | 125.42      | 122.70   |
| 1   | 2A    | 2207    | G    | N7-C8-N9   | 5.42  | 115.81      | 113.10   |
| 32  | 2a    | 1158    | C    | C2-N1-C1'  | 5.42  | 124.76      | 118.80   |
| 1   | 2A    | 2321    | G    | P-O3'-C3'  | 5.41  | 126.19      | 119.70   |
| 1   | 1A    | 2183    | C    | C5-C6-N1   | 5.41  | 123.70      | 121.00   |
| 1   | 2A    | 513     | A    | N1-C6-N6   | 5.39  | 121.83      | 118.60   |
| 1   | 1A    | 215     | G    | N3-C4-N9   | -5.39 | 122.77      | 126.00   |
| 1   | 1A    | 223     | C    | N1-C2-O2   | 5.38  | 122.13      | 118.90   |
| 1   | 1A    | 184     | A    | P-O3'-C3'  | 5.38  | 126.16      | 119.70   |
| 1   | 1A    | 2057    | G    | O5'-P-OP1  | -5.37 | 100.86      | 105.70   |
| 32  | 2a    | 404     | U    | C5-C6-N1   | 5.37  | 125.39      | 122.70   |
| 1   | 1A    | 2390    | A    | N1-C6-N6   | 5.37  | 121.82      | 118.60   |
| 1   | 2A    | 2120    | G    | N3-C4-N9   | 5.36  | 129.22      | 126.00   |
| 32  | 2a    | 901     | A    | N1-C6-N6   | 5.36  | 121.82      | 118.60   |
| 1   | 1A    | 854     | U    | N1-C2-N3   | 5.36  | 118.12      | 114.90   |
| 1   | 1A    | 82      | G    | C8-N9-C4   | 5.36  | 108.54      | 106.40   |
| 1   | 1A    | 2459    | G    | C5-C6-N1   | 5.35  | 114.18      | 111.50   |
| 1   | 1A    | 1418    | U    | C5-C4-O4   | -5.35 | 122.69      | 125.90   |
| 1   | 2A    | 784     | A    | P-O3'-C3'  | 5.34  | 126.11      | 119.70   |
| 32  | 1a    | 1201    | A    | P-O3'-C3'  | 5.34  | 126.11      | 119.70   |
| 1   | 1A    | 2627    | U    | O5'-P-OP1  | -5.33 | 100.90      | 105.70   |
| 1   | 1A    | 1020    | C    | O5'-P-OP1  | -5.33 | 100.90      | 105.70   |
| 1   | 1A    | 1815    | A    | O5'-P-OP2  | -5.33 | 100.90      | 105.70   |
| 32  | 1a    | 299     | G    | N9-C4-C5   | -5.33 | 103.27      | 105.40   |
| 32  | 1a    | 404     | U    | N3-C2-O2   | -5.33 | 118.47      | 122.20   |
| 1   | 1A    | 2188    | G    | N3-C4-C5   | 5.33  | 131.26      | 128.60   |
| 32  | 1a    | 754     | C    | C2-N1-C1'  | 5.32  | 124.65      | 118.80   |
| 32  | 2a    | 343     | U    | O4'-C1'-N1 | 5.32  | 112.45      | 108.20   |
| 1   | 2A    | 1992    | G    | N3-C4-C5   | -5.30 | 125.95      | 128.60   |
| 1   | 2A    | 1351    | C    | OP1-P-O3'  | 5.29  | 116.85      | 105.20   |
| 32  | 2a    | 1030(B) | C    | C5-C6-N1   | 5.29  | 123.65      | 121.00   |
| 32  | 1a    | 404     | U    | C2-N1-C1'  | 5.29  | 124.05      | 117.70   |
| 1   | 1A    | 906     | G    | C8-N9-C4   | 5.29  | 108.52      | 106.40   |
| 1   | 2A    | 2144    | U    | C2-N1-C1'  | 5.29  | 124.04      | 117.70   |
| 1   | 1A    | 697     | C    | C5-C6-N1   | 5.28  | 123.64      | 121.00   |
| 1   | 2A    | 1359    | A    | C2-N3-C4   | 5.28  | 113.24      | 110.60   |
| 32  | 1a    | 1024    | G    | C6-C5-N7   | -5.28 | 127.23      | 130.40   |
| 1   | 1A    | 2587    | C    | O5'-P-OP2  | -5.27 | 100.95      | 105.70   |
| 32  | 2a    | 60      | A    | P-O3'-C3'  | 5.27  | 126.02      | 119.70   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | 1A    | 854  | U    | C5-C4-O4    | -5.26 | 122.74      | 125.90   |
| 1   | 1A    | 2457 | G    | N1-C6-O6    | -5.26 | 116.74      | 119.90   |
| 1   | 1A    | 2134 | G    | N3-C4-C5    | -5.26 | 125.97      | 128.60   |
| 1   | 1A    | 1162 | C    | C2-N1-C1'   | 5.25  | 124.58      | 118.80   |
| 32  | 1a    | 975  | A    | O4'-C1'-N9  | -5.25 | 104.00      | 108.20   |
| 1   | 1A    | 236  | G    | C8-N9-C4    | 5.25  | 108.50      | 106.40   |
| 1   | 1A    | 2045 | G    | O5'-P-OP1   | -5.25 | 100.98      | 105.70   |
| 1   | 1A    | 1220 | U    | P-O3'-C3'   | 5.25  | 125.99      | 119.70   |
| 32  | 1a    | 346  | G    | C5-C6-O6    | -5.24 | 125.45      | 128.60   |
| 1   | 2A    | 2318 | G    | C4-N9-C1'   | 5.24  | 133.31      | 126.50   |
| 1   | 2A    | 1045 | A    | C2-N3-C4    | 5.23  | 113.22      | 110.60   |
| 1   | 2A    | 2146 | C    | O4'-C1'-N1  | 5.23  | 112.38      | 108.20   |
| 32  | 2a    | 404  | U    | C2-N3-C4    | 5.23  | 130.14      | 127.00   |
| 1   | 1A    | 1716 | A    | C8-N9-C4    | -5.23 | 103.71      | 105.80   |
| 1   | 2A    | 386  | G    | C6-N1-C2    | -5.22 | 121.97      | 125.10   |
| 12  | 1Q    | 41   | TRP  | CD2-CE2-CZ2 | 5.22  | 128.56      | 122.30   |
| 1   | 1A    | 82   | G    | C4-C5-N7    | 5.22  | 112.89      | 110.80   |
| 1   | 1A    | 697  | C    | N1-C2-O2    | 5.21  | 122.03      | 118.90   |
| 32  | 1a    | 353  | A    | OP2-P-O3'   | 5.21  | 116.67      | 105.20   |
| 32  | 2a    | 1027 | C    | N3-C2-O2    | -5.21 | 118.25      | 121.90   |
| 1   | 1A    | 1119 | A    | C2-N3-C4    | 5.21  | 113.21      | 110.60   |
| 1   | 2A    | 2114 | A    | C8-N9-C4    | -5.21 | 103.72      | 105.80   |
| 1   | 1A    | 2194 | U    | C5-C4-O4    | 5.20  | 129.02      | 125.90   |
| 32  | 2a    | 1026 | G    | C8-N9-C4    | -5.20 | 104.32      | 106.40   |
| 54  | 2x    | 46   | G    | C6-N1-C2    | -5.20 | 121.98      | 125.10   |
| 32  | 2a    | 1036 | G    | C8-N9-C4    | -5.20 | 104.32      | 106.40   |
| 1   | 1A    | 1687 | C    | O4'-C1'-N1  | 5.20  | 112.36      | 108.20   |
| 1   | 1A    | 847  | A    | N1-C6-N6    | -5.20 | 115.48      | 118.60   |
| 32  | 1a    | 1213 | A    | N1-C6-N6    | -5.19 | 115.48      | 118.60   |
| 1   | 1A    | 1239 | A    | N1-C6-N6    | -5.19 | 115.49      | 118.60   |
| 32  | 1a    | 1067 | A    | C8-N9-C4    | -5.19 | 103.72      | 105.80   |
| 1   | 1A    | 2155 | G    | O4'-C1'-N9  | 5.18  | 112.35      | 108.20   |
| 1   | 1A    | 1110 | C    | C2-N1-C1'   | 5.18  | 124.50      | 118.80   |
| 1   | 1A    | 215  | G    | C4-N9-C1'   | -5.18 | 119.77      | 126.50   |
| 1   | 1A    | 599  | U    | O5'-P-OP1   | -5.18 | 101.04      | 105.70   |
| 1   | 1A    | 1388 | A    | O5'-P-OP2   | -5.17 | 101.04      | 105.70   |
| 1   | 1A    | 665  | C    | C6-N1-C2    | -5.17 | 118.23      | 120.30   |
| 1   | 1A    | 1707 | C    | N3-C4-N4    | -5.17 | 114.38      | 118.00   |
| 32  | 1a    | 1442 | G    | P-O3'-C3'   | 5.17  | 125.90      | 119.70   |
| 1   | 1A    | 752  | A    | N1-C6-N6    | 5.16  | 121.70      | 118.60   |
| 32  | 2a    | 1397 | C    | C6-N1-C1'   | -5.16 | 114.61      | 120.80   |
| 1   | 1A    | 1220 | U    | OP1-P-O3'   | 5.15  | 116.54      | 105.20   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | 1A    | 952  | G    | O4'-C1'-N9 | 5.14  | 112.31      | 108.20   |
| 1   | 1A    | 2192 | A    | O4'-C1'-N9 | 5.14  | 112.31      | 108.20   |
| 32  | 2a    | 266  | G    | C4-N9-C1'  | 5.14  | 133.18      | 126.50   |
| 32  | 1a    | 533  | A    | C4-C5-C6   | 5.13  | 119.57      | 117.00   |
| 1   | 2A    | 2378 | A    | N1-C6-N6   | 5.13  | 121.68      | 118.60   |
| 1   | 1A    | 101  | A    | N9-C4-C5   | -5.13 | 103.75      | 105.80   |
| 32  | 2a    | 1257 | U    | O4'-C1'-N1 | 5.13  | 112.30      | 108.20   |
| 1   | 1A    | 1255 | A    | P-O3'-C3'  | 5.13  | 125.85      | 119.70   |
| 12  | 1Q    | 41   | TRP  | CE2-CD2-CG | 5.13  | 111.40      | 107.30   |
| 1   | 2A    | 458  | G    | O4'-C1'-N9 | 5.12  | 112.29      | 108.20   |
| 1   | 2A    | 277  | C    | C2-N1-C1'  | 5.11  | 124.42      | 118.80   |
| 1   | 2A    | 1416 | G    | C4-N9-C1'  | -5.11 | 119.86      | 126.50   |
| 32  | 2a    | 520  | A    | C8-N9-C4   | -5.11 | 103.76      | 105.80   |
| 32  | 1a    | 1026 | G    | O4'-C1'-N9 | 5.11  | 112.29      | 108.20   |
| 1   | 1A    | 1142 | A    | O4'-C1'-N9 | 5.10  | 112.28      | 108.20   |
| 32  | 1a    | 1027 | C    | C5-C6-N1   | 5.10  | 123.55      | 121.00   |
| 1   | 2A    | 2187 | G    | N3-C4-N9   | 5.10  | 129.06      | 126.00   |
| 1   | 1A    | 1134 | A    | C4-N9-C1'  | 5.09  | 135.47      | 126.30   |
| 3   | 1D    | 155  | LEU  | CA-CB-CG   | 5.09  | 127.02      | 115.30   |
| 32  | 1a    | 78   | G    | N3-C4-N9   | -5.09 | 122.95      | 126.00   |
| 32  | 1a    | 1036 | G    | C4-N9-C1'  | 5.09  | 133.12      | 126.50   |
| 1   | 1A    | 203  | G    | O4'-C1'-N9 | 5.08  | 112.27      | 108.20   |
| 1   | 1A    | 2597 | U    | OP1-P-O3'  | 5.08  | 116.37      | 105.20   |
| 1   | 2A    | 2318 | G    | C8-N9-C4   | -5.08 | 104.37      | 106.40   |
| 1   | 1A    | 637  | U    | C2-N1-C1'  | 5.08  | 123.79      | 117.70   |
| 1   | 1A    | 1218 | G    | O4'-C1'-N9 | 5.08  | 112.26      | 108.20   |
| 1   | 1A    | 1738 | C    | N3-C2-O2   | -5.08 | 118.35      | 121.90   |
| 1   | 1A    | 2155 | G    | C4-N9-C1'  | -5.07 | 119.91      | 126.50   |
| 32  | 2a    | 1016 | A    | N1-C6-N6   | 5.07  | 121.64      | 118.60   |
| 2   | 1B    | 24   | G    | C4-N9-C1'  | 5.07  | 133.09      | 126.50   |
| 32  | 1a    | 115  | G    | P-O3'-C3'  | 5.07  | 125.78      | 119.70   |
| 1   | 2A    | 614  | U    | C2-N1-C1'  | 5.06  | 123.78      | 117.70   |
| 1   | 2A    | 2585 | U    | OP1-P-O3'  | 5.06  | 116.34      | 105.20   |
| 32  | 1a    | 533  | A    | C6-N1-C2   | -5.06 | 115.56      | 118.60   |
| 1   | 2A    | 2238 | G    | N3-C4-C5   | -5.06 | 126.07      | 128.60   |
| 32  | 2a    | 913  | A    | P-O3'-C3'  | 5.06  | 125.77      | 119.70   |
| 1   | 1A    | 137  | G    | C8-N9-C1'  | -5.06 | 120.43      | 127.00   |
| 1   | 1A    | 2014 | G    | O5'-P-OP1  | -5.05 | 101.15      | 105.70   |
| 32  | 2a    | 687  | A    | P-O3'-C3'  | 5.05  | 125.76      | 119.70   |
| 1   | 1A    | 2513 | C    | C2-N1-C1'  | -5.05 | 113.25      | 118.80   |
| 1   | 1A    | 2903 | G    | N3-C2-N2   | -5.05 | 116.37      | 119.90   |
| 1   | 1A    | 101  | A    | C8-N9-C1'  | -5.05 | 118.61      | 127.70   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | 2A    | 1835 | G    | O4'-C1'-N9 | -5.05 | 104.16      | 108.20   |
| 32  | 2a    | 1465 | C    | N3-C4-C5   | 5.04  | 123.92      | 121.90   |
| 1   | 1A    | 1007 | G    | OP1-P-O3'  | 5.04  | 116.29      | 105.20   |
| 1   | 1A    | 1098 | C    | C6-N1-C2   | -5.04 | 118.28      | 120.30   |
| 1   | 2A    | 1420 | U    | P-O3'-C3'  | 5.04  | 125.75      | 119.70   |
| 1   | 1A    | 2614 | A    | P-O3'-C3'  | 5.04  | 125.74      | 119.70   |
| 32  | 2a    | 1004 | A    | O4'-C1'-N9 | 5.03  | 112.23      | 108.20   |
| 1   | 1A    | 894  | U    | C2-N1-C1'  | 5.03  | 123.73      | 117.70   |
| 24  | 12    | 69   | ARG  | N-CA-C     | 5.03  | 124.58      | 111.00   |
| 1   | 1A    | 1332 | A    | C8-N9-C4   | 5.02  | 107.81      | 105.80   |
| 1   | 1A    | 611  | U    | O5'-P-OP2  | -5.02 | 101.18      | 105.70   |
| 1   | 1A    | 279  | G    | O4'-C1'-N9 | -5.02 | 104.19      | 108.20   |
| 1   | 1A    | 765  | A    | N1-C6-N6   | 5.01  | 121.61      | 118.60   |
| 1   | 2A    | 906  | G    | N9-C4-C5   | 5.01  | 107.41      | 105.40   |
| 1   | 2A    | 1131 | G    | O4'-C1'-N9 | 5.01  | 112.21      | 108.20   |
| 1   | 1A    | 399  | G    | O4'-C1'-N9 | 5.01  | 112.21      | 108.20   |
| 1   | 2A    | 226  | G    | C8-N9-C1'  | 5.01  | 133.51      | 127.00   |
| 1   | 2A    | 800  | A    | O5'-P-OP1  | -5.01 | 101.19      | 105.70   |
| 1   | 2A    | 2114 | A    | N7-C8-N9   | 5.01  | 116.30      | 113.80   |
| 1   | 2A    | 391  | G    | C6-N1-C2   | -5.00 | 122.10      | 125.10   |
| 32  | 1a    | 993  | G    | N3-C4-N9   | 5.00  | 129.00      | 126.00   |
| 1   | 2A    | 1210 | A    | P-O3'-C3'  | 5.00  | 125.70      | 119.70   |

There are no chirality outliers.

All (4) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 33  | 1b    | 231 | GLU  | Peptide   |
| 55  | 1y    | 15  | PRO  | Mainchain |
| 26  | 24    | 59  | PHE  | Peptide   |
| 55  | 2y    | 15  | PRO  | Mainchain |

## 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    | 61872 | 0        | 31199    | 649     | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | 2A    | 61761 | 0        | 31142    | 691     | 0            |
| 2   | 1B    | 2575  | 0        | 1304     | 19      | 0            |
| 2   | 2B    | 2571  | 0        | 1308     | 29      | 0            |
| 3   | 1D    | 2131  | 0        | 2207     | 50      | 0            |
| 3   | 2D    | 2136  | 0        | 2218     | 42      | 0            |
| 4   | 1E    | 1559  | 0        | 1618     | 35      | 0            |
| 4   | 2E    | 1559  | 0        | 1618     | 33      | 0            |
| 5   | 1F    | 1584  | 0        | 1625     | 30      | 0            |
| 5   | 2F    | 1580  | 0        | 1619     | 46      | 0            |
| 6   | 1G    | 1426  | 0        | 1445     | 61      | 0            |
| 6   | 2G    | 1424  | 0        | 1441     | 60      | 0            |
| 7   | 1H    | 1330  | 0        | 1407     | 37      | 0            |
| 7   | 2H    | 1324  | 0        | 1402     | 42      | 0            |
| 8   | 1I    | 1094  | 0        | 1127     | 20      | 0            |
| 8   | 2I    | 1076  | 0        | 1094     | 26      | 0            |
| 9   | 1N    | 1121  | 0        | 1195     | 28      | 0            |
| 9   | 2N    | 1117  | 0        | 1184     | 23      | 0            |
| 10  | 1O    | 933   | 0        | 996      | 8       | 0            |
| 10  | 2O    | 933   | 0        | 996      | 20      | 0            |
| 11  | 1P    | 1135  | 0        | 1212     | 30      | 0            |
| 11  | 2P    | 1135  | 0        | 1212     | 26      | 0            |
| 12  | 1Q    | 1122  | 0        | 1179     | 26      | 0            |
| 12  | 2Q    | 1122  | 0        | 1178     | 29      | 0            |
| 13  | 1R    | 968   | 0        | 1033     | 16      | 0            |
| 13  | 2R    | 968   | 0        | 1032     | 17      | 0            |
| 14  | 1S    | 877   | 0        | 938      | 23      | 0            |
| 14  | 2S    | 870   | 0        | 923      | 22      | 0            |
| 15  | 1T    | 1091  | 0        | 1151     | 25      | 0            |
| 15  | 2T    | 1083  | 0        | 1136     | 20      | 0            |
| 16  | 1U    | 959   | 0        | 1019     | 15      | 0            |
| 16  | 2U    | 959   | 0        | 1019     | 17      | 0            |
| 17  | 1V    | 775   | 0        | 841      | 10      | 0            |
| 17  | 2V    | 771   | 0        | 830      | 14      | 0            |
| 18  | 1W    | 886   | 0        | 940      | 9       | 0            |
| 18  | 2W    | 886   | 0        | 940      | 13      | 0            |
| 19  | 1X    | 750   | 0        | 814      | 19      | 0            |
| 19  | 2X    | 750   | 0        | 814      | 15      | 0            |
| 20  | 1Y    | 810   | 0        | 892      | 18      | 0            |
| 20  | 2Y    | 810   | 0        | 887      | 18      | 0            |
| 21  | 1Z    | 1587  | 0        | 1598     | 36      | 0            |
| 21  | 2Z    | 1557  | 0        | 1564     | 51      | 0            |
| 22  | 10    | 608   | 0        | 622      | 16      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 22  | 20    | 608   | 0        | 621      | 10      | 0            |
| 23  | 11    | 754   | 0        | 823      | 11      | 0            |
| 23  | 21    | 759   | 0        | 837      | 24      | 0            |
| 24  | 12    | 588   | 0        | 643      | 8       | 0            |
| 24  | 22    | 592   | 0        | 654      | 7       | 0            |
| 25  | 13    | 469   | 0        | 518      | 9       | 0            |
| 25  | 23    | 464   | 0        | 514      | 12      | 0            |
| 26  | 14    | 546   | 0        | 522      | 19      | 0            |
| 26  | 24    | 536   | 0        | 514      | 27      | 0            |
| 27  | 15    | 459   | 0        | 476      | 12      | 0            |
| 27  | 25    | 455   | 0        | 465      | 8       | 0            |
| 28  | 16    | 453   | 0        | 473      | 10      | 0            |
| 28  | 26    | 449   | 0        | 469      | 12      | 0            |
| 29  | 17    | 418   | 0        | 467      | 10      | 0            |
| 29  | 27    | 418   | 0        | 467      | 9       | 0            |
| 30  | 18    | 517   | 0        | 582      | 18      | 0            |
| 30  | 28    | 517   | 0        | 582      | 11      | 0            |
| 31  | 19    | 307   | 0        | 335      | 6       | 0            |
| 31  | 29    | 307   | 0        | 335      | 7       | 0            |
| 32  | 1a    | 32246 | 0        | 16295    | 0       | 0            |
| 32  | 2a    | 32331 | 0        | 16339    | 0       | 0            |
| 33  | 1b    | 1842  | 0        | 1862     | 0       | 0            |
| 33  | 2b    | 1825  | 0        | 1828     | 0       | 0            |
| 34  | 1c    | 1558  | 0        | 1557     | 0       | 0            |
| 34  | 2c    | 1542  | 0        | 1517     | 0       | 0            |
| 35  | 1d    | 1665  | 0        | 1687     | 0       | 0            |
| 35  | 2d    | 1668  | 0        | 1703     | 0       | 0            |
| 36  | 1e    | 1133  | 0        | 1190     | 0       | 0            |
| 36  | 2e    | 1133  | 0        | 1191     | 0       | 0            |
| 37  | 1f    | 814   | 0        | 808      | 0       | 0            |
| 37  | 2f    | 816   | 0        | 808      | 0       | 0            |
| 38  | 1g    | 1235  | 0        | 1249     | 0       | 0            |
| 38  | 2g    | 1229  | 0        | 1238     | 0       | 0            |
| 39  | 1h    | 1098  | 0        | 1143     | 0       | 0            |
| 39  | 2h    | 1088  | 0        | 1126     | 0       | 0            |
| 40  | 1i    | 986   | 0        | 990      | 0       | 0            |
| 40  | 2i    | 966   | 0        | 953      | 0       | 0            |
| 41  | 1j    | 719   | 0        | 672      | 0       | 0            |
| 41  | 2j    | 710   | 0        | 661      | 0       | 0            |
| 42  | 1k    | 834   | 0        | 838      | 0       | 0            |
| 42  | 2k    | 833   | 0        | 836      | 0       | 0            |
| 43  | 1l    | 932   | 0        | 981      | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 43  | 2l    | 932   | 0        | 981      | 0       | 0            |
| 44  | 1m    | 914   | 0        | 954      | 0       | 0            |
| 44  | 2m    | 895   | 0        | 920      | 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    | 648   | 0        | 658      | 0       | 0            |
| 50  | 2s    | 645   | 0        | 635      | 0       | 0            |
| 51  | 1t    | 732   | 0        | 809      | 0       | 0            |
| 51  | 2t    | 733   | 0        | 795      | 0       | 0            |
| 52  | 1u    | 199   | 0        | 208      | 0       | 0            |
| 52  | 2u    | 199   | 0        | 208      | 0       | 0            |
| 53  | 1v    | 65    | 0        | 33       | 0       | 0            |
| 53  | 2v    | 65    | 0        | 33       | 0       | 0            |
| 54  | 1x    | 1625  | 0        | 829      | 0       | 0            |
| 54  | 2x    | 1625  | 0        | 829      | 0       | 0            |
| 55  | 1y    | 147   | 0        | 170      | 0       | 0            |
| 55  | 2y    | 147   | 0        | 170      | 0       | 0            |
| 56  | 10    | 8     | 0        | 0        | 0       | 0            |
| 56  | 11    | 2     | 0        | 0        | 0       | 0            |
| 56  | 13    | 2     | 0        | 0        | 0       | 0            |
| 56  | 15    | 7     | 0        | 0        | 0       | 0            |
| 56  | 17    | 2     | 0        | 0        | 0       | 0            |
| 56  | 18    | 1     | 0        | 0        | 0       | 0            |
| 56  | 19    | 3     | 0        | 0        | 0       | 0            |
| 56  | 1A    | 973   | 0        | 0        | 0       | 0            |
| 56  | 1B    | 27    | 0        | 0        | 0       | 0            |
| 56  | 1D    | 14    | 0        | 0        | 0       | 0            |
| 56  | 1E    | 7     | 0        | 0        | 0       | 0            |
| 56  | 1F    | 10    | 0        | 0        | 0       | 0            |
| 56  | 1G    | 3     | 0        | 0        | 0       | 0            |
| 56  | 1H    | 2     | 0        | 0        | 0       | 0            |
| 56  | 1N    | 4     | 0        | 0        | 0       | 0            |
| 56  | 1P    | 4     | 0        | 0        | 0       | 0            |
| 56  | 1Q    | 6     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 56  | 1R    | 4     | 0        | 0        | 0       | 0            |
| 56  | 1S    | 1     | 0        | 0        | 0       | 0            |
| 56  | 1T    | 1     | 0        | 0        | 0       | 0            |
| 56  | 1U    | 3     | 0        | 0        | 0       | 0            |
| 56  | 1V    | 3     | 0        | 0        | 0       | 0            |
| 56  | 1W    | 3     | 0        | 0        | 0       | 0            |
| 56  | 1X    | 1     | 0        | 0        | 0       | 0            |
| 56  | 1a    | 240   | 0        | 0        | 0       | 0            |
| 56  | 1b    | 1     | 0        | 0        | 0       | 0            |
| 56  | 1d    | 5     | 0        | 0        | 0       | 0            |
| 56  | 1e    | 1     | 0        | 0        | 0       | 0            |
| 56  | 1f    | 1     | 0        | 0        | 0       | 0            |
| 56  | 1g    | 1     | 0        | 0        | 0       | 0            |
| 56  | 1h    | 1     | 0        | 0        | 0       | 0            |
| 56  | 1i    | 1     | 0        | 0        | 0       | 0            |
| 56  | 1l    | 3     | 0        | 0        | 0       | 0            |
| 56  | 1n    | 1     | 0        | 0        | 0       | 0            |
| 56  | 1o    | 2     | 0        | 0        | 0       | 0            |
| 56  | 1q    | 1     | 0        | 0        | 0       | 0            |
| 56  | 1t    | 1     | 0        | 0        | 0       | 0            |
| 56  | 1x    | 13    | 0        | 0        | 0       | 0            |
| 56  | 20    | 5     | 0        | 0        | 0       | 0            |
| 56  | 23    | 2     | 0        | 0        | 0       | 0            |
| 56  | 25    | 3     | 0        | 0        | 0       | 0            |
| 56  | 27    | 2     | 0        | 0        | 0       | 0            |
| 56  | 28    | 1     | 0        | 0        | 0       | 0            |
| 56  | 29    | 2     | 0        | 0        | 0       | 0            |
| 56  | 2A    | 986   | 0        | 0        | 0       | 0            |
| 56  | 2B    | 25    | 0        | 0        | 0       | 0            |
| 56  | 2D    | 17    | 0        | 0        | 0       | 0            |
| 56  | 2E    | 6     | 0        | 0        | 0       | 0            |
| 56  | 2F    | 9     | 0        | 0        | 0       | 0            |
| 56  | 2G    | 3     | 0        | 0        | 0       | 0            |
| 56  | 2H    | 2     | 0        | 0        | 0       | 0            |
| 56  | 2N    | 3     | 0        | 0        | 0       | 0            |
| 56  | 2P    | 3     | 0        | 0        | 0       | 0            |
| 56  | 2Q    | 4     | 0        | 0        | 0       | 0            |
| 56  | 2R    | 2     | 0        | 0        | 0       | 0            |
| 56  | 2S    | 1     | 0        | 0        | 0       | 0            |
| 56  | 2U    | 7     | 0        | 0        | 0       | 0            |
| 56  | 2V    | 1     | 0        | 0        | 0       | 0            |
| 56  | 2W    | 1     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 56  | 2X    | 2     | 0        | 0        | 0       | 0            |
| 56  | 2Y    | 2     | 0        | 0        | 0       | 0            |
| 56  | 2a    | 221   | 0        | 0        | 0       | 0            |
| 56  | 2b    | 1     | 0        | 0        | 0       | 0            |
| 56  | 2d    | 4     | 0        | 0        | 0       | 0            |
| 56  | 2e    | 1     | 0        | 0        | 0       | 0            |
| 56  | 2f    | 1     | 0        | 0        | 0       | 0            |
| 56  | 2g    | 1     | 0        | 0        | 0       | 0            |
| 56  | 2h    | 2     | 0        | 0        | 0       | 0            |
| 56  | 2i    | 1     | 0        | 0        | 0       | 0            |
| 56  | 2j    | 1     | 0        | 0        | 0       | 0            |
| 56  | 2l    | 2     | 0        | 0        | 0       | 0            |
| 56  | 2n    | 1     | 0        | 0        | 0       | 0            |
| 56  | 2o    | 1     | 0        | 0        | 0       | 0            |
| 56  | 2t    | 1     | 0        | 0        | 0       | 0            |
| 56  | 2v    | 1     | 0        | 0        | 0       | 0            |
| 56  | 2x    | 12    | 0        | 0        | 0       | 0            |
| 57  | 14    | 1     | 0        | 0        | 0       | 0            |
| 57  | 15    | 1     | 0        | 0        | 0       | 0            |
| 57  | 16    | 1     | 0        | 0        | 0       | 0            |
| 57  | 19    | 1     | 0        | 0        | 0       | 0            |
| 57  | 1Y    | 1     | 0        | 0        | 0       | 0            |
| 57  | 1n    | 1     | 0        | 0        | 0       | 0            |
| 57  | 24    | 1     | 0        | 0        | 0       | 0            |
| 57  | 25    | 1     | 0        | 0        | 0       | 0            |
| 57  | 26    | 1     | 0        | 0        | 0       | 0            |
| 57  | 29    | 1     | 0        | 0        | 0       | 0            |
| 57  | 2Y    | 1     | 0        | 0        | 0       | 0            |
| 57  | 2n    | 1     | 0        | 0        | 0       | 0            |
| 58  | 1d    | 8     | 0        | 0        | 0       | 0            |
| 58  | 2d    | 8     | 0        | 0        | 0       | 0            |
| 59  | 1x    | 1     | 0        | 0        | 0       | 0            |
| 59  | 2A    | 1     | 0        | 0        | 0       | 0            |
| 60  | 10    | 5     | 0        | 0        | 0       | 0            |
| 60  | 11    | 5     | 0        | 0        | 0       | 0            |
| 60  | 13    | 1     | 0        | 0        | 0       | 0            |
| 60  | 15    | 3     | 0        | 0        | 0       | 0            |
| 60  | 16    | 1     | 0        | 0        | 0       | 0            |
| 60  | 17    | 2     | 0        | 0        | 0       | 0            |
| 60  | 18    | 8     | 0        | 0        | 0       | 0            |
| 60  | 19    | 2     | 0        | 0        | 0       | 0            |
| 60  | 1A    | 1795  | 0        | 0        | 7       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 60  | 1B    | 49    | 0        | 0        | 1       | 0            |
| 60  | 1D    | 23    | 0        | 0        | 0       | 0            |
| 60  | 1E    | 16    | 0        | 0        | 0       | 0            |
| 60  | 1F    | 9     | 0        | 0        | 0       | 0            |
| 60  | 1G    | 2     | 0        | 0        | 0       | 0            |
| 60  | 1H    | 4     | 0        | 0        | 0       | 0            |
| 60  | 1N    | 8     | 0        | 0        | 0       | 0            |
| 60  | 1P    | 14    | 0        | 0        | 0       | 0            |
| 60  | 1Q    | 6     | 0        | 0        | 0       | 0            |
| 60  | 1R    | 6     | 0        | 0        | 1       | 0            |
| 60  | 1T    | 5     | 0        | 0        | 0       | 0            |
| 60  | 1U    | 3     | 0        | 0        | 0       | 0            |
| 60  | 1V    | 6     | 0        | 0        | 0       | 0            |
| 60  | 1W    | 1     | 0        | 0        | 0       | 0            |
| 60  | 1X    | 6     | 0        | 0        | 0       | 0            |
| 60  | 1Y    | 4     | 0        | 0        | 0       | 0            |
| 60  | 1a    | 408   | 0        | 0        | 0       | 0            |
| 60  | 1d    | 8     | 0        | 0        | 0       | 0            |
| 60  | 1e    | 3     | 0        | 0        | 0       | 0            |
| 60  | 1f    | 1     | 0        | 0        | 0       | 0            |
| 60  | 1h    | 1     | 0        | 0        | 0       | 0            |
| 60  | 1j    | 1     | 0        | 0        | 0       | 0            |
| 60  | 1l    | 4     | 0        | 0        | 0       | 0            |
| 60  | 1m    | 1     | 0        | 0        | 0       | 0            |
| 60  | 1o    | 2     | 0        | 0        | 0       | 0            |
| 60  | 1p    | 1     | 0        | 0        | 0       | 0            |
| 60  | 1t    | 2     | 0        | 0        | 0       | 0            |
| 60  | 1v    | 2     | 0        | 0        | 0       | 0            |
| 60  | 1x    | 5     | 0        | 0        | 0       | 0            |
| 60  | 1y    | 2     | 0        | 0        | 0       | 0            |
| 60  | 20    | 9     | 0        | 0        | 1       | 0            |
| 60  | 21    | 2     | 0        | 0        | 0       | 0            |
| 60  | 23    | 2     | 0        | 0        | 0       | 0            |
| 60  | 25    | 2     | 0        | 0        | 0       | 0            |
| 60  | 26    | 1     | 0        | 0        | 0       | 0            |
| 60  | 27    | 2     | 0        | 0        | 0       | 0            |
| 60  | 28    | 9     | 0        | 0        | 0       | 0            |
| 60  | 29    | 4     | 0        | 0        | 0       | 0            |
| 60  | 2A    | 1787  | 0        | 0        | 16      | 0            |
| 60  | 2B    | 46    | 0        | 0        | 2       | 0            |
| 60  | 2D    | 20    | 0        | 0        | 0       | 0            |
| 60  | 2E    | 15    | 0        | 0        | 1       | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 60  | 2F    | 11     | 0        | 0        | 0       | 0            |
| 60  | 2G    | 2      | 0        | 0        | 0       | 0            |
| 60  | 2H    | 4      | 0        | 0        | 0       | 0            |
| 60  | 2N    | 8      | 0        | 0        | 0       | 0            |
| 60  | 2P    | 17     | 0        | 0        | 0       | 0            |
| 60  | 2Q    | 4      | 0        | 0        | 0       | 0            |
| 60  | 2R    | 6      | 0        | 0        | 0       | 0            |
| 60  | 2T    | 4      | 0        | 0        | 0       | 0            |
| 60  | 2U    | 5      | 0        | 0        | 0       | 0            |
| 60  | 2V    | 3      | 0        | 0        | 0       | 0            |
| 60  | 2W    | 1      | 0        | 0        | 0       | 0            |
| 60  | 2X    | 5      | 0        | 0        | 0       | 0            |
| 60  | 2Y    | 8      | 0        | 0        | 0       | 0            |
| 60  | 2a    | 408    | 0        | 0        | 0       | 0            |
| 60  | 2d    | 7      | 0        | 0        | 0       | 0            |
| 60  | 2e    | 4      | 0        | 0        | 0       | 0            |
| 60  | 2f    | 1      | 0        | 0        | 0       | 0            |
| 60  | 2h    | 1      | 0        | 0        | 0       | 0            |
| 60  | 2j    | 2      | 0        | 0        | 0       | 0            |
| 60  | 2l    | 7      | 0        | 0        | 0       | 0            |
| 60  | 2m    | 1      | 0        | 0        | 0       | 0            |
| 60  | 2n    | 1      | 0        | 0        | 0       | 0            |
| 60  | 2t    | 1      | 0        | 0        | 0       | 0            |
| 60  | 2v    | 3      | 0        | 0        | 0       | 0            |
| 60  | 2x    | 4      | 0        | 0        | 0       | 0            |
| 60  | 2y    | 4      | 0        | 0        | 0       | 0            |
| All | All   | 296108 | 0        | 194899   | 2305    | 0            |

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

All (2305) 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:2564:OMU:C4 | 1:1A:2564:OMU:C5 | 1.78                     | 1.62              |
| 1:2A:2552:OMU:C5 | 1:2A:2552:OMU:C4 | 1.77                     | 1.56              |
| 1:1A:1085:G:H1   | 1:1A:1162:C:N4   | 1.37                     | 1.23              |
| 1:2A:2119:A:H61  | 1:2A:2168:G:N2   | 1.40                     | 1.17              |
| 1:2A:2119:A:N6   | 1:2A:2168:G:H21  | 1.43                     | 1.14              |
| 1:1A:1405:A:N6   | 1:1A:1418:U:H3   | 1.46                     | 1.11              |
| 1:1A:1005:A:C6   | 1:1A:1024:G:N2   | 29.55                    | 1.08              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:2A:2131:G:H5''  | 1:2A:2132:U:H5'   | 1.38                     | 1.05              |
| 1:2A:2123:G:H1    | 1:2A:2175:C:H42   | 1.08                     | 0.99              |
| 1:2A:2102:U:O2    | 1:2A:2187:G:O6    | 1.81                     | 0.98              |
| 1:1A:1578:C:H42   | 1:1A:1585:G:H1    | 1.04                     | 0.97              |
| 1:2A:1065:U:H3    | 1:2A:1073:A:N6    | 1.61                     | 0.97              |
| 21:1Z:198:LYS:HB3 | 21:1Z:202:GLU:HB2 | 1.47                     | 0.96              |
| 1:2A:1041:C:H42   | 1:2A:1114:G:H1    | 1.03                     | 0.96              |
| 1:1A:1405:A:N1    | 1:1A:1418:U:O4    | 2.01                     | 0.94              |
| 1:1A:303:C:H42    | 1:1A:385:G:H1     | 1.00                     | 0.93              |
| 1:2A:1047:G:H21   | 1:2A:1111:A:H62   | 0.98                     | 0.93              |
| 1:1A:1005:A:N6    | 1:1A:1024:G:N2    | 30.10                    | 0.92              |
| 1:1A:354:A:H2     | 1:1A:1255:A:HO2'  | 0.97                     | 0.92              |
| 1:1A:2331:G:H22   | 14:1S:3:ARG:HD3   | 1.35                     | 0.90              |
| 1:2A:1064:C:H3'   | 1:2A:1065:U:H5''  | 1.53                     | 0.89              |
| 1:1A:1110:C:H3'   | 1:1A:1111:U:H5''  | 1.53                     | 0.89              |
| 12:1Q:8:LYS:HA    | 21:1Z:197:ILE:HB  | 1.56                     | 0.87              |
| 20:1Y:92:ASN:HB2  | 20:1Y:94:LYS:H    | 1.39                     | 0.86              |
| 1:2A:1264:G:OP1   | 27:25:19:ARG:NH2  | 2.08                     | 0.86              |
| 1:2A:272(G):C:H42 | 1:2A:363(C):G:H1  | 1.23                     | 0.85              |
| 19:2X:2:LYS:NZ    | 19:2X:38:GLU:OE2  | 2.09                     | 0.85              |
| 1:2A:2123:G:H1    | 1:2A:2175:C:N4    | 1.72                     | 0.85              |
| 1:2A:1063:G:N2    | 1:2A:1076:C:O2'   | 2.09                     | 0.85              |
| 1:1A:303:C:N4     | 1:1A:385:G:H1     | 1.74                     | 0.84              |
| 1:2A:2123:G:N2    | 1:2A:2175:C:N3    | 2.25                     | 0.84              |
| 1:2A:817:C:H42    | 1:2A:1529:G:H1    | 113.65                   | 0.84              |
| 1:1A:922:G:H1     | 1:1A:948:C:H42    | 1.21                     | 0.83              |
| 1:2A:1065:U:H3    | 1:2A:1073:A:H61   | 0.87                     | 0.83              |
| 1:2A:2111:C:H42   | 1:2A:2147:G:H22   | 1.27                     | 0.82              |
| 1:1A:1766:G:H8    | 1:1A:1770:A:H62   | 1.28                     | 0.81              |
| 1:1A:1847:G:O6    | 3:1D:35:LYS:NZ    | 2.13                     | 0.81              |
| 1:2A:2285:C:OP2   | 28:26:6:ARG:NH1   | 2.13                     | 0.81              |
| 17:2V:72:VAL:HG13 | 17:2V:85:LYS:HB3  | 1.62                     | 0.81              |
| 1:1A:11:G:H2'     | 1:1A:12:U:H5''    | 1.63                     | 0.80              |
| 1:2A:1047:G:N2    | 1:2A:1111:A:H62   | 1.77                     | 0.80              |
| 2:2B:60:C:N4      | 60:2B:3101:HOH:O  | 2.13                     | 0.80              |
| 1:1A:1087:C:H42   | 1:1A:1160:G:H1    | 1.28                     | 0.80              |
| 1:2A:1864:U:OP1   | 1:2A:2410:G:O2'   | 1.98                     | 0.80              |
| 1:1A:2702:C:OP1   | 13:1R:17:ARG:NH2  | 2.15                     | 0.80              |
| 1:1A:1578:C:N4    | 1:1A:1585:G:H1    | 1.79                     | 0.80              |
| 1:1A:1305:G:H22   | 1:1A:1331:G:H1'   | 40.05                    | 0.80              |
| 1:2A:1041:C:N4    | 1:2A:1114:G:H1    | 1.79                     | 0.80              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 21:2Z:144:LEU:HD21 | 21:2Z:150:LEU:HD13 | 1.63                     | 0.80              |
| 7:1H:149:ARG:NH1   | 7:1H:167:GLU:OE2   | 2.14                     | 0.79              |
| 5:2F:120:GLU:HB3   | 5:2F:122:LYS:HG2   | 1.63                     | 0.79              |
| 18:2W:2:GLU:OE2    | 18:2W:72:LYS:NZ    | 2.15                     | 0.79              |
| 1:2A:1073:A:H2'    | 1:2A:1074:G:H8     | 1.45                     | 0.79              |
| 1:1A:2138:G:OP2    | 1:1A:2188:G:N2     | 2.15                     | 0.79              |
| 2:2B:16:G:H1       | 2:2B:68:C:H42      | 1.26                     | 0.79              |
| 1:2A:2141:G:H1     | 1:2A:2150:U:H3     | 1.27                     | 0.79              |
| 6:1G:41:GLN:HB3    | 6:1G:43:LEU:HD13   | 1.65                     | 0.79              |
| 2:2B:18:G:H1       | 2:2B:65:C:H42      | 1.29                     | 0.79              |
| 8:1I:38:LEU:HB3    | 8:1I:40:THR:HG23   | 1.65                     | 0.78              |
| 1:2A:1046:A:N6     | 1:2A:1211:U:O2     | 148.97                   | 0.78              |
| 1:1A:1102:G:N1     | 1:1A:1148:C:OP2    | 2.13                     | 0.78              |
| 1:1A:1039:G:OP1    | 16:1U:50:ARG:NH2   | 2.17                     | 0.78              |
| 24:12:65:ASN:OD1   | 24:12:69:ARG:NH1   | 2.17                     | 0.77              |
| 2:2B:16:G:H1       | 2:2B:68:C:N4       | 1.81                     | 0.77              |
| 1:1A:1140:U:H1'    | 1:1A:1143:U:H5     | 1.48                     | 0.77              |
| 1:1A:138:G:H1      | 1:1A:225:C:H42     | 82.05                    | 0.77              |
| 12:1Q:21:THR:HG21  | 12:1Q:101:ARG:HB2  | 1.66                     | 0.77              |
| 1:2A:1466:G:HO2'   | 1:2A:1546:C:HO2'   | 1.31                     | 0.77              |
| 1:1A:2188:G:O6     | 1:1A:2194:U:O4     | 2.01                     | 0.77              |
| 1:1A:2798:C:OP1    | 4:1E:41:LYS:NZ     | 2.18                     | 0.77              |
| 23:21:51:VAL:HG11  | 23:21:74:VAL:HG21  | 1.66                     | 0.77              |
| 1:2A:1202:C:H42    | 1:2A:1243:G:H1     | 1.29                     | 0.77              |
| 19:2X:40:LYS:HG3   | 19:2X:51:VAL:HB    | 1.67                     | 0.76              |
| 12:2Q:6:ARG:HE     | 21:2Z:197:ILE:HD11 | 1.51                     | 0.76              |
| 1:2A:2079:U:OP1    | 23:21:21:ARG:NH2   | 2.19                     | 0.76              |
| 6:2G:3:LEU:HD11    | 6:2G:97:ASP:HB3    | 1.68                     | 0.76              |
| 1:1A:2188:G:O6     | 1:1A:2194:U:C4     | 2.38                     | 0.76              |
| 1:2A:65:C:O2       | 1:2A:456:C:N4      | 2.18                     | 0.76              |
| 26:14:40:HIS:HB3   | 26:14:43:TYR:HB2   | 1.68                     | 0.75              |
| 1:1A:909:G:OP1     | 12:1Q:18:LYS:NZ    | 2.18                     | 0.75              |
| 12:2Q:8:LYS:HA     | 21:2Z:197:ILE:HB   | 1.68                     | 0.75              |
| 1:1A:2188:G:O6     | 1:1A:2194:U:C5     | 2.39                     | 0.75              |
| 1:2A:1359:A:N6     | 1:2A:1372:U:O4     | 2.19                     | 0.75              |
| 5:1F:120:GLU:HB3   | 5:1F:122:LYS:HG2   | 1.67                     | 0.75              |
| 1:1A:1121:C:OP1    | 12:1Q:59:ARG:NE    | 2.18                     | 0.75              |
| 13:2R:67:LEU:HD13  | 13:2R:76:VAL:HG21  | 1.67                     | 0.75              |
| 11:1P:100:LEU:HD12 | 11:1P:112:LEU:HD11 | 1.69                     | 0.75              |
| 5:2F:29:ASN:H      | 5:2F:112:MET:HE2   | 1.50                     | 0.75              |
| 1:2A:2319:G:H22    | 14:2S:3:ARG:HD3    | 1.50                     | 0.75              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:1A:1310:G:OP1    | 27:15:19:ARG:NH2   | 2.18                     | 0.75              |
| 1:2A:11:G:H2'      | 1:2A:12:U:H5''     | 1.69                     | 0.75              |
| 1:2A:1047:G:H21    | 1:2A:1111:A:N6     | 1.81                     | 0.75              |
| 1:1A:2188:G:C6     | 1:1A:2194:U:O4     | 2.39                     | 0.74              |
| 3:2D:164:GLN:OE1   | 3:2D:176:ARG:NH2   | 2.19                     | 0.74              |
| 2:2B:8:U:H3        | 2:2B:113:G:H1      | 1.35                     | 0.74              |
| 1:2A:2292:C:OP1    | 14:2S:17:ARG:NH2   | 2.19                     | 0.74              |
| 17:2V:100:ARG:HH11 | 17:2V:100:ARG:HB2  | 1.51                     | 0.74              |
| 3:1D:242:ARG:HH11  | 3:1D:242:ARG:HG3   | 1.51                     | 0.74              |
| 1:1A:2324:U:H5'    | 6:1G:88:ILE:HD11   | 1.69                     | 0.74              |
| 19:1X:60:ARG:HH12  | 29:17:47:ARG:HH22  | 1.33                     | 0.74              |
| 1:1A:1305:G:N2     | 1:1A:1331:G:H1'    | 39.79                    | 0.74              |
| 1:2A:2640:G:O3'    | 9:2N:74:ARG:NH2    | 2.21                     | 0.74              |
| 26:24:16:CYS:SG    | 26:24:17:GLY:N     | 2.60                     | 0.74              |
| 12:2Q:59:ARG:HA    | 21:2Z:180:VAL:HG23 | 1.69                     | 0.74              |
| 1:1A:1071:G:O2'    | 60:1A:9001:HOH:O   | 2.05                     | 0.74              |
| 1:1A:1112:U:H3     | 1:1A:1119:A:H62    | 1.36                     | 0.73              |
| 1:1A:2766:A:N3     | 31:19:15:LYS:NZ    | 2.33                     | 0.73              |
| 1:1A:215:G:N2      | 1:1A:217:A:H62     | 1.86                     | 0.73              |
| 3:1D:4:LYS:HB3     | 3:1D:18:VAL:HG23   | 1.69                     | 0.73              |
| 1:2A:1914:C:O2'    | 1:2A:1915:5MU:OP1  | 2.06                     | 0.73              |
| 26:24:59:PHE:HA    | 26:24:61:ARG:N     | 2.03                     | 0.73              |
| 4:1E:47:VAL:HG21   | 4:1E:86:PRO:HD2    | 1.70                     | 0.73              |
| 27:15:33:CYS:HB2   | 27:15:40:LYS:HD3   | 1.71                     | 0.73              |
| 1:1A:2701:U:H4'    | 1:1A:2702:C:H5'    | 1.71                     | 0.72              |
| 1:1A:1219:A:H1'    | 1:1A:1220:U:H5''   | 1.71                     | 0.72              |
| 1:2A:1514:U:H2'    | 1:2A:1515:G:H8     | 1.55                     | 0.72              |
| 7:2H:64:LEU:O      | 7:2H:68:THR:OG1    | 2.08                     | 0.72              |
| 1:1A:1218:G:O2'    | 1:1A:1219:A:O5'    | 2.06                     | 0.72              |
| 1:1A:215:G:H21     | 1:1A:217:A:H62     | 1.36                     | 0.72              |
| 1:2A:2144:U:OP1    | 1:2A:2145:C:N4     | 2.23                     | 0.72              |
| 1:2A:2224:G:OP1    | 3:2D:268:ARG:NE    | 2.23                     | 0.72              |
| 8:2I:4:ILE:HD11    | 8:2I:44:LEU:HD12   | 1.71                     | 0.72              |
| 1:2A:220:G:O2'     | 1:2A:233:A:N3      | 2.20                     | 0.71              |
| 5:1F:165:ARG:HA    | 5:1F:168:ARG:HD3   | 1.72                     | 0.71              |
| 5:1F:28:ILE:HG23   | 5:1F:112:MET:HB3   | 1.71                     | 0.71              |
| 1:1A:1005:A:N6     | 1:1A:1024:G:H21    | 30.49                    | 0.71              |
| 1:2A:1430:C:H42    | 1:2A:1563:G:H1     | 1.37                     | 0.71              |
| 1:2A:568:U:O2'     | 60:2A:4002:HOH:O   | 2.06                     | 0.71              |
| 1:1A:542:C:OP1     | 27:15:16:ARG:NH2   | 2.24                     | 0.71              |
| 5:1F:157:VAL:HB    | 5:1F:194:MET:HG2   | 1.71                     | 0.71              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 13:1R:3:HIS:NE2   | 60:1R:301:HOH:O   | 2.23                     | 0.71              |
| 13:2R:57:ARG:NE   | 13:2R:59:ASP:OD2  | 2.21                     | 0.71              |
| 1:2A:1842:G:O2'   | 3:2D:253:GLN:NE2  | 2.24                     | 0.70              |
| 1:2A:1798:U:OP2   | 3:2D:274:ARG:NH2  | 2.24                     | 0.70              |
| 1:2A:2180:U:H2'   | 1:2A:2181:G:C8    | 2.26                     | 0.70              |
| 1:2A:2207:G:O2'   | 1:2A:2208:A:OP1   | 2.09                     | 0.70              |
| 1:2A:2552:OMU:C6  | 1:2A:2552:OMU:C4  | 2.46                     | 0.70              |
| 28:26:43:CYS:HB3  | 28:26:45:LYS:HE2  | 1.73                     | 0.70              |
| 1:1A:2228:G:O2'   | 1:1A:2229:A:OP1   | 2.09                     | 0.70              |
| 25:13:29:ARG:HG3  | 25:13:30:ARG:HG3  | 1.74                     | 0.70              |
| 1:1A:1005:A:C5    | 1:1A:1024:G:N2    | 28.23                    | 0.70              |
| 1:2A:272(G):C:N4  | 1:2A:363(C):G:H1  | 1.90                     | 0.70              |
| 27:25:16:ARG:NH1  | 27:25:17:ASP:OD1  | 2.24                     | 0.70              |
| 1:2A:79:G:N2      | 1:2A:90:U:O2      | 30.88                    | 0.70              |
| 1:1A:656:A:OP1    | 11:1P:65:ARG:NH1  | 2.25                     | 0.69              |
| 1:1A:922:G:H1     | 1:1A:948:C:N4     | 1.89                     | 0.69              |
| 1:2A:652(T):C:H2' | 1:2A:652(U):G:C8  | 2.27                     | 0.69              |
| 1:2A:2302:G:N2    | 6:2G:126:ASP:OD1  | 2.24                     | 0.69              |
| 8:2I:130:TYR:HB3  | 8:2I:138:ILE:HB   | 1.72                     | 0.69              |
| 1:1A:2695:C:O2    | 10:1O:70:LYS:NZ   | 2.19                     | 0.69              |
| 1:2A:817:C:N4     | 1:2A:1529:G:H1    | 114.24                   | 0.69              |
| 14:1S:27:SER:HA   | 14:1S:88:ASP:HB3  | 1.73                     | 0.69              |
| 6:1G:15:VAL:HG22  | 6:1G:175:LEU:HB3  | 1.74                     | 0.69              |
| 18:2W:65:LEU:HD12 | 18:2W:68:ARG:HE   | 1.56                     | 0.69              |
| 1:2A:2357:U:OP1   | 22:20:20:ARG:NE   | 2.23                     | 0.69              |
| 13:1R:67:LEU:HD13 | 13:1R:76:VAL:HG21 | 1.75                     | 0.69              |
| 11:1P:59:LEU:HD11 | 30:18:10:ALA:HB2  | 1.75                     | 0.68              |
| 30:28:33:ASN:HA   | 30:28:36:LYS:HD2  | 1.75                     | 0.68              |
| 1:2A:2206:G:H3'   | 1:2A:2207:G:H8    | 1.58                     | 0.68              |
| 1:1A:2658:C:OP2   | 1:1A:2745:G:O2'   | 2.11                     | 0.68              |
| 1:2A:2143:C:N3    | 1:2A:2148:G:O6    | 2.26                     | 0.68              |
| 1:1A:1085:G:N2    | 1:1A:1162:C:N3    | 2.37                     | 0.68              |
| 16:2U:85:LYS:HB3  | 16:2U:116:ALA:HB1 | 1.73                     | 0.68              |
| 1:1A:268:G:HO2'   | 1:1A:269:G:H8     | 1.41                     | 0.68              |
| 1:1A:2183:C:H2'   | 1:1A:2184:G:H5''  | 1.76                     | 0.68              |
| 1:2A:1062:G:N7    | 1:2A:1070:A:H1'   | 2.08                     | 0.68              |
| 24:22:35:LEU:HD21 | 24:22:49:LYS:HE2  | 1.75                     | 0.68              |
| 1:2A:1286:A:H2'   | 1:2A:1287:A:H4'   | 6.71                     | 0.68              |
| 1:2A:2689:U:H4'   | 1:2A:2690:C:H5'   | 1.75                     | 0.68              |
| 1:1A:268:G:O2'    | 1:1A:269:G:H8     | 1.77                     | 0.68              |
| 1:2A:2134:A:N6    | 1:2A:2156:G:O2'   | 2.22                     | 0.68              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:1A:2081:A:H2'   | 1:1A:2515:2MA:HM23 | 1.76                     | 0.67              |
| 6:2G:41:GLN:HB3   | 6:2G:43:LEU:HD22   | 1.74                     | 0.67              |
| 1:1A:921:G:H1     | 1:1A:949:C:H42     | 1.42                     | 0.67              |
| 1:1A:2304:C:OP1   | 14:1S:17:ARG:NH2   | 2.27                     | 0.67              |
| 3:1D:17:THR:O     | 3:1D:211:ARG:NH2   | 2.26                     | 0.67              |
| 1:2A:1245:G:OP1   | 11:2P:13:ASN:ND2   | 2.23                     | 0.67              |
| 7:1H:7:LEU:HD12   | 7:1H:8:PRO:HD2     | 1.75                     | 0.67              |
| 26:24:41:PRO:HG3  | 26:24:49:PHE:HE2   | 1.59                     | 0.67              |
| 8:2I:3:VAL:HG12   | 8:2I:38:LEU:HA     | 1.75                     | 0.67              |
| 8:1I:72:LEU:O     | 8:1I:74:ASN:N      | 2.26                     | 0.67              |
| 1:1A:467:U:O2     | 5:1F:46:ARG:NH2    | 2.27                     | 0.67              |
| 1:2A:2134:A:O2'   | 1:2A:2159:G:N3     | 2.27                     | 0.67              |
| 12:1Q:45:GLN:N    | 12:1Q:45:GLN:OE1   | 2.28                     | 0.67              |
| 1:1A:1700:G:H3'   | 13:1R:2:ARG:HD3    | 1.77                     | 0.67              |
| 6:1G:67:LYS:HD3   | 26:14:5:ILE:HB     | 1.77                     | 0.66              |
| 1:1A:1405:A:H61   | 1:1A:1418:U:H3     | 0.73                     | 0.66              |
| 1:1A:2391:G:O2'   | 14:1S:17:ARG:NH1   | 2.28                     | 0.66              |
| 12:2Q:39:PRO:HD3  | 12:2Q:99:PRO:HG3   | 1.77                     | 0.66              |
| 1:1A:1085:G:H1    | 1:1A:1162:C:H42    | 0.70                     | 0.66              |
| 22:10:10:THR:HG22 | 22:10:12:ASN:H     | 1.60                     | 0.66              |
| 29:17:24:THR:HG22 | 29:17:27:GLY:H     | 1.61                     | 0.66              |
| 1:2A:1065:U:O2'   | 1:2A:1066:U:OP2    | 2.11                     | 0.66              |
| 1:2A:2445:G:OP1   | 5:2F:74:ARG:NH2    | 2.29                     | 0.66              |
| 6:2G:122:PRO:HB3  | 6:2G:170:ARG:HH12  | 1.59                     | 0.66              |
| 1:1A:1346:U:H4'   | 1:1A:1347:A:H5''   | 1.78                     | 0.66              |
| 27:25:40:LYS:NZ   | 27:25:44:THR:O     | 2.23                     | 0.66              |
| 1:2A:1073:A:H2'   | 1:2A:1074:G:C8     | 2.29                     | 0.66              |
| 1:2A:1607:C:N4    | 1:2A:1622:G:OP2    | 2.26                     | 0.66              |
| 1:1A:2877:G:OP2   | 15:1T:119:LYS:NZ   | 2.23                     | 0.66              |
| 23:11:76:ARG:HB3  | 23:11:97:LEU:HD13  | 1.76                     | 0.66              |
| 1:1A:611:U:H2'    | 1:1A:612:C:C6      | 2.30                     | 0.66              |
| 1:1A:1873:G:O2'   | 3:1D:253:GLN:NE2   | 2.29                     | 0.66              |
| 1:1A:976:G:H5'    | 1:1A:1358:U:O2'    | 103.46                   | 0.66              |
| 15:1T:54:ARG:HA   | 15:1T:59:THR:HG22  | 1.78                     | 0.66              |
| 1:2A:864:G:H1'    | 1:2A:914:C:H42     | 1.61                     | 0.66              |
| 13:2R:97:VAL:HG22 | 13:2R:114:VAL:HG22 | 1.78                     | 0.66              |
| 6:1G:136:ARG:HB2  | 6:1G:136:ARG:HH11  | 1.60                     | 0.66              |
| 1:1A:1261:G:OP2   | 16:1U:12:ARG:NH2   | 2.25                     | 0.66              |
| 1:2A:2111:C:N4    | 1:2A:2147:G:H22    | 1.94                     | 0.66              |
| 1:1A:2762:A:OP1   | 7:1H:3:ARG:NH1     | 2.30                     | 0.65              |
| 8:1I:77:LEU:HD12  | 8:1I:104:GLN:HE21  | 1.60                     | 0.65              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:2A:2483:C:N3    | 12:2Q:124:LYS:NZ   | 2.41                     | 0.65              |
| 4:2E:174:ASP:OD1  | 4:2E:175:VAL:N     | 2.29                     | 0.65              |
| 13:2R:103:ARG:NH1 | 13:2R:108:GLY:O    | 2.29                     | 0.65              |
| 1:2A:106:C:H1'    | 20:2Y:1:MET:HG3    | 1.78                     | 0.65              |
| 1:1A:2149:G:H21   | 1:1A:2195:A:H1'    | 1.61                     | 0.65              |
| 1:2A:2059:A:H2'   | 1:2A:2503:2MA:HM23 | 1.77                     | 0.65              |
| 1:2A:1066:U:O2'   | 1:2A:1067:A:H5''   | 1.96                     | 0.65              |
| 5:1F:53:THR:HG23  | 5:1F:55:GLY:H      | 1.61                     | 0.65              |
| 24:22:65:ASN:OD1  | 24:22:69:ARG:NH1   | 2.30                     | 0.65              |
| 1:2A:1064:C:H3'   | 1:2A:1065:U:C5'    | 2.25                     | 0.65              |
| 1:2A:2849:U:O4    | 15:2T:23:ARG:NH2   | 2.29                     | 0.65              |
| 3:2D:69:ARG:NH2   | 3:2D:128:GLY:O     | 2.20                     | 0.65              |
| 4:2E:52:LEU:HB3   | 4:2E:53:PRO:HD2    | 1.79                     | 0.65              |
| 1:1A:1117:G:H1'   | 1:1A:1135:G:H2'    | 1.77                     | 0.65              |
| 1:2A:2218:U:O4'   | 23:21:52:ARG:NH2   | 2.23                     | 0.64              |
| 1:2A:2638:G:P     | 4:2E:82:ARG:HH12   | 2.20                     | 0.64              |
| 1:2A:1041:C:N3    | 1:2A:1114:G:N2     | 2.37                     | 0.64              |
| 5:2F:157:VAL:HB   | 5:2F:194:MET:HG2   | 1.78                     | 0.64              |
| 14:2S:27:SER:HA   | 14:2S:88:ASP:HB3   | 1.78                     | 0.64              |
| 1:1A:1219:A:H4'   | 1:1A:1220:U:OP1    | 1.98                     | 0.64              |
| 1:2A:2186:G:H2'   | 1:2A:2187:G:H5''   | 1.79                     | 0.64              |
| 1:2A:276:A:H5''   | 1:2A:277:C:H5'     | 1.80                     | 0.64              |
| 7:2H:159:GLU:HG3  | 7:2H:169:VAL:HG11  | 1.79                     | 0.64              |
| 1:2A:2313:C:H5''  | 6:2G:91:ARG:HD3    | 1.80                     | 0.64              |
| 21:2Z:10:ARG:NH1  | 21:2Z:26:GLY:O     | 2.31                     | 0.64              |
| 1:2A:362:U:O2'    | 1:2A:363:G:H5''    | 1.98                     | 0.64              |
| 26:14:61:ARG:HG3  | 26:14:62:ARG:H     | 1.63                     | 0.64              |
| 1:2A:2012:G:OP1   | 18:2W:11:ARG:NH2   | 2.30                     | 0.64              |
| 1:2A:2291:U:H2'   | 1:2A:2292:C:C6     | 2.33                     | 0.64              |
| 1:2A:958:U:OP2    | 12:2Q:14:ARG:NH1   | 2.31                     | 0.64              |
| 4:1E:9:VAL:HB     | 15:1T:3:ARG:HG2    | 1.80                     | 0.64              |
| 22:20:10:THR:HG22 | 22:20:12:ASN:H     | 1.62                     | 0.64              |
| 1:2A:2327:A:H2'   | 1:2A:2328:A:C8     | 2.32                     | 0.64              |
| 1:1A:1094:A:OP2   | 1:1A:1155:C:N4     | 2.32                     | 0.63              |
| 1:1A:2642:G:H21   | 1:1A:2901:A:H1'    | 1.62                     | 0.63              |
| 15:1T:55:ASN:H    | 15:1T:59:THR:HG22  | 1.63                     | 0.63              |
| 1:2A:2573:C:C2    | 20:2Y:2:ARG:HG3    | 100.24                   | 0.63              |
| 1:2A:856:C:H2'    | 1:2A:857:C:C6      | 2.34                     | 0.63              |
| 12:2Q:45:GLN:N    | 12:2Q:45:GLN:OE1   | 2.30                     | 0.63              |
| 1:1A:85:C:H4'     | 1:1A:102:U:H1'     | 1.80                     | 0.63              |
| 6:1G:27:ASN:HB3   | 6:1G:30:GLU:HG3    | 1.80                     | 0.63              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 3:2D:206:LEU:HD22 | 3:2D:211:ARG:HG2   | 1.80                     | 0.63              |
| 4:2E:98:PRO:HG3   | 4:2E:174:ASP:HA    | 1.81                     | 0.63              |
| 4:2E:9:VAL:HB     | 15:2T:3:ARG:HG2    | 1.80                     | 0.63              |
| 1:1A:1474:C:O2'   | 1:1A:1616:A:OP2    | 2.14                     | 0.63              |
| 7:1H:40:GLU:OE1   | 7:1H:61:HIS:NE2    | 2.30                     | 0.63              |
| 19:1X:60:ARG:HH22 | 29:17:47:ARG:HH12  | 1.46                     | 0.63              |
| 1:2A:1202:C:N4    | 1:2A:1243:G:H1     | 1.95                     | 0.63              |
| 1:2A:2547:U:O2    | 10:2O:23:ARG:NH2   | 2.27                     | 0.63              |
| 12:2Q:111:GLU:O   | 12:2Q:115:MET:HG2  | 1.98                     | 0.63              |
| 26:14:56:VAL:HB   | 26:14:60:GLN:HG2   | 1.81                     | 0.63              |
| 1:2A:301:G:OP2    | 20:2Y:84:ARG:NH2   | 2.32                     | 0.63              |
| 1:1A:2457:G:OP1   | 5:1F:74:ARG:NH2    | 2.32                     | 0.63              |
| 1:2A:530:G:N1     | 1:2A:2023:G:OP1    | 2.27                     | 0.62              |
| 1:1A:2757:G:N2    | 7:1H:143:GLN:OE1   | 2.32                     | 0.62              |
| 22:20:27:GLU:HG3  | 22:20:68:GLU:HA    | 1.79                     | 0.62              |
| 4:2E:47:VAL:HG11  | 4:2E:86:PRO:HD2    | 1.81                     | 0.62              |
| 3:2D:108:PRO:HB3  | 3:2D:143:HIS:HE1   | 1.63                     | 0.62              |
| 20:2Y:77:PRO:HD2  | 20:2Y:106:LEU:HD23 | 1.81                     | 0.62              |
| 20:2Y:87:LYS:HB3  | 20:2Y:95:LYS:HD2   | 1.81                     | 0.62              |
| 1:1A:2156:A:H1'   | 1:1A:2180:A:H1'    | 1.80                     | 0.62              |
| 3:1D:147:LEU:HD13 | 3:1D:155:LEU:HD11  | 1.81                     | 0.62              |
| 1:2A:2206:G:H3'   | 1:2A:2207:G:C8     | 2.34                     | 0.62              |
| 1:1A:2160:C:H2'   | 1:1A:2161:C:C6     | 2.35                     | 0.62              |
| 5:2F:24:LEU:HD23  | 5:2F:115:ALA:HA    | 1.82                     | 0.62              |
| 1:2A:528:A:OP2    | 9:2N:114:ARG:NH2   | 2.32                     | 0.62              |
| 1:2A:1081:U:H2'   | 1:2A:1082:U:H5''   | 1.81                     | 0.62              |
| 1:2A:79:G:H1      | 1:2A:90:U:H3       | 29.54                    | 0.62              |
| 1:1A:1578:C:N3    | 1:1A:1585:G:N2     | 2.40                     | 0.62              |
| 1:1A:1147:U:H2'   | 1:1A:1148:C:C6     | 2.34                     | 0.62              |
| 2:2B:5:C:OP1      | 2:2B:61:G:O2'      | 2.15                     | 0.62              |
| 1:1A:2303:U:H2'   | 1:1A:2304:C:C6     | 2.35                     | 0.61              |
| 8:2I:72:LEU:HD21  | 8:2I:107:VAL:HG11  | 1.81                     | 0.61              |
| 8:1I:31:LEU:HD21  | 8:1I:38:LEU:HD13   | 1.81                     | 0.61              |
| 1:2A:1216:G:OP2   | 16:2U:12:ARG:NH2   | 2.26                     | 0.61              |
| 1:2A:2753:A:N3    | 31:29:15:LYS:NZ    | 2.48                     | 0.61              |
| 1:1A:1087:C:N4    | 1:1A:1160:G:H1     | 1.99                     | 0.61              |
| 1:1A:630:U:OP1    | 5:1F:102:PRO:HA    | 2.00                     | 0.61              |
| 1:1A:559:U:O2'    | 16:1U:49:HIS:ND1   | 2.24                     | 0.61              |
| 1:2A:2561:A:H2    | 10:2O:23:ARG:HH21  | 1.49                     | 0.61              |
| 1:1A:941:U:H5'    | 1:1A:942:A:OP2     | 2.00                     | 0.61              |
| 26:24:34:GLU:HG2  | 26:24:35:VAL:HG12  | 1.82                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:2B:39:A:O2'     | 2:2B:46:A:N1      | 2.33                     | 0.61              |
| 21:2Z:19:ARG:NH1  | 21:2Z:84:GLU:O    | 2.32                     | 0.61              |
| 1:1A:2149:G:OP2   | 1:1A:2184:G:N2    | 2.32                     | 0.61              |
| 16:1U:83:LEU:HD12 | 16:1U:113:ALA:HB2 | 1.82                     | 0.61              |
| 1:1A:2585:C:C2    | 20:1Y:2:ARG:HG3   | 99.66                    | 0.61              |
| 25:13:3:ARG:NH1   | 25:13:60:GLU:OE2  | 2.34                     | 0.61              |
| 1:1A:1435:G:H2'   | 1:1A:1436:U:C6    | 2.96                     | 0.61              |
| 1:1A:555:G:N1     | 1:1A:2045:G:OP1   | 2.28                     | 0.61              |
| 8:1I:9:LEU:HD11   | 8:1I:35:LEU:HD13  | 1.82                     | 0.61              |
| 1:1A:2897:U:H2'   | 1:1A:2898:C:H6    | 1.66                     | 0.61              |
| 11:1P:121:LYS:O   | 11:1P:123:LEU:N   | 2.34                     | 0.61              |
| 1:2A:577:G:O2'    | 1:2A:1254:A:OP1   | 2.17                     | 0.61              |
| 1:2A:607:U:OP1    | 5:2F:102:PRO:HA   | 1.99                     | 0.61              |
| 1:1A:1451:U:H2'   | 1:1A:1452:U:C6    | 2.35                     | 0.61              |
| 1:1A:769:A:H2'    | 1:1A:770:G:C8     | 2.36                     | 0.61              |
| 11:1P:95:VAL:HA   | 11:1P:99:LEU:HD12 | 1.82                     | 0.61              |
| 1:2A:2543:G:H21   | 1:2A:2646:C:H5''  | 1.65                     | 0.61              |
| 24:12:23:LYS:O    | 24:12:27:GLU:HG3  | 2.01                     | 0.61              |
| 1:1A:1071:G:C4    | 1:1A:1180:C:H1'   | 2.36                     | 0.61              |
| 1:1A:2163:G:H1    | 1:1A:2172:U:H3    | 1.48                     | 0.61              |
| 1:1A:2897:U:H2'   | 1:1A:2898:C:C6    | 2.36                     | 0.61              |
| 1:1A:2892:A:OP1   | 13:1R:96:ARG:NH1  | 2.33                     | 0.61              |
| 1:1A:2136:A:H2    | 1:1A:2189:U:HO2'  | 1.49                     | 0.60              |
| 7:1H:27:LYS:HG2   | 7:1H:32:GLU:HB3   | 1.83                     | 0.60              |
| 30:28:6:THR:HG22  | 30:28:63:PRO:HD2  | 1.83                     | 0.60              |
| 1:2A:1025:G:C4    | 1:2A:1135:C:H1'   | 2.35                     | 0.60              |
| 1:2A:2585:U:H4'   | 1:2A:2586:C:OP1   | 2.01                     | 0.60              |
| 5:2F:197:ASP:OD1  | 5:2F:198:ALA:N    | 2.33                     | 0.60              |
| 11:2P:91:PHE:O    | 11:2P:121:LYS:NZ  | 2.29                     | 0.60              |
| 1:2A:2319:G:N2    | 14:2S:3:ARG:HD3   | 2.16                     | 0.60              |
| 1:2A:271(K):U:O2  | 8:2I:50:ARG:NH2   | 2.34                     | 0.60              |
| 1:1A:331:G:H21    | 1:1A:354:A:H62    | 1.48                     | 0.60              |
| 1:2A:1069:A:H5'   | 1:2A:1096:A:H5'   | 1.84                     | 0.60              |
| 4:2E:14:ILE:HG13  | 4:2E:21:VAL:HG23  | 1.84                     | 0.60              |
| 2:2B:31:C:H4'     | 6:2G:29:TRP:CH2   | 2.36                     | 0.60              |
| 1:1A:406:G:N2     | 23:11:42:GLN:OE1  | 2.26                     | 0.60              |
| 1:2A:1268:A:H5'   | 60:2A:5440:HOH:O  | 2.01                     | 0.60              |
| 1:2A:2390:U:P     | 30:28:35:GLN:HE22 | 2.25                     | 0.60              |
| 1:2A:615:G:OP2    | 5:2F:43:LYS:NZ    | 2.29                     | 0.60              |
| 4:2E:98:PRO:HD3   | 4:2E:175:VAL:HG12 | 1.82                     | 0.60              |
| 6:2G:113:ARG:HD2  | 6:2G:140:ILE:HA   | 1.84                     | 0.60              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:1A:1110:C:H3'   | 1:1A:1111:U:C5'    | 2.31                     | 0.60              |
| 1:1A:1218:G:O2'   | 1:1A:1219:A:O4'    | 2.18                     | 0.60              |
| 11:2P:88:LEU:HD11 | 11:2P:114:ILE:HD12 | 1.83                     | 0.60              |
| 5:1F:10:PRO:HB3   | 5:1F:17:ARG:NH2    | 2.16                     | 0.60              |
| 3:2D:109:ASP:HB2  | 3:2D:197:GLY:HA2   | 1.83                     | 0.60              |
| 4:2E:28:ALA:HB3   | 4:2E:93:VAL:HG12   | 1.84                     | 0.60              |
| 1:1A:747:G:O2'    | 1:1A:1679:A:N3     | 2.25                     | 0.60              |
| 1:1A:302:A:H2'    | 1:1A:303:C:C6      | 2.36                     | 0.60              |
| 8:1I:109:ILE:HG13 | 8:1I:130:TYR:CZ    | 2.37                     | 0.60              |
| 9:1N:58:ASP:OD1   | 9:1N:58:ASP:N      | 2.34                     | 0.60              |
| 26:14:24:THR:OG1  | 26:14:25:TYR:N     | 2.35                     | 0.59              |
| 1:1A:2442:A:N3    | 1:1A:2442:A:H2'    | 2.17                     | 0.59              |
| 9:1N:73:THR:HG23  | 9:1N:82:LEU:HD11   | 1.83                     | 0.59              |
| 1:2A:153:C:OP2    | 23:21:92:LYS:NZ    | 2.35                     | 0.59              |
| 19:2X:11:PRO:HG2  | 19:2X:13:LEU:HD21  | 1.84                     | 0.59              |
| 21:2Z:108:PRO:HA  | 21:2Z:142:SER:HA   | 1.83                     | 0.59              |
| 22:10:27:GLU:HG3  | 22:10:68:GLU:HA    | 1.83                     | 0.59              |
| 1:2A:1420:U:O2'   | 1:2A:1421:G:OP1    | 2.19                     | 0.59              |
| 8:2I:62:LYS:HG2   | 8:2I:133:HIS:CD2   | 2.37                     | 0.59              |
| 1:1A:1116:A:C8    | 1:1A:1143:U:H4'    | 2.37                     | 0.59              |
| 1:1A:1410:G:N7    | 23:11:3:LYS:HE2    | 2.16                     | 0.59              |
| 1:2A:143:G:H4'    | 19:2X:35:THR:HG21  | 1.84                     | 0.59              |
| 21:2Z:40:ASP:HB3  | 21:2Z:43:GLU:HB2   | 1.85                     | 0.59              |
| 1:1A:1911:A:H2'   | 1:1A:1912:A:C8     | 2.37                     | 0.59              |
| 6:1G:60:LEU:HD23  | 6:1G:63:ILE:HD12   | 1.85                     | 0.59              |
| 7:1H:20:ALA:HB3   | 7:1H:23:ARG:HG3    | 1.83                     | 0.59              |
| 21:1Z:198:LYS:CB  | 21:1Z:202:GLU:HB2  | 2.27                     | 0.59              |
| 13:2R:33:ARG:NH2  | 27:25:57:VAL:O     | 2.30                     | 0.59              |
| 1:2A:1514:U:H2'   | 1:2A:1515:G:C8     | 2.36                     | 0.59              |
| 1:2A:624:C:H2'    | 1:2A:625:G:H8      | 2.69                     | 0.59              |
| 1:2A:1803:A:O2'   | 3:2D:259:THR:HG21  | 2.02                     | 0.59              |
| 1:2A:2785:C:OP1   | 4:2E:41:LYS:NZ     | 2.35                     | 0.59              |
| 1:2A:1028:A:N6    | 1:2A:1125:G:H2'    | 2.17                     | 0.59              |
| 9:2N:58:ASP:N     | 9:2N:58:ASP:OD1    | 2.35                     | 0.59              |
| 1:2A:2105:C:H42   | 1:2A:2184:G:H1     | 1.50                     | 0.59              |
| 6:2G:97:ASP:HA    | 6:2G:100:TRP:HD1   | 1.67                     | 0.59              |
| 1:2A:2748:A:H5'   | 7:2H:4:ILE:HD12    | 1.84                     | 0.59              |
| 1:2A:1007:C:OP1   | 9:2N:35:ARG:NH1    | 2.36                     | 0.59              |
| 6:2G:101:ILE:HG22 | 6:2G:105:LYS:HE2   | 1.85                     | 0.59              |
| 22:10:11:ARG:O    | 22:10:14:ARG:NH2   | 2.36                     | 0.59              |
| 1:1A:1318:A:H5''  | 14:1S:3:ARG:HH12   | 126.97                   | 0.59              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:1A:2155:G:C2    | 1:1A:2179:G:H2'    | 2.38                     | 0.59              |
| 6:1G:11:TYR:OH    | 6:1G:32:PRO:O      | 2.20                     | 0.59              |
| 7:1H:3:ARG:NH1    | 7:1H:4:ILE:H       | 2.00                     | 0.59              |
| 8:1I:4:ILE:HG12   | 8:1I:18:VAL:HG22   | 1.84                     | 0.59              |
| 1:1A:184:A:OP1    | 11:1P:46:LYS:NZ    | 2.35                     | 0.59              |
| 1:2A:1991:U:H2'   | 1:2A:1992:G:H5''   | 1.85                     | 0.59              |
| 1:2A:2115:G:H1'   | 1:2A:2171:A:N6     | 2.18                     | 0.59              |
| 1:2A:2406:U:OP1   | 1:2A:2411:A:N6     | 2.36                     | 0.59              |
| 21:2Z:99:TYR:HB3  | 21:2Z:123:ASP:HB2  | 1.85                     | 0.59              |
| 1:1A:2650:G:P     | 4:1E:82:ARG:HH12   | 2.25                     | 0.59              |
| 5:1F:185:ASP:HA   | 5:1F:188:ARG:HD3   | 1.85                     | 0.59              |
| 6:1G:77:ILE:HG22  | 6:1G:80:PHE:H      | 1.68                     | 0.59              |
| 18:1W:25:ARG:NH2  | 18:1W:74:ALA:O     | 2.26                     | 0.59              |
| 21:1Z:110:GLY:HA3 | 21:1Z:174:VAL:HG11 | 1.84                     | 0.59              |
| 1:2A:2126:A:H4'   | 1:2A:2127:G:O5'    | 2.01                     | 0.59              |
| 1:2A:2189:U:H2'   | 1:2A:2190:G:C8     | 2.37                     | 0.59              |
| 1:1A:142:G:H4'    | 19:1X:35:THR:HG21  | 1.83                     | 0.58              |
| 21:1Z:145:GLU:H   | 21:1Z:148:ASP:HB2  | 1.66                     | 0.58              |
| 4:2E:201:THR:HG23 | 4:2E:203:LYS:H     | 1.67                     | 0.58              |
| 6:2G:125:PHE:HB3  | 6:2G:166:ASP:CG    | 2.24                     | 0.58              |
| 26:24:41:PRO:HG3  | 26:24:49:PHE:CE2   | 2.37                     | 0.58              |
| 1:2A:2396:G:OP1   | 23:21:25:LYS:NZ    | 2.34                     | 0.58              |
| 1:2A:2526:G:H5'   | 1:2A:2742:C:O2'    | 2.04                     | 0.58              |
| 1:2A:481:G:O5'    | 20:2Y:47:LYS:NZ    | 2.30                     | 0.58              |
| 1:1A:2208:G:H2'   | 1:1A:2209:G:H5''   | 1.86                     | 0.58              |
| 1:1A:2320:G:O2'   | 1:1A:2322:A:N7     | 2.34                     | 0.58              |
| 21:1Z:118:GLN:N   | 21:1Z:173:ALA:O    | 2.36                     | 0.58              |
| 1:2A:671:C:N4     | 60:2A:4014:HOH:O   | 2.36                     | 0.58              |
| 21:2Z:153:SER:HB3 | 21:2Z:167:PRO:HB3  | 1.84                     | 0.58              |
| 1:1A:1513:G:HO2'  | 1:1A:1593:C:HO2'   | 1.34                     | 0.58              |
| 1:1A:196:A:H2'    | 1:1A:197:C:O4'     | 2.03                     | 0.58              |
| 20:1Y:17:SER:OG   | 20:1Y:71:LYS:NZ    | 2.28                     | 0.58              |
| 12:1Q:93:TYR:OH   | 21:1Z:194:PRO:HG2  | 2.03                     | 0.58              |
| 1:2A:952:G:OP1    | 12:2Q:16:ARG:NH2   | 2.36                     | 0.58              |
| 12:2Q:11:LYS:NZ   | 12:2Q:88:GLY:O     | 2.28                     | 0.58              |
| 1:1A:2108:U:H2'   | 1:1A:2109:G:C8     | 2.38                     | 0.58              |
| 1:1A:2904:U:H2'   | 1:1A:2905:C:C6     | 2.39                     | 0.58              |
| 1:1A:532:A:N6     | 1:1A:1206:G:O2'    | 79.98                    | 0.58              |
| 18:1W:65:LEU:HD12 | 18:1W:68:ARG:HE    | 1.69                     | 0.58              |
| 1:2A:2816:C:N4    | 60:2A:4013:HOH:O   | 2.35                     | 0.58              |
| 4:2E:121:ASN:ND2  | 60:2E:401:HOH:O    | 2.36                     | 0.58              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 5:2F:20:LEU:HD23  | 5:2F:22:ALA:HB2    | 1.86                     | 0.58              |
| 21:2Z:53:ILE:HG22 | 21:2Z:71:VAL:HB    | 1.85                     | 0.58              |
| 1:1A:10:G:N2      | 1:1A:2813:G:OP1    | 2.36                     | 0.58              |
| 21:1Z:128:VAL:HB  | 21:1Z:161:VAL:HG23 | 1.86                     | 0.58              |
| 1:2A:226:G:N2     | 1:2A:228:A:H62     | 2.02                     | 0.58              |
| 6:1G:170:ARG:NH1  | 6:1G:174:GLU:OE1   | 2.36                     | 0.58              |
| 23:21:83:GLU:N    | 23:21:83:GLU:OE1   | 2.37                     | 0.58              |
| 1:1A:2148:A:H4'   | 1:1A:2149:G:O5'    | 2.04                     | 0.58              |
| 6:1G:16:ARG:HG3   | 6:1G:16:ARG:HH11   | 1.69                     | 0.58              |
| 26:24:24:THR:OG1  | 26:24:25:TYR:N     | 2.36                     | 0.58              |
| 1:2A:1915:5MU:H3' | 1:2A:1916:A:H8     | 1.68                     | 0.58              |
| 1:2A:2163:C:OP2   | 1:2A:2164:C:N4     | 2.36                     | 0.58              |
| 1:1A:1825:U:H2'   | 1:1A:1826:C:C6     | 2.39                     | 0.58              |
| 1:2A:271(E):U:H2' | 1:2A:271(F):C:C6   | 2.39                     | 0.58              |
| 1:2A:76:C:H42     | 1:2A:93:G:H1       | 27.25                    | 0.58              |
| 9:1N:46:VAL:HG23  | 9:1N:48:MET:HG2    | 1.86                     | 0.58              |
| 1:1A:1261:G:P     | 16:1U:12:ARG:HH21  | 2.27                     | 0.58              |
| 17:1V:40:LEU:HB2  | 17:1V:46:VAL:HG13  | 1.86                     | 0.58              |
| 1:1A:142:G:H1'    | 19:1X:37:THR:HG21  | 1.85                     | 0.58              |
| 19:1X:40:LYS:HG3  | 19:1X:51:VAL:HB    | 1.84                     | 0.58              |
| 1:2A:1741:A:H2'   | 1:2A:1742:G:O4'    | 2.04                     | 0.58              |
| 1:2A:473:G:H2'    | 1:2A:474:G:H8      | 2.89                     | 0.57              |
| 1:2A:994:C:OP1    | 16:2U:53:ARG:NH2   | 2.36                     | 0.57              |
| 1:1A:2044:U:O2'   | 1:1A:2629:C:H5'    | 2.04                     | 0.57              |
| 8:2I:75:LEU:HD11  | 8:2I:105:HIS:ND1   | 2.19                     | 0.57              |
| 1:2A:2162:G:H4'   | 1:2A:2172:U:O2'    | 2.03                     | 0.57              |
| 25:23:8:LEU:HG    | 25:23:31:LEU:HD22  | 1.87                     | 0.57              |
| 1:2A:2430:A:H2'   | 1:2A:2430:A:N3     | 2.19                     | 0.57              |
| 1:2A:302:C:H42    | 1:2A:315:G:H1      | 1.51                     | 0.57              |
| 6:2G:47:LYS:HG3   | 6:2G:48:GLU:H      | 1.69                     | 0.57              |
| 1:1A:1091:A:H5'   | 1:1A:1092:A:H5''   | 1.87                     | 0.57              |
| 1:2A:2727:G:O2'   | 10:2O:70:LYS:NZ    | 2.38                     | 0.57              |
| 2:2B:40:U:H2'     | 26:24:2:LYS:HE3    | 1.85                     | 0.57              |
| 7:2H:59:ARG:O     | 7:2H:63:SER:OG     | 2.23                     | 0.57              |
| 8:1I:4:ILE:HD11   | 8:1I:44:LEU:HD13   | 1.85                     | 0.57              |
| 1:2A:2347:C:HO2'  | 28:26:21:TYR:HH    | 1.52                     | 0.57              |
| 3:2D:79:VAL:HG21  | 3:2D:111:LEU:HD11  | 1.85                     | 0.57              |
| 1:1A:2136:A:O2'   | 1:1A:2189:U:H5''   | 2.04                     | 0.57              |
| 1:1A:831:A:H5'    | 1:1A:832:G:OP1     | 2.05                     | 0.57              |
| 2:1B:59:A:N6      | 60:1B:3101:HOH:O   | 2.16                     | 0.57              |
| 7:1H:85:LYS:HE2   | 7:1H:142:GLY:HA2   | 1.87                     | 0.57              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:13:44:ARG:O     | 25:13:48:GLU:HG3   | 2.04                     | 0.57              |
| 1:1A:953:U:H4'     | 12:1Q:101:ARG:HH22 | 1.69                     | 0.57              |
| 11:1P:126:VAL:HG12 | 11:1P:148:LEU:HD11 | 1.87                     | 0.57              |
| 1:2A:1076:C:H4'    | 1:2A:1077:A:OP1    | 2.04                     | 0.57              |
| 1:2A:2189:U:H2'    | 1:2A:2190:G:H8     | 1.68                     | 0.57              |
| 26:14:57:GLU:HB2   | 26:14:58:ARG:HA    | 1.87                     | 0.57              |
| 12:1Q:37:LEU:HD21  | 12:1Q:130:LYS:HB2  | 1.86                     | 0.57              |
| 19:1X:53:LYS:HB3   | 19:1X:82:GLN:HB3   | 1.85                     | 0.57              |
| 1:2A:1006:C:N4     | 1:2A:1022:G:O6     | 13.29                    | 0.57              |
| 1:2A:2666:C:N4     | 7:2H:108:GLY:O     | 2.33                     | 0.57              |
| 11:1P:97:PRO:HA    | 11:1P:112:LEU:HD12 | 1.87                     | 0.57              |
| 1:1A:2710:U:H2'    | 1:1A:2711:C:C6     | 2.40                     | 0.56              |
| 1:1A:402:C:H2'     | 1:1A:403:C:C6      | 2.40                     | 0.56              |
| 1:1A:843:C:H2'     | 1:1A:844:C:C6      | 2.39                     | 0.56              |
| 1:2A:729:G:C6      | 3:2D:208:LYS:HB2   | 2.40                     | 0.56              |
| 1:1A:326:C:OP2     | 20:1Y:73:ARG:NH2   | 2.38                     | 0.56              |
| 1:1A:424:G:H2'     | 1:1A:425:G:H8      | 2.28                     | 0.56              |
| 9:1N:34:LEU:HD21   | 9:1N:120:LEU:HB2   | 1.87                     | 0.56              |
| 25:23:6:VAL:HG13   | 25:23:56:VAL:HG13  | 1.85                     | 0.56              |
| 7:2H:89:ILE:O      | 7:2H:129:THR:HG23  | 2.05                     | 0.56              |
| 1:2A:631:A:OP1     | 11:2P:65:ARG:NH1   | 2.37                     | 0.56              |
| 15:2T:22:PHE:HE1   | 15:2T:49:VAL:HG11  | 1.69                     | 0.56              |
| 26:14:16:CYS:SG    | 26:14:17:GLY:N     | 2.78                     | 0.56              |
| 1:1A:7:G:H2'       | 1:1A:8:A:O4'       | 2.05                     | 0.56              |
| 3:1D:242:ARG:HD2   | 3:1D:246:PRO:HG3   | 1.87                     | 0.56              |
| 1:2A:2129:C:N3     | 1:2A:2159:G:O6     | 2.38                     | 0.56              |
| 1:2A:2819:G:H1     | 1:2A:2827:C:H42    | 1.51                     | 0.56              |
| 1:1A:1055:A:OP2    | 9:1N:37:LYS:NZ     | 2.39                     | 0.56              |
| 3:1D:145:VAL:HG11  | 3:1D:175:LEU:HD11  | 1.86                     | 0.56              |
| 5:1F:8:GLN:HE22    | 5:1F:21:ALA:HB2    | 1.71                     | 0.56              |
| 11:1P:50:ARG:HD3   | 30:18:7:HIS:CD2    | 2.39                     | 0.56              |
| 1:1A:2858:G:H8     | 15:1T:97:ALA:HB2   | 1.70                     | 0.56              |
| 28:26:13:CYS:SG    | 28:26:47:THR:HG21  | 2.45                     | 0.56              |
| 1:2A:2001:A:H2'    | 1:2A:2002:G:C8     | 2.40                     | 0.56              |
| 1:2A:300:A:OP1     | 20:2Y:86:ARG:NH2   | 2.38                     | 0.56              |
| 1:1A:2348:A:H61    | 22:10:43:THR:CG2   | 2.18                     | 0.56              |
| 1:1A:242:C:OP2     | 30:18:5:LYS:NZ     | 2.27                     | 0.56              |
| 1:1A:673:G:H2'     | 1:1A:674:G:C8      | 3.07                     | 0.56              |
| 7:1H:137:ASP:HB3   | 7:1H:140:LYS:HB3   | 1.87                     | 0.56              |
| 1:2A:1525:G:H2'    | 1:2A:1526:G:C8     | 2.41                     | 0.56              |
| 1:2A:2657:A:O3'    | 7:2H:160:LYS:NZ    | 2.38                     | 0.56              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:13:10:LYS:NZ    | 25:13:15:TYR:OH    | 2.38                     | 0.56              |
| 1:1A:989:G:H5''    | 1:1A:990:A:O5'     | 2.05                     | 0.56              |
| 10:1O:115:VAL:HG13 | 10:1O:121:VAL:HG21 | 1.88                     | 0.56              |
| 1:2A:2110:G:OP1    | 1:2A:2118:U:N3     | 2.36                     | 0.56              |
| 1:1A:2236:G:OP1    | 3:1D:268:ARG:NE    | 2.39                     | 0.56              |
| 1:2A:2079:U:O3'    | 23:21:35:THR:OG1   | 2.24                     | 0.56              |
| 17:2V:52:VAL:HG23  | 17:2V:55:ALA:HB3   | 1.87                     | 0.56              |
| 23:11:64:ALA:HA    | 23:11:67:ILE:HG13  | 1.87                     | 0.56              |
| 1:1A:605:G:H2'     | 1:1A:606:G:C8      | 2.40                     | 0.56              |
| 4:1E:105:THR:OG1   | 4:1E:199:ARG:NH2   | 2.38                     | 0.56              |
| 26:24:46:GLN:HE21  | 26:24:48:ARG:HH22  | 1.53                     | 0.56              |
| 1:2A:453:C:O2      | 1:2A:457:A:O2'     | 2.23                     | 0.56              |
| 6:1G:62:LEU:HD13   | 26:14:28:LYS:HZ1   | 1.70                     | 0.56              |
| 3:1D:69:ARG:HE     | 3:1D:130:ALA:HB2   | 1.71                     | 0.56              |
| 11:2P:59:LEU:HD11  | 30:28:10:ALA:HB2   | 1.88                     | 0.56              |
| 1:2A:2137:C:H2'    | 1:2A:2138:C:O4'    | 2.05                     | 0.56              |
| 7:2H:33:LEU:HD11   | 7:2H:75:ALA:HB1    | 1.87                     | 0.56              |
| 12:2Q:29:PHE:O     | 21:2Z:122:ARG:NH2  | 2.38                     | 0.56              |
| 30:18:33:ASN:HA    | 30:18:36:LYS:HD2   | 1.88                     | 0.56              |
| 5:1F:56:GLU:OE1    | 5:1F:93:LYS:NZ     | 2.38                     | 0.56              |
| 1:2A:1155:A:H5''   | 16:2U:55:ARG:HD3   | 1.87                     | 0.56              |
| 1:2A:1165:U:H2'    | 1:2A:1166:C:C6     | 2.40                     | 0.56              |
| 1:2A:1442:G:H2'    | 1:2A:1442:G:N3     | 3.11                     | 0.56              |
| 1:2A:1996:C:H4'    | 1:2A:1997:G:OP1    | 2.05                     | 0.56              |
| 1:2A:2417:C:OP1    | 11:2P:65:ARG:NH2   | 2.38                     | 0.56              |
| 1:2A:332:A:O2'     | 1:2A:334:C:OP2     | 2.24                     | 0.56              |
| 15:2T:30:VAL:HG22  | 15:2T:86:ILE:HG12  | 1.88                     | 0.56              |
| 1:1A:1091:A:H1'    | 1:1A:1093:G:N3     | 2.21                     | 0.56              |
| 28:26:6:ARG:NH1    | 28:26:26:ASN:HB2   | 2.20                     | 0.56              |
| 1:2A:1063:G:H1     | 1:2A:1075:C:H42    | 1.54                     | 0.56              |
| 7:2H:17:VAL:HG22   | 7:2H:26:VAL:HG22   | 1.88                     | 0.56              |
| 2:1B:91:C:OP2      | 12:1Q:16:ARG:NH1   | 2.39                     | 0.55              |
| 6:1G:40:ASN:HB3    | 6:1G:156:ASP:HB2   | 1.87                     | 0.55              |
| 1:2A:857:C:H4'     | 22:20:23:VAL:HG21  | 1.89                     | 0.55              |
| 1:2A:2788:C:OP1    | 4:2E:61:ARG:NH2    | 2.39                     | 0.55              |
| 1:1A:2579:G:H2'    | 1:1A:2580:C:C6     | 2.41                     | 0.55              |
| 1:1A:1186:U:OP1    | 9:1N:25:ARG:NH1    | 2.39                     | 0.55              |
| 1:2A:1048:A:N1     | 1:2A:1112:G:O2'    | 2.33                     | 0.55              |
| 2:2B:5:C:H42       | 2:2B:116:G:H1      | 1.54                     | 0.55              |
| 1:2A:662:G:H5''    | 11:2P:16:ARG:HG2   | 1.88                     | 0.55              |
| 1:2A:1278:A:OP1    | 13:2R:36:THR:HG23  | 2.05                     | 0.55              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:1A:1219:A:H1'   | 1:1A:1220:U:C5'    | 2.36                     | 0.55              |
| 13:1R:97:VAL:HG22 | 13:1R:114:VAL:HG22 | 1.88                     | 0.55              |
| 20:1Y:87:LYS:HB3  | 20:1Y:95:LYS:HD2   | 1.89                     | 0.55              |
| 1:2A:2747:G:O6    | 1:2A:2755:C:H5''   | 2.06                     | 0.55              |
| 3:2D:108:PRO:HG2  | 3:2D:111:LEU:HB2   | 1.89                     | 0.55              |
| 14:2S:14:VAL:O    | 14:2S:18:ILE:HG12  | 2.06                     | 0.55              |
| 1:1A:1766:G:N2    | 1:1A:1768:U:OP2    | 2.40                     | 0.55              |
| 5:1F:183:VAL:O    | 5:1F:187:VAL:HG23  | 2.07                     | 0.55              |
| 1:2A:2128:C:H2'   | 1:2A:2129:C:H5''   | 1.89                     | 0.55              |
| 1:2A:2165:G:H2'   | 1:2A:2166:G:O4'    | 2.07                     | 0.55              |
| 1:1A:1091:A:H8    | 1:1A:1157:A:C6     | 2.25                     | 0.55              |
| 1:1A:138:G:H1     | 1:1A:225:C:N4      | 81.47                    | 0.55              |
| 1:1A:606:G:OP2    | 16:1U:10:ARG:NH1   | 2.39                     | 0.55              |
| 1:1A:1855:G:OP1   | 3:1D:52:ARG:NH1    | 2.39                     | 0.55              |
| 7:1H:72:ILE:O     | 7:1H:76:VAL:HG23   | 2.06                     | 0.55              |
| 1:2A:2693:A:H2'   | 1:2A:2694:G:H8     | 1.71                     | 0.55              |
| 1:1A:733:G:N2     | 1:1A:835:A:H61     | 2.05                     | 0.55              |
| 1:2A:1297:C:O2'   | 1:2A:1302:A:N1     | 2.34                     | 0.55              |
| 1:2A:1796:U:H2'   | 1:2A:1797:C:C6     | 2.42                     | 0.55              |
| 1:1A:1562:U:H2'   | 1:1A:1563:G:H8     | 1.72                     | 0.55              |
| 8:2I:77:LEU:HD21  | 8:2I:100:ALA:HB3   | 1.88                     | 0.55              |
| 1:1A:1889:G:N2    | 1:1A:1905:G:H2'    | 2.21                     | 0.55              |
| 7:1H:88:LEU:HD23  | 7:1H:130:ARG:HG3   | 1.89                     | 0.55              |
| 1:2A:2224:G:H4'   | 1:2A:2226:C:C2     | 2.41                     | 0.55              |
| 6:2G:173:LEU:HA   | 6:2G:176:LEU:HD12  | 1.88                     | 0.55              |
| 6:2G:55:LYS:HZ2   | 6:2G:153:ARG:HH22  | 1.55                     | 0.55              |
| 1:1A:1093:G:H2'   | 1:1A:1156:G:H22    | 1.71                     | 0.55              |
| 1:1A:240:A:C5     | 1:1A:241:G:H1'     | 2.41                     | 0.55              |
| 2:1B:91:C:H5'     | 12:1Q:18:LYS:HA    | 1.88                     | 0.55              |
| 7:1H:86:GLU:OE2   | 7:1H:132:ARG:NH2   | 2.40                     | 0.55              |
| 7:2H:149:ARG:NH1  | 7:2H:167:GLU:OE2   | 2.40                     | 0.55              |
| 14:2S:78:LEU:HD11 | 14:2S:108:GLY:O    | 2.07                     | 0.55              |
| 9:1N:72:TYR:HE2   | 9:1N:87:LEU:HD23   | 1.72                     | 0.54              |
| 21:1Z:58:VAL:HG12 | 21:1Z:68:PRO:HA    | 1.88                     | 0.54              |
| 1:1A:1114:G:C8    | 1:1A:1115:A:N7     | 2.76                     | 0.54              |
| 1:1A:2348:A:H61   | 22:10:43:THR:HG22  | 1.72                     | 0.54              |
| 1:1A:385:G:C6     | 1:1A:386:U:O4      | 2.60                     | 0.54              |
| 6:1G:16:ARG:HE    | 6:1G:31:VAL:HG21   | 1.71                     | 0.54              |
| 11:1P:90:ARG:HH11 | 11:1P:105:LEU:HD11 | 1.72                     | 0.54              |
| 15:1T:109:GLU:O   | 15:1T:113:LYS:HG2  | 2.07                     | 0.54              |
| 18:1W:18:ARG:NH1  | 18:1W:76:VAL:O     | 2.39                     | 0.54              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:2A:323:G:C8     | 5:2F:171:PRO:HG3   | 2.42                     | 0.54              |
| 1:1A:1142:A:OP2   | 1:1A:1142:A:H8     | 1.91                     | 0.54              |
| 1:2A:1430:C:N4    | 1:2A:1563:G:H1     | 2.02                     | 0.54              |
| 1:2A:2119:A:H61   | 1:2A:2168:G:H21    | 0.65                     | 0.54              |
| 1:2A:984:A:H5''   | 1:2A:985:C:H5      | 1.72                     | 0.54              |
| 4:2E:116:VAL:HG13 | 4:2E:122:PHE:HB2   | 1.88                     | 0.54              |
| 7:2H:90:LYS:NZ    | 7:2H:159:GLU:OE2   | 2.40                     | 0.54              |
| 12:2Q:55:VAL:HG11 | 21:2Z:183:LEU:HD21 | 1.89                     | 0.54              |
| 1:1A:1068:G:OP2   | 1:1A:1068:G:H8     | 6.98                     | 0.54              |
| 1:1A:591:U:O2'    | 60:1A:9004:HOH:O   | 2.18                     | 0.54              |
| 17:1V:43:GLU:N    | 17:1V:43:GLU:OE1   | 2.40                     | 0.54              |
| 1:2A:1210:A:O2'   | 60:2A:4005:HOH:O   | 2.17                     | 0.54              |
| 1:2A:207:A:H2'    | 1:2A:208:C:O4'     | 2.08                     | 0.54              |
| 1:1A:1288:A:N1    | 1:1A:1371:G:H1'    | 71.69                    | 0.54              |
| 1:2A:1034:G:H5'   | 31:29:18:ARG:HD3   | 1.90                     | 0.54              |
| 11:2P:97:PRO:HD3  | 11:2P:126:VAL:O    | 2.06                     | 0.54              |
| 1:1A:1539:C:H5    | 1:1A:2227:G:HO2'   | 1.55                     | 0.54              |
| 1:1A:2418:U:H2'   | 1:1A:2418:U:OP2    | 2.07                     | 0.54              |
| 4:1E:7:VAL:HG12   | 4:1E:27:LEU:HB3    | 1.90                     | 0.54              |
| 1:1A:509:A:H5''   | 20:1Y:50:ARG:HD3   | 1.89                     | 0.54              |
| 1:2A:1200:C:H5'   | 60:2A:4003:HOH:O   | 2.08                     | 0.54              |
| 1:2A:1412:A:H2'   | 1:2A:1413:G:C8     | 2.42                     | 0.54              |
| 1:2A:1792:G:O2'   | 1:2A:1830:C:OP1    | 2.25                     | 0.54              |
| 1:2A:2641:G:P     | 9:2N:74:ARG:HH22   | 2.31                     | 0.54              |
| 14:2S:46:VAL:HG12 | 14:2S:48:LEU:HD12  | 1.90                     | 0.54              |
| 15:2T:60:THR:HG22 | 15:2T:77:PRO:HA    | 1.90                     | 0.54              |
| 20:2Y:20:TYR:CE2  | 20:2Y:43:ASN:HA    | 2.42                     | 0.54              |
| 1:1A:1827:U:H2'   | 1:1A:1828:C:C6     | 2.42                     | 0.54              |
| 1:1A:2155:G:HO2'  | 1:1A:2180:A:H2     | 1.56                     | 0.54              |
| 1:1A:2250:G:H2'   | 1:1A:2250:G:N3     | 2.23                     | 0.54              |
| 7:1H:12:PRO:O     | 7:1H:15:VAL:HG13   | 2.07                     | 0.54              |
| 9:1N:67:LEU:HD12  | 9:1N:87:LEU:HD12   | 1.88                     | 0.54              |
| 10:1O:68:GLU:HB3  | 10:1O:78:ARG:HD3   | 1.90                     | 0.54              |
| 21:1Z:182:LYS:O   | 21:1Z:185:GLU:HG3  | 2.07                     | 0.54              |
| 1:2A:1069:A:H5'   | 1:2A:1096:A:C5'    | 2.38                     | 0.54              |
| 17:2V:5:VAL:HG11  | 17:2V:57:VAL:HG21  | 1.90                     | 0.54              |
| 1:1A:167:G:H2'    | 1:1A:168:G:H8      | 2.37                     | 0.54              |
| 1:1A:599:U:H2'    | 1:1A:600:G:C8      | 2.43                     | 0.54              |
| 9:1N:9:VAL:HG21   | 9:1N:39:ARG:NH2    | 2.22                     | 0.54              |
| 1:2A:1072:C:N4    | 1:2A:1093:G:H1     | 2.06                     | 0.54              |
| 1:2A:579:G:H2'    | 1:2A:580:C:C6      | 2.42                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:2B:16:G:N2      | 2:2B:68:C:N3      | 2.44                     | 0.54              |
| 5:2F:185:ASP:HA   | 5:2F:188:ARG:HD3  | 1.89                     | 0.54              |
| 9:2N:34:LEU:HD21  | 9:2N:120:LEU:HB2  | 1.90                     | 0.54              |
| 1:1A:2149:G:N2    | 1:1A:2195:A:H1'   | 2.23                     | 0.54              |
| 1:1A:2340:A:H2'   | 1:1A:2341:G:C8    | 2.43                     | 0.54              |
| 1:1A:265:U:H2'    | 1:1A:266:C:C6     | 2.43                     | 0.54              |
| 1:2A:1300:U:H4'   | 1:2A:1301:A:H5'   | 1.89                     | 0.54              |
| 1:2A:1946:U:H2'   | 1:2A:1947:C:C6    | 2.43                     | 0.54              |
| 1:2A:807:U:OP2    | 11:2P:41:ARG:NH2  | 2.40                     | 0.54              |
| 6:2G:139:LEU:HD21 | 6:2G:152:LEU:HD23 | 1.90                     | 0.54              |
| 8:2I:101:LEU:HD21 | 8:2I:140:LEU:HD11 | 1.89                     | 0.54              |
| 6:1G:142:PRO:HB2  | 26:14:31:ILE:HG21 | 1.90                     | 0.53              |
| 1:1A:965:G:N2     | 1:1A:2281:A:OP2   | 2.41                     | 0.53              |
| 15:1T:22:PHE:CE1  | 15:1T:49:VAL:HG11 | 2.42                     | 0.53              |
| 1:2A:1786:A:H1'   | 1:2A:1938:A:N6    | 2.24                     | 0.53              |
| 1:2A:2155:G:H2'   | 1:2A:2156:G:O4'   | 2.07                     | 0.53              |
| 1:2A:2315:G:H2'   | 1:2A:2316:C:C6    | 2.42                     | 0.53              |
| 1:2A:2438:U:O2'   | 1:2A:2440:C:OP1   | 2.16                     | 0.53              |
| 2:2B:18:G:H1      | 2:2B:65:C:N4      | 2.02                     | 0.53              |
| 6:2G:166:ASP:O    | 6:2G:170:ARG:N    | 2.40                     | 0.53              |
| 30:28:26:LYS:HE3  | 30:28:46:ARG:HH12 | 1.72                     | 0.53              |
| 12:2Q:16:ARG:HG3  | 12:2Q:17:LEU:H    | 1.74                     | 0.53              |
| 13:2R:26:LYS:HE2  | 13:2R:70:LEU:O    | 2.08                     | 0.53              |
| 9:1N:67:LEU:O     | 9:1N:88:GLU:HG3   | 2.08                     | 0.53              |
| 1:2A:1789:A:N6    | 60:2A:4018:HOH:O  | 2.42                     | 0.53              |
| 1:2A:1835:G:H5'   | 1:2A:1836:C:OP2   | 2.08                     | 0.53              |
| 1:1A:1211:U:H2'   | 1:1A:1212:C:C6    | 2.43                     | 0.53              |
| 6:1G:67:LYS:H     | 26:14:6:HIS:CE1   | 2.26                     | 0.53              |
| 6:1G:79:ASN:N     | 6:1G:79:ASN:OD1   | 2.42                     | 0.53              |
| 14:1S:14:VAL:O    | 14:1S:18:ILE:HG12 | 2.08                     | 0.53              |
| 1:2A:1078:U:O2'   | 1:2A:1079:C:OP2   | 2.26                     | 0.53              |
| 1:2A:2296:U:OP2   | 14:2S:9:ARG:NH2   | 2.42                     | 0.53              |
| 2:2B:22:U:H3      | 2:2B:61:G:H1      | 1.56                     | 0.53              |
| 14:2S:66:ALA:O    | 14:2S:69:VAL:HG12 | 2.08                     | 0.53              |
| 1:1A:2185:C:OP2   | 1:1A:2186:C:N4    | 2.40                     | 0.53              |
| 8:1I:57:ARG:O     | 8:1I:61:ARG:HG2   | 2.09                     | 0.53              |
| 25:23:5:LYS:HG3   | 25:23:36:VAL:HG22 | 1.90                     | 0.53              |
| 1:2A:1579:A:H2'   | 1:2A:1580:A:C8    | 2.44                     | 0.53              |
| 19:1X:60:ARG:NH1  | 29:17:47:ARG:HH22 | 2.04                     | 0.53              |
| 1:1A:1117:G:H4'   | 1:1A:1135:G:OP2   | 2.09                     | 0.53              |
| 1:1A:2339:A:H2'   | 1:1A:2340:A:C8    | 2.42                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1A:2801:C:O2'   | 1:1A:2819:A:N3    | 2.40                     | 0.53              |
| 16:1U:76:TYR:CZ   | 16:1U:80:ILE:HG13 | 2.43                     | 0.53              |
| 1:2A:61:G:OP1     | 24:22:51:ARG:NH1  | 2.41                     | 0.53              |
| 1:1A:1005:A:N6    | 1:1A:1024:G:C2    | 30.82                    | 0.53              |
| 1:1A:1085:G:N1    | 1:1A:1162:C:N4    | 2.16                     | 0.53              |
| 5:1F:95:ARG:HD3   | 5:1F:97:TYR:CZ    | 2.43                     | 0.53              |
| 18:1W:67:ASP:N    | 18:1W:67:ASP:OD1  | 2.41                     | 0.53              |
| 1:2A:1071:G:N2    | 60:2A:4017:HOH:O  | 2.42                     | 0.53              |
| 1:1A:1139:G:C2'   | 1:1A:1144:A:H61   | 2.22                     | 0.53              |
| 15:1T:96:ARG:HH11 | 15:1T:96:ARG:HB2  | 1.74                     | 0.53              |
| 17:1V:72:VAL:HG13 | 17:1V:85:LYS:HB3  | 1.90                     | 0.53              |
| 1:2A:1153:C:H2'   | 1:2A:1154:G:O4'   | 2.09                     | 0.53              |
| 1:2A:606:U:H4'    | 1:2A:658:C:H4'    | 1.91                     | 0.53              |
| 4:2E:36:ARG:HG2   | 4:2E:47:VAL:HG12  | 1.90                     | 0.53              |
| 21:2Z:30:ASN:ND2  | 21:2Z:90:VAL:HB   | 2.23                     | 0.53              |
| 20:1Y:92:ASN:N    | 20:1Y:93:GLY:HA2  | 2.23                     | 0.53              |
| 1:2A:581:C:H2'    | 1:2A:582:G:C8     | 2.44                     | 0.53              |
| 1:2A:793:A:OP2    | 1:2A:2071:A:O2'   | 2.26                     | 0.53              |
| 25:13:3:ARG:HD3   | 25:13:60:GLU:CD   | 2.29                     | 0.53              |
| 1:1A:1525:G:O2'   | 1:1A:1605:A:N7    | 2.40                     | 0.53              |
| 1:1A:1815:A:H4'   | 1:1A:1816:A:O5'   | 2.09                     | 0.53              |
| 1:1A:2806:G:H2'   | 1:1A:2807:C:O4'   | 2.09                     | 0.53              |
| 1:1A:602:G:H2'    | 1:1A:603:C:C6     | 2.44                     | 0.53              |
| 1:2A:1044:G:H1'   | 1:2A:1048:A:H1'   | 1.91                     | 0.53              |
| 1:2A:1839:G:C8    | 1:2A:1927:A:H1'   | 2.44                     | 0.53              |
| 5:2F:135:LYS:HG2  | 5:2F:137:LYS:HG2  | 1.90                     | 0.53              |
| 8:2I:38:LEU:HB3   | 8:2I:40:THR:HG23  | 1.90                     | 0.53              |
| 14:2S:71:ARG:NE   | 14:2S:107:GLU:OE1 | 2.39                     | 0.53              |
| 1:1A:116:A:C8     | 1:1A:117:A:C8     | 2.97                     | 0.52              |
| 1:1A:625:G:O2'    | 1:1A:702:A:N6     | 2.42                     | 0.52              |
| 7:1H:125:VAL:HG22 | 7:1H:131:VAL:HG22 | 1.90                     | 0.52              |
| 12:1Q:37:LEU:HD21 | 12:1Q:130:LYS:HD2 | 1.91                     | 0.52              |
| 1:2A:1056:G:H5''  | 1:2A:1057:A:O4'   | 2.09                     | 0.52              |
| 1:2A:1316:U:H2'   | 1:2A:1317:A:C8    | 2.44                     | 0.52              |
| 1:2A:2641:G:P     | 9:2N:74:ARG:HH12  | 2.32                     | 0.52              |
| 5:2F:11:VAL:HB    | 5:2F:18:ARG:HG2   | 1.91                     | 0.52              |
| 7:2H:55:PRO:HG2   | 7:2H:61:HIS:CG    | 2.43                     | 0.52              |
| 1:1A:441:C:H2'    | 1:1A:442:A:C8     | 2.43                     | 0.52              |
| 1:1A:946:A:H2'    | 1:1A:947:A:H8     | 1.72                     | 0.52              |
| 6:2G:101:ILE:HD13 | 26:24:25:TYR:HB2  | 1.91                     | 0.52              |
| 1:2A:2626:C:H2'   | 1:2A:2627:G:O4'   | 2.10                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:2E:21:VAL:HG12   | 4:2E:185:LYS:HD2   | 1.92                     | 0.52              |
| 6:2G:36:LYS:HE2    | 6:2G:160:VAL:HG21  | 1.92                     | 0.52              |
| 1:1A:2584:A:N7     | 4:1E:144:ARG:HD2   | 2.24                     | 0.52              |
| 1:2A:1316:U:H2'    | 1:2A:1317:A:H8     | 1.73                     | 0.52              |
| 1:2A:2167:U:H2'    | 1:2A:2168:G:C8     | 2.45                     | 0.52              |
| 1:1A:1004:A:C5     | 1:1A:1037:C:C2     | 54.00                    | 0.52              |
| 1:1A:1133:G:N2     | 1:1A:1149:A:H1'    | 2.24                     | 0.52              |
| 1:1A:236:G:H4'     | 1:1A:413:G:C5      | 2.45                     | 0.52              |
| 1:1A:811:A:N3      | 3:1D:213:ARG:NH1   | 2.56                     | 0.52              |
| 9:1N:67:LEU:HA     | 9:1N:87:LEU:HD12   | 1.90                     | 0.52              |
| 12:1Q:41:TRP:HZ3   | 12:1Q:74:TYR:HE1   | 1.58                     | 0.52              |
| 1:2A:140:G:N2      | 1:2A:1596:A:H4'    | 2.23                     | 0.52              |
| 10:2O:35:VAL:HG11  | 10:2O:103:ALA:HB3  | 1.92                     | 0.52              |
| 1:1A:174:U:H4'     | 1:1A:207:A:H4'     | 1.90                     | 0.52              |
| 21:1Z:144:LEU:HD11 | 21:1Z:150:LEU:HD22 | 1.91                     | 0.52              |
| 1:2A:2461:C:H2'    | 1:2A:2462:U:C6     | 2.43                     | 0.52              |
| 1:1A:2182:G:H2'    | 1:1A:2183:C:C6     | 2.44                     | 0.52              |
| 1:1A:2118:U:H3     | 1:1A:2215:G:H1     | 1.57                     | 0.52              |
| 1:1A:2495:C:N3     | 12:1Q:124:LYS:NZ   | 2.53                     | 0.52              |
| 1:1A:704:U:H2'     | 1:1A:705:C:C6      | 2.45                     | 0.52              |
| 1:2A:2250:G:O2'    | 1:2A:2496:C:OP1    | 2.24                     | 0.52              |
| 14:2S:36:TYR:HA    | 14:2S:52:SER:HB3   | 1.90                     | 0.52              |
| 17:2V:33:VAL:HG23  | 17:2V:59:ALA:HB3   | 1.91                     | 0.52              |
| 23:11:51:VAL:HG11  | 23:11:74:VAL:HG21  | 1.91                     | 0.52              |
| 1:1A:1121:C:H2'    | 1:1A:1122:C:H3'    | 1.91                     | 0.52              |
| 4:1E:78:LEU:O      | 4:1E:79:ARG:NH1    | 2.43                     | 0.52              |
| 6:1G:50:ALA:C      | 6:1G:52:ILE:H      | 2.13                     | 0.52              |
| 13:1R:44:LEU:HD22  | 13:1R:48:VAL:HG23  | 1.91                     | 0.52              |
| 19:1X:60:ARG:HH12  | 29:17:47:ARG:NH2   | 2.04                     | 0.52              |
| 1:2A:1794:U:H2'    | 1:2A:1795:C:C6     | 2.45                     | 0.52              |
| 1:2A:322:A:OP2     | 5:2F:169:ASN:HB2   | 2.09                     | 0.52              |
| 5:2F:183:VAL:O     | 5:2F:187:VAL:HG23  | 2.09                     | 0.52              |
| 7:2H:20:ALA:HB1    | 7:2H:21:PRO:HD2    | 1.92                     | 0.52              |
| 1:2A:1009:A:OP2    | 9:2N:37:LYS:NZ     | 2.43                     | 0.52              |
| 13:2R:79:LEU:HA    | 13:2R:83:ILE:HD12  | 1.91                     | 0.52              |
| 21:2Z:150:LEU:HB3  | 21:2Z:171:ILE:HD11 | 1.92                     | 0.52              |
| 28:16:14:THR:HG21  | 28:16:48:VAL:HG13  | 1.92                     | 0.52              |
| 1:1A:2227:G:H5''   | 1:1A:2228:G:N7     | 2.24                     | 0.52              |
| 15:1T:126:ALA:HA   | 15:1T:129:ARG:NH1  | 2.24                     | 0.52              |
| 1:2A:2119:A:N6     | 1:2A:2168:G:N2     | 2.21                     | 0.52              |
| 1:2A:588:U:H2'     | 1:2A:589:C:C6      | 2.44                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:2A:762:U:H5''   | 60:2A:4243:HOH:O  | 2.09                     | 0.52              |
| 1:2A:878:A:H2'    | 1:2A:879:G:H5'    | 1.91                     | 0.52              |
| 6:2G:141:PHE:HB3  | 6:2G:142:PRO:HD2  | 1.91                     | 0.52              |
| 8:2I:26:ALA:HA    | 8:2I:30:LEU:HB2   | 1.91                     | 0.52              |
| 1:2A:2318:G:H22   | 14:2S:3:ARG:NE    | 2.07                     | 0.52              |
| 21:1Z:24:LEU:HD12 | 21:1Z:25:PRO:HD2  | 1.91                     | 0.52              |
| 1:2A:1658:C:OP1   | 4:2E:135:HIS:NE2  | 2.42                     | 0.52              |
| 1:2A:2010:G:H5''  | 18:2W:42:ARG:HB2  | 1.91                     | 0.52              |
| 1:2A:2471:C:N4    | 1:2A:2476:A:O2'   | 2.42                     | 0.52              |
| 1:2A:729:G:OP1    | 3:2D:10:THR:OG1   | 2.20                     | 0.52              |
| 2:2B:50:G:OP1     | 14:2S:63:THR:OG1  | 2.23                     | 0.52              |
| 6:2G:15:VAL:HG22  | 6:2G:175:LEU:HB3  | 1.92                     | 0.52              |
| 1:1A:2589:A:O4'   | 27:15:3:LYS:HB2   | 2.09                     | 0.52              |
| 1:1A:2134:G:O6    | 1:1A:2191:A:N7    | 2.43                     | 0.52              |
| 1:1A:2240:G:OP1   | 3:1D:261:LYS:NZ   | 2.20                     | 0.52              |
| 1:1A:2597:U:H4'   | 1:1A:2598:C:OP1   | 2.08                     | 0.52              |
| 1:2A:458:G:O2'    | 29:27:39:ARG:HD3  | 2.10                     | 0.52              |
| 1:2A:1495:A:H2'   | 1:2A:1496:A:C8    | 2.45                     | 0.52              |
| 1:2A:2378:A:H8    | 1:2A:2378:A:O5'   | 1.93                     | 0.52              |
| 30:18:23:VAL:HG22 | 30:18:47:LYS:HB3  | 1.92                     | 0.51              |
| 30:18:62:LEU:HB3  | 30:18:65:GLU:HG3  | 1.92                     | 0.51              |
| 1:1A:1276:C:H2'   | 1:1A:1277:G:C8    | 2.45                     | 0.51              |
| 1:1A:2879:G:H2'   | 1:1A:2880:C:O4'   | 2.10                     | 0.51              |
| 1:1A:721:G:O2'    | 5:1F:74:ARG:HD3   | 2.10                     | 0.51              |
| 1:2A:2320:A:H2'   | 1:2A:2320:A:N3    | 2.25                     | 0.51              |
| 1:2A:2836:U:H2'   | 1:2A:2837:G:C8    | 2.46                     | 0.51              |
| 1:2A:2316:C:O2'   | 6:2G:128:ARG:NH1  | 2.43                     | 0.51              |
| 1:2A:2495:G:H5''  | 12:2Q:82:ARG:HG2  | 1.91                     | 0.51              |
| 1:1A:2018:C:H4'   | 1:1A:2019:G:OP1   | 2.10                     | 0.51              |
| 1:1A:2086:C:H2'   | 1:1A:2087:C:C6    | 2.45                     | 0.51              |
| 1:1A:2131:U:O2    | 1:1A:2202:U:O4    | 2.28                     | 0.51              |
| 1:1A:2211:U:H2'   | 1:1A:2212:G:C8    | 2.45                     | 0.51              |
| 1:1A:2291:G:O6    | 22:10:14:ARG:HG3  | 2.10                     | 0.51              |
| 1:2A:2172:U:H4'   | 1:2A:2173:A:OP2   | 2.11                     | 0.51              |
| 1:2A:226:G:H21    | 1:2A:228:A:H62    | 1.56                     | 0.51              |
| 1:2A:756:C:H2'    | 1:2A:757:U:O4'    | 2.58                     | 0.51              |
| 5:2F:118:ALA:HA   | 5:2F:123:LEU:HB3  | 1.92                     | 0.51              |
| 20:2Y:86:ARG:HB2  | 20:2Y:98:VAL:HG23 | 1.92                     | 0.51              |
| 1:2A:300:A:H8     | 1:2A:300:A:O5'    | 2.76                     | 0.51              |
| 3:2D:4:LYS:HB3    | 3:2D:18:VAL:HG23  | 1.93                     | 0.51              |
| 5:2F:197:ASP:O    | 5:2F:201:VAL:HG12 | 2.10                     | 0.51              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:1A:1140:U:H1'   | 1:1A:1143:U:C5     | 2.36                     | 0.51              |
| 1:1A:1556:A:H2'   | 1:1A:1557:A:O4'    | 2.11                     | 0.51              |
| 1:1A:1825:U:H2'   | 1:1A:1826:C:H6     | 1.75                     | 0.51              |
| 1:1A:2184:G:H4'   | 1:1A:2194:U:O2'    | 2.11                     | 0.51              |
| 3:1D:71:ASP:OD2   | 3:1D:103:ARG:NH2   | 2.41                     | 0.51              |
| 1:1A:2800:C:H1'   | 4:1E:62:PRO:HG3    | 1.91                     | 0.51              |
| 6:1G:135:LEU:O    | 6:1G:154:GLY:HA3   | 2.10                     | 0.51              |
| 10:1O:35:VAL:HG11 | 10:1O:103:ALA:HB3  | 1.91                     | 0.51              |
| 21:1Z:152:ALA:HB3 | 21:1Z:167:PRO:HA   | 1.92                     | 0.51              |
| 1:2A:2250:G:C8    | 1:2A:2496:C:H5''   | 2.45                     | 0.51              |
| 1:2A:247:G:H4'    | 1:2A:386:G:C5      | 2.45                     | 0.51              |
| 5:2F:184:TYR:HE1  | 11:2P:3:LEU:HD21   | 1.75                     | 0.51              |
| 5:2F:21:ALA:HB3   | 5:2F:22:ALA:HA     | 1.90                     | 0.51              |
| 10:2O:107:ARG:HG2 | 10:2O:115:VAL:HG21 | 1.93                     | 0.51              |
| 1:1A:1119:A:N3    | 1:1A:1119:A:H3'    | 2.25                     | 0.51              |
| 1:1A:2023:A:H2'   | 1:1A:2024:G:C8     | 2.46                     | 0.51              |
| 14:1S:15:ARG:O    | 14:1S:19:LYS:HG2   | 2.11                     | 0.51              |
| 23:21:75:GLU:O    | 23:21:78:LYS:HG2   | 2.11                     | 0.51              |
| 1:2A:2074:U:H2'   | 1:2A:2075:U:C6     | 2.46                     | 0.51              |
| 1:2A:2139:C:H42   | 1:2A:2152:G:H1     | 1.58                     | 0.51              |
| 2:2B:90:A:C5      | 2:2B:91:C:H1'      | 2.45                     | 0.51              |
| 23:11:72:GLU:OE2  | 23:11:76:ARG:NH2   | 2.44                     | 0.51              |
| 6:1G:143:GLU:HG3  | 26:14:31:ILE:HD11  | 1.93                     | 0.51              |
| 1:1A:2623:U:C4    | 27:15:3:LYS:HG3    | 2.46                     | 0.51              |
| 1:1A:643:C:H2'    | 1:1A:644:G:H8      | 2.76                     | 0.51              |
| 1:2A:2336:A:H61   | 22:20:43:THR:CG2   | 2.24                     | 0.51              |
| 1:2A:271(H):G:H2' | 1:2A:271(I):G:C8   | 2.45                     | 0.51              |
| 2:2B:84:C:H42     | 2:2B:93:G:H1       | 1.57                     | 0.51              |
| 27:15:16:ARG:HG3  | 27:15:17:ASP:N     | 2.25                     | 0.51              |
| 1:1A:2096:U:H2'   | 1:1A:2097:U:C6     | 2.46                     | 0.51              |
| 2:1B:24:G:N7      | 2:1B:56:G:H2'      | 2.26                     | 0.51              |
| 1:1A:2328:C:O2'   | 6:1G:128:ARG:NH2   | 2.44                     | 0.51              |
| 1:2A:1264:G:H2'   | 1:2A:2014:A:N6     | 2.26                     | 0.51              |
| 1:2A:876:C:H2'    | 1:2A:877:U:O4'     | 2.11                     | 0.51              |
| 8:2I:98:ALA:HA    | 8:2I:101:LEU:HD12  | 1.92                     | 0.51              |
| 1:1A:1101:G:N2    | 1:1A:1150:C:O2     | 2.34                     | 0.51              |
| 1:1A:1362:U:H2'   | 1:1A:1363:A:C8     | 2.46                     | 0.51              |
| 1:1A:2699:U:H2'   | 1:1A:2700:U:O4'    | 2.11                     | 0.51              |
| 1:1A:733:G:H21    | 1:1A:835:A:H61     | 1.58                     | 0.51              |
| 7:1H:3:ARG:HH11   | 7:1H:4:ILE:H       | 1.59                     | 0.51              |
| 15:1T:16:ARG:NH2  | 15:1T:18:ASP:OD2   | 2.42                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 17:1V:76:LYS:HB2  | 17:1V:81:TYR:HB3  | 1.91                     | 0.51              |
| 1:1A:1425:A:H4'   | 1:1A:1426:G:OP2   | 2.10                     | 0.51              |
| 1:1A:1879:A:H2'   | 1:1A:1880:G:H8    | 1.76                     | 0.51              |
| 1:1A:826:U:OP1    | 3:1D:49:ILE:HG13  | 2.11                     | 0.51              |
| 3:1D:242:ARG:HG3  | 3:1D:242:ARG:NH1  | 2.22                     | 0.51              |
| 21:1Z:7:ALA:O     | 21:1Z:62:PRO:HD3  | 2.11                     | 0.51              |
| 23:21:40:ARG:NH2  | 23:21:42:GLN:HG2  | 2.25                     | 0.51              |
| 1:2A:2125:G:H1'   | 1:2A:2173:A:N6    | 2.26                     | 0.51              |
| 1:2A:993:G:OP1    | 16:2U:50:ARG:NH2  | 2.44                     | 0.51              |
| 17:2V:25:LEU:H    | 17:2V:92:THR:HG1  | 1.59                     | 0.51              |
| 1:1A:1037:C:H2'   | 1:1A:1038:C:C6    | 2.84                     | 0.50              |
| 1:1A:469:A:C6     | 5:1F:45:ARG:HD2   | 2.46                     | 0.50              |
| 6:1G:82:LEU:HD21  | 6:1G:88:ILE:HG21  | 1.93                     | 0.50              |
| 12:1Q:93:TYR:CZ   | 21:1Z:194:PRO:HG2 | 2.47                     | 0.50              |
| 1:2A:2206:G:H5''  | 1:2A:2207:G:N7    | 2.25                     | 0.50              |
| 1:2A:2660:A:N7    | 7:2H:175:LYS:NZ   | 2.50                     | 0.50              |
| 15:2T:120:ARG:HA  | 15:2T:123:GLN:HB3 | 1.92                     | 0.50              |
| 1:2A:1188:U:H4'   | 17:2V:79:VAL:HG22 | 1.94                     | 0.50              |
| 19:2X:53:LYS:HB3  | 19:2X:82:GLN:HB3  | 1.93                     | 0.50              |
| 1:1A:1077:G:H5''  | 31:19:8:LYS:HE3   | 1.93                     | 0.50              |
| 1:1A:1338:U:H2'   | 1:1A:1339:C:C6    | 2.46                     | 0.50              |
| 1:1A:1562:U:H2'   | 1:1A:1563:G:C8    | 2.46                     | 0.50              |
| 13:1R:28:LEU:HD23 | 13:1R:48:VAL:HG21 | 1.93                     | 0.50              |
| 19:1X:2:LYS:NZ    | 19:1X:38:GLU:OE2  | 2.33                     | 0.50              |
| 22:20:70:GLN:HG2  | 22:20:80:HIS:HE2  | 1.76                     | 0.50              |
| 1:2A:1221(A):C:C2 | 1:2A:1229:G:C2    | 3.00                     | 0.50              |
| 1:2A:2324:C:H5''  | 1:2A:2325:G:H5'   | 1.93                     | 0.50              |
| 1:2A:2785:C:O2'   | 4:2E:66:HIS:ND1   | 2.43                     | 0.50              |
| 5:2F:164:ARG:HD2  | 5:2F:175:THR:HG23 | 1.93                     | 0.50              |
| 1:1A:1112:U:H3    | 1:1A:1119:A:N6    | 2.05                     | 0.50              |
| 1:1A:167:G:H2'    | 1:1A:168:G:C8     | 3.07                     | 0.50              |
| 1:1A:1857:G:H4'   | 3:1D:242:ARG:CZ   | 2.40                     | 0.50              |
| 6:1G:11:TYR:CZ    | 6:1G:16:ARG:HD3   | 2.46                     | 0.50              |
| 6:1G:47:LYS:HG3   | 6:1G:48:GLU:H     | 1.77                     | 0.50              |
| 13:1R:44:LEU:HD11 | 13:1R:79:LEU:HD13 | 10.47                    | 0.50              |
| 1:2A:2815:C:C5'   | 27:25:29:THR:HG21 | 2.41                     | 0.50              |
| 1:2A:2321:G:O2'   | 1:2A:2322:A:OP1   | 2.26                     | 0.50              |
| 1:2A:2576:G:H1'   | 60:2A:4759:HOH:O  | 2.10                     | 0.50              |
| 5:2F:117:ARG:NH2  | 5:2F:189:THR:O    | 2.28                     | 0.50              |
| 1:1A:2188:G:O6    | 1:1A:2194:U:H5    | 1.93                     | 0.50              |
| 1:1A:442:A:H2'    | 1:1A:443:C:H6     | 1.76                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:1B:50:G:OP1     | 14:1S:63:THR:OG1  | 2.18                     | 0.50              |
| 7:1H:97:ARG:HG2   | 7:1H:104:GLU:HB3  | 1.94                     | 0.50              |
| 10:1O:64:ARG:NH1  | 10:1O:81:ASP:OD1  | 2.45                     | 0.50              |
| 15:1T:107:ASP:O   | 15:1T:111:ARG:HG3 | 2.12                     | 0.50              |
| 15:1T:24:PRO:HD3  | 15:1T:52:ILE:HD12 | 1.93                     | 0.50              |
| 1:2A:1108:U:H2'   | 1:2A:1109:C:C6    | 2.46                     | 0.50              |
| 1:2A:1115:G:H2'   | 1:2A:1116:C:C6    | 2.46                     | 0.50              |
| 1:2A:774:A:N3     | 1:2A:774:A:H2'    | 2.26                     | 0.50              |
| 6:2G:19:LEU:HD11  | 6:2G:172:LEU:HA   | 1.94                     | 0.50              |
| 15:2T:51:ARG:HG3  | 15:2T:98:LYS:HE3  | 1.93                     | 0.50              |
| 1:1A:217:A:H8     | 1:1A:218:A:H5'    | 1.77                     | 0.50              |
| 6:1G:3:LEU:HD22   | 26:14:25:TYR:CZ   | 2.47                     | 0.50              |
| 8:1I:10:GLU:O     | 8:1I:12:LEU:N     | 2.44                     | 0.50              |
| 1:2A:1084:A:H3'   | 1:2A:1085:A:C4'   | 2.42                     | 0.50              |
| 4:2E:36:ARG:NH2   | 4:2E:88:GLY:O     | 2.44                     | 0.50              |
| 5:2F:184:TYR:CE2  | 5:2F:188:ARG:HD2  | 2.47                     | 0.50              |
| 7:2H:121:ILE:HD11 | 7:2H:140:LYS:HG2  | 1.93                     | 0.50              |
| 21:2Z:7:ALA:O     | 21:2Z:62:PRO:HD3  | 2.10                     | 0.50              |
| 1:1A:1231:G:H2'   | 1:1A:1232:G:O4'   | 2.12                     | 0.50              |
| 1:1A:801:C:H2'    | 1:1A:802:C:H6     | 1.76                     | 0.50              |
| 8:1I:92:VAL:HG13  | 8:1I:120:ILE:HB   | 1.94                     | 0.50              |
| 1:2A:2009:G:N3    | 13:2R:107:ASP:HA  | 2.27                     | 0.50              |
| 1:2A:783:A:O2'    | 1:2A:785:G:OP1    | 2.27                     | 0.50              |
| 1:1A:9:U:N3       | 1:1A:2641:A:C2    | 2.78                     | 0.50              |
| 8:1I:117:GLU:HG3  | 8:1I:118:LYS:N    | 2.27                     | 0.50              |
| 1:2A:1799:G:O2'   | 3:2D:183:ARG:NH1  | 2.43                     | 0.50              |
| 1:2A:2138:C:H2'   | 1:2A:2139:C:C6    | 2.47                     | 0.50              |
| 1:2A:2875:C:O2'   | 15:2T:2:ASN:OD1   | 2.30                     | 0.50              |
| 15:1T:60:THR:HG22 | 15:1T:77:PRO:HA   | 1.93                     | 0.50              |
| 1:2A:1012:U:H5    | 9:2N:28:THR:HG21  | 1.77                     | 0.50              |
| 1:2A:1066:U:O2'   | 1:2A:1068:G:OP2   | 2.29                     | 0.50              |
| 1:2A:1889:A:H2'   | 1:2A:1890:A:C8    | 2.47                     | 0.50              |
| 2:2B:86:G:H1      | 2:2B:91:C:H42     | 1.59                     | 0.50              |
| 8:2I:77:LEU:HD11  | 8:2I:100:ALA:HB1  | 1.94                     | 0.50              |
| 1:1A:714:U:O2     | 30:18:2:PRO:HD2   | 2.12                     | 0.50              |
| 3:1D:75:ILE:HG21  | 3:1D:99:ASP:HB2   | 1.94                     | 0.50              |
| 1:2A:1999:C:H4'   | 1:2A:2723:C:O2    | 2.11                     | 0.50              |
| 1:2A:26:G:C6      | 1:2A:27:G:N1      | 2.80                     | 0.50              |
| 1:2A:2012:G:P     | 18:2W:11:ARG:HH22 | 2.35                     | 0.50              |
| 1:1A:2131:U:O5'   | 1:1A:2131:U:H6    | 1.94                     | 0.49              |
| 1:1A:233:A:C2     | 1:1A:244:A:C4     | 3.00                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:1A:27:G:N2       | 1:1A:537:G:H1'     | 2.27                     | 0.49              |
| 4:1E:18:ASP:HB3    | 15:1T:82:LEU:HD21  | 1.94                     | 0.49              |
| 22:20:14:ARG:NE    | 60:20:201:HOH:O    | 2.44                     | 0.49              |
| 1:2A:1593:G:H2'    | 1:2A:1594:G:C8     | 2.46                     | 0.49              |
| 1:2A:2567:G:H2'    | 1:2A:2568:C:C6     | 2.47                     | 0.49              |
| 1:2A:538:G:H2'     | 1:2A:539:G:H8      | 1.76                     | 0.49              |
| 1:2A:657:U:H2'     | 1:2A:658:C:C6      | 2.46                     | 0.49              |
| 3:2D:275:LYS:HE3   | 3:2D:276:LYS:HA    | 1.94                     | 0.49              |
| 6:2G:14:GLU:C      | 6:2G:17:PRO:HD2    | 2.33                     | 0.49              |
| 17:2V:43:GLU:OE1   | 17:2V:43:GLU:N     | 2.45                     | 0.49              |
| 1:1A:2117:C:H2'    | 1:1A:2118:U:O4'    | 2.12                     | 0.49              |
| 1:1A:2331:G:N1     | 14:1S:3:ARG:HA     | 2.27                     | 0.49              |
| 7:1H:113:VAL:HG11  | 7:1H:151:ILE:HD13  | 1.93                     | 0.49              |
| 14:1S:20:ARG:HH21  | 22:10:47:PRO:HB2   | 1.77                     | 0.49              |
| 20:1Y:35:TYR:CE2   | 20:1Y:69:ALA:HB3   | 2.47                     | 0.49              |
| 1:2A:2119:A:N1     | 1:2A:2170:A:H2'    | 2.26                     | 0.49              |
| 1:2A:2121:G:O6     | 1:2A:2176:A:N6     | 2.44                     | 0.49              |
| 1:2A:2286:A:H4'    | 1:2A:2287:A:O4'    | 2.12                     | 0.49              |
| 1:2A:271(Z):C:H1'  | 1:2A:272(C):G:H1'  | 1.94                     | 0.49              |
| 1:2A:1187:G:H5'    | 17:2V:81:TYR:CE1   | 2.47                     | 0.49              |
| 21:2Z:39:VAL:HG21  | 21:2Z:44:PHE:HB2   | 1.94                     | 0.49              |
| 1:1A:1604:C:H5''   | 1:1A:1605:A:OP2    | 2.12                     | 0.49              |
| 1:1A:173:C:H2'     | 1:1A:174:U:C6      | 2.47                     | 0.49              |
| 1:1A:1890:A:N6     | 1:1A:1905:G:O2'    | 2.45                     | 0.49              |
| 1:1A:1936:C:H2'    | 1:1A:1937:5MU:O4'  | 2.13                     | 0.49              |
| 4:1E:120:TRP:CD1   | 4:1E:155:LYS:HB3   | 2.48                     | 0.49              |
| 12:1Q:109:VAL:HG22 | 12:1Q:113:GLN:OE1  | 2.12                     | 0.49              |
| 12:1Q:30:GLY:O     | 12:1Q:134:ARG:NH1  | 2.45                     | 0.49              |
| 23:21:35:THR:OG1   | 23:21:35:THR:O     | 2.31                     | 0.49              |
| 1:2A:1509(A):A:H2' | 1:2A:1509(B):A:O4' | 2.12                     | 0.49              |
| 1:2A:576:U:H2'     | 1:2A:577:G:C8      | 2.47                     | 0.49              |
| 1:1A:2402:U:P      | 30:18:35:GLN:HE22  | 2.35                     | 0.49              |
| 3:1D:37:LEU:HD12   | 3:1D:62:TYR:HB2    | 1.92                     | 0.49              |
| 17:1V:19:LYS:HG2   | 17:1V:95:LEU:HD12  | 1.95                     | 0.49              |
| 30:28:22:VAL:HG12  | 30:28:50:LEU:HD12  | 1.95                     | 0.49              |
| 1:2A:1067:A:H4'    | 1:2A:1068:G:OP2    | 2.12                     | 0.49              |
| 1:2A:2291:U:OP1    | 1:2A:2380:C:O2'    | 2.30                     | 0.49              |
| 1:2A:922:U:H2'     | 1:2A:923:C:C6      | 2.46                     | 0.49              |
| 7:2H:6:ARG:NH2     | 7:2H:54:ARG:HH12   | 2.11                     | 0.49              |
| 1:1A:1114:G:HO2'   | 1:1A:1142:A:HO2'   | 1.54                     | 0.49              |
| 1:1A:1475:G:H2'    | 1:1A:1476:C:C6     | 2.47                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:1G:59:GLU:OE1   | 6:1G:153:ARG:HD2  | 2.12                     | 0.49              |
| 8:1I:40:THR:O     | 8:1I:44:LEU:HB2   | 2.12                     | 0.49              |
| 9:1N:128:HIS:O    | 9:1N:131:GLN:NE2  | 2.46                     | 0.49              |
| 11:1P:116:GLY:O   | 11:1P:137:LYS:NZ  | 2.37                     | 0.49              |
| 15:1T:56:GLY:O    | 15:1T:59:THR:HG23 | 2.11                     | 0.49              |
| 16:1U:85:LYS:HB2  | 16:1U:116:ALA:HB1 | 1.95                     | 0.49              |
| 20:1Y:8:LYS:HA    | 20:1Y:30:VAL:HG21 | 1.94                     | 0.49              |
| 1:2A:1791:A:H3'   | 1:2A:1792:G:H8    | 1.78                     | 0.49              |
| 1:2A:27:G:N2      | 1:2A:512:G:H1'    | 2.28                     | 0.49              |
| 1:1A:178:G:H2'    | 1:1A:194:G:N2     | 2.27                     | 0.49              |
| 1:1A:2133:C:N3    | 1:1A:2169:G:N2    | 2.60                     | 0.49              |
| 1:2A:1069:A:C2    | 1:2A:1073:A:H5'   | 2.48                     | 0.49              |
| 1:2A:1360:A:OP1   | 1:2A:1360:A:H8    | 5.06                     | 0.49              |
| 1:2A:1798:U:H5'   | 3:2D:259:THR:CG2  | 2.41                     | 0.49              |
| 1:2A:272(B):G:H2' | 1:2A:272(C):G:H8  | 1.78                     | 0.49              |
| 15:2T:22:PHE:CE1  | 15:2T:49:VAL:HG11 | 2.47                     | 0.49              |
| 21:2Z:24:LEU:HD12 | 21:2Z:25:PRO:HD2  | 1.94                     | 0.49              |
| 21:2Z:59:LEU:N    | 21:2Z:67:LEU:O    | 2.43                     | 0.49              |
| 26:14:34:GLU:HG2  | 26:14:35:VAL:HG12 | 1.94                     | 0.49              |
| 1:1A:1002:A:H4'   | 12:1Q:74:TYR:OH   | 2.13                     | 0.49              |
| 4:1E:116:VAL:HG13 | 4:1E:122:PHE:HB2  | 1.95                     | 0.49              |
| 2:1B:57:A:H1'     | 6:1G:29:TRP:HB2   | 1.95                     | 0.49              |
| 11:1P:89:ALA:O    | 11:1P:121:LYS:NZ  | 2.40                     | 0.49              |
| 1:2A:2690:C:H5''  | 1:2A:2872:G:N2    | 2.28                     | 0.49              |
| 1:2A:622:G:H2'    | 1:2A:623:G:H8     | 1.76                     | 0.49              |
| 1:2A:637:A:H4'    | 1:2A:638:G:O5'    | 2.13                     | 0.49              |
| 5:2F:161:GLU:O    | 5:2F:165:ARG:HG3  | 2.13                     | 0.49              |
| 1:1A:2291:G:N7    | 22:10:14:ARG:NH1  | 2.60                     | 0.49              |
| 1:1A:27:G:C2      | 1:1A:537:G:N3     | 2.81                     | 0.49              |
| 1:1A:769:A:H2'    | 1:1A:770:G:H8     | 1.78                     | 0.49              |
| 4:1E:170:LEU:HB3  | 4:1E:184:VAL:HG22 | 1.95                     | 0.49              |
| 1:2A:1045:A:H2'   | 1:2A:1045:A:N3    | 2.27                     | 0.49              |
| 1:2A:1077:A:C5    | 1:2A:1078:U:O4    | 2.65                     | 0.49              |
| 1:2A:1384:A:N3    | 1:2A:1405:U:H1'   | 2.28                     | 0.49              |
| 3:2D:145:VAL:HG12 | 3:2D:146:GLU:O    | 2.13                     | 0.49              |
| 1:1A:1143:U:H2'   | 1:1A:1144:A:O4'   | 2.13                     | 0.49              |
| 1:1A:1577:C:O2'   | 1:1A:1578:C:O5'   | 2.29                     | 0.49              |
| 1:1A:2745:G:H3'   | 1:1A:2746:A:O4'   | 2.13                     | 0.49              |
| 1:2A:1096:A:C8    | 1:2A:1097:U:H5    | 2.30                     | 0.49              |
| 1:2A:1448:G:O2'   | 1:2A:1528(A):A:N1 | 2.39                     | 0.49              |
| 1:2A:2103:C:O2    | 1:2A:2186:G:N1    | 2.44                     | 0.49              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:2A:602:G:O2'    | 1:2A:655:A:N6      | 2.46                     | 0.49              |
| 12:2Q:34:LEU:HB2  | 12:2Q:118:LEU:HD22 | 1.94                     | 0.49              |
| 1:2A:1266:G:O5'   | 18:2W:15:ARG:NH2   | 2.46                     | 0.49              |
| 27:15:45:VAL:HA   | 27:15:52:TYR:HB2   | 1.95                     | 0.49              |
| 1:1A:1560:U:H2'   | 1:1A:1561:C:C6     | 2.47                     | 0.49              |
| 1:1A:1889:G:H22   | 1:1A:1905:G:H2'    | 1.78                     | 0.49              |
| 14:1S:39:ILE:HB   | 14:1S:49:VAL:HG13  | 1.94                     | 0.49              |
| 1:2A:2064:C:H1'   | 1:2A:2450:A:C2     | 2.48                     | 0.49              |
| 1:2A:434:U:H2'    | 1:2A:435:C:C6      | 6.67                     | 0.49              |
| 5:2F:39:TRP:NE1   | 5:2F:99:TYR:O      | 2.45                     | 0.49              |
| 10:2O:119:PRO:HB2 | 15:2T:68:TYR:CE2   | 2.47                     | 0.49              |
| 1:1A:2135:U:O4    | 1:1A:2190:G:H4'    | 2.13                     | 0.48              |
| 1:2A:1006:C:H2'   | 1:2A:1007:C:C6     | 3.37                     | 0.48              |
| 1:2A:1104:C:H2'   | 1:2A:1105:U:C6     | 2.48                     | 0.48              |
| 1:2A:10:G:H2'     | 1:2A:11:G:H8       | 1.77                     | 0.48              |
| 1:2A:2166:G:O5'   | 1:2A:2166:G:H8     | 1.96                     | 0.48              |
| 1:2A:2441:C:OP2   | 1:2A:2586:C:O2'    | 2.31                     | 0.48              |
| 1:2A:272(G):C:N3  | 1:2A:363(C):G:N2   | 2.50                     | 0.48              |
| 10:2O:34:THR:OG1  | 10:2O:35:VAL:N     | 2.45                     | 0.48              |
| 23:11:95:LEU:O    | 23:11:98:LEU:HB2   | 2.13                     | 0.48              |
| 1:1A:1829:U:H5'   | 3:1D:259:THR:CG2   | 2.43                     | 0.48              |
| 21:1Z:54:HIS:HD2  | 21:1Z:99:TYR:O     | 1.95                     | 0.48              |
| 1:2A:2529:G:O6    | 31:29:31:LYS:NZ    | 2.46                     | 0.48              |
| 1:2A:2347:C:O2'   | 28:26:21:TYR:OH    | 2.25                     | 0.48              |
| 1:2A:2635:C:O2    | 4:2E:37:ARG:NH2    | 2.46                     | 0.48              |
| 1:2A:2693:A:H2'   | 1:2A:2694:G:C8     | 2.48                     | 0.48              |
| 1:2A:856:C:H2'    | 1:2A:857:C:H6      | 1.76                     | 0.48              |
| 6:2G:96:ARG:O     | 6:2G:99:MET:HB3    | 2.12                     | 0.48              |
| 1:1A:2141:A:N6    | 1:1A:2190:G:H1'    | 2.27                     | 0.48              |
| 1:1A:2149:G:H5''  | 1:1A:2149:G:H8     | 1.79                     | 0.48              |
| 1:1A:505:A:N3     | 1:1A:507:G:H5''    | 2.28                     | 0.48              |
| 1:2A:1131:G:O6    | 1:2A:2040:C:H1'    | 2.13                     | 0.48              |
| 1:2A:620:G:H5'    | 1:2A:620:G:N3      | 2.29                     | 0.48              |
| 1:2A:192:C:O2'    | 1:2A:802:A:N3      | 2.43                     | 0.48              |
| 1:2A:2773:C:H5''  | 4:2E:164:ARG:HG2   | 1.95                     | 0.48              |
| 7:2H:137:ASP:HB3  | 7:2H:140:LYS:HB3   | 1.95                     | 0.48              |
| 12:2Q:108:GLY:HA3 | 21:2Z:116:VAL:HG13 | 1.96                     | 0.48              |
| 1:1A:2032:G:H5''  | 18:1W:42:ARG:HB2   | 1.95                     | 0.48              |
| 1:1A:745:C:O2'    | 1:1A:781:A:N6      | 2.47                     | 0.48              |
| 6:1G:16:ARG:O     | 6:1G:20:ILE:HG13   | 2.13                     | 0.48              |
| 26:24:18:CYS:HB2  | 26:24:20:ASN:HB2   | 1.95                     | 0.48              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:2A:2156:G:O6     | 1:2A:2157:G:N2    | 2.35                     | 0.48              |
| 1:2A:2537:U:H2'    | 1:2A:2538:C:C6    | 2.48                     | 0.48              |
| 1:2A:658:C:H2'     | 1:2A:659:C:C6     | 2.49                     | 0.48              |
| 7:2H:7:LEU:HB3     | 7:2H:69:ARG:HH21  | 1.78                     | 0.48              |
| 10:2O:2:ILE:HD12   | 10:2O:6:THR:HG21  | 1.94                     | 0.48              |
| 15:1T:55:ASN:N     | 15:1T:59:THR:HG22 | 2.28                     | 0.48              |
| 1:2A:2294:C:OP2    | 14:2S:89:ARG:NH2  | 2.39                     | 0.48              |
| 1:2A:2889:C:H3'    | 1:2A:2891:G:H8    | 1.78                     | 0.48              |
| 5:2F:11:VAL:HG22   | 5:2F:125:LEU:HB2  | 1.96                     | 0.48              |
| 25:13:39:ASP:OD2   | 25:13:44:ARG:NH2  | 2.34                     | 0.48              |
| 1:1A:1554:A:H4'    | 1:1A:1556:A:C5    | 2.49                     | 0.48              |
| 1:1A:553:A:OP2     | 9:1N:114:ARG:NH1  | 2.47                     | 0.48              |
| 1:2A:848:G:H2'     | 1:2A:849:A:C8     | 2.49                     | 0.48              |
| 6:2G:122:PRO:HA    | 6:2G:180:PHE:CD1  | 2.49                     | 0.48              |
| 7:2H:98:LEU:HD22   | 7:2H:125:VAL:HG23 | 1.95                     | 0.48              |
| 14:2S:34:HIS:ND1   | 14:2S:53:SER:OG   | 2.38                     | 0.48              |
| 1:1A:1766:G:H5'    | 1:1A:1767:A:OP2   | 2.14                     | 0.48              |
| 1:1A:1895:U:OP1    | 1:1A:2422:G:O2'   | 2.23                     | 0.48              |
| 1:1A:265:U:H2'     | 1:1A:266:C:H6     | 1.77                     | 0.48              |
| 1:1A:275:C:H2'     | 1:1A:276:C:C6     | 2.48                     | 0.48              |
| 3:1D:70:TRP:CE2    | 3:1D:150:LYS:HD3  | 2.49                     | 0.48              |
| 6:1G:161:THR:HG22  | 6:1G:163:ALA:H    | 1.77                     | 0.48              |
| 23:21:72:GLU:HG2   | 23:21:76:ARG:HD2  | 1.94                     | 0.48              |
| 1:2A:1365:A:O4'    | 23:21:41:ARG:NH2  | 2.47                     | 0.48              |
| 1:2A:1472:A:N6     | 1:2A:1519:G:H1'   | 2.28                     | 0.48              |
| 1:2A:2086:U:H2'    | 1:2A:2087:G:C8    | 2.48                     | 0.48              |
| 1:2A:2105:C:N4     | 1:2A:2184:G:H1    | 2.11                     | 0.48              |
| 1:2A:320:A:H4'     | 1:2A:322:A:C8     | 2.49                     | 0.48              |
| 1:2A:1130:U:O2     | 4:2E:149:ARG:NH2  | 2.46                     | 0.48              |
| 6:2G:122:PRO:HA    | 6:2G:180:PHE:HD1  | 1.78                     | 0.48              |
| 20:2Y:43:ASN:ND2   | 20:2Y:65:ALA:HB3  | 2.29                     | 0.48              |
| 27:15:35:GLU:N     | 27:15:35:GLU:OE1  | 2.47                     | 0.48              |
| 1:1A:211:A:H5''    | 1:1A:448:U:OP1    | 2.14                     | 0.48              |
| 1:1A:2136:A:H2'    | 1:1A:2137:G:O4'   | 2.14                     | 0.48              |
| 12:1Q:110:THR:HG23 | 12:1Q:113:GLN:OE1 | 2.14                     | 0.48              |
| 1:2A:1379:A:H4'    | 1:2A:1380:G:OP2   | 2.14                     | 0.48              |
| 1:2A:2135:A:H3'    | 1:2A:2136:C:H5'   | 1.95                     | 0.48              |
| 1:2A:2144:U:H1'    | 1:2A:2147:G:O6    | 2.14                     | 0.48              |
| 1:2A:2309:A:H61    | 6:2G:79:ASN:ND2   | 2.11                     | 0.48              |
| 1:2A:2386:C:H2'    | 1:2A:2387:U:C6    | 2.48                     | 0.48              |
| 1:2A:536:A:H2'     | 1:2A:537:C:C6     | 2.49                     | 0.48              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:2A:923:C:H4'    | 22:20:29:GLN:HG3   | 1.94                     | 0.48              |
| 1:2A:833:U:O2     | 11:2P:55:ARG:NH1   | 2.47                     | 0.48              |
| 11:1P:63:PRO:HD3  | 30:18:27:THR:HG22  | 1.94                     | 0.48              |
| 31:19:32:HIS:O    | 31:19:34:GLN:HG3   | 2.13                     | 0.48              |
| 1:1A:217:A:H2'    | 1:1A:219:U:O4'     | 2.13                     | 0.48              |
| 1:1A:2236:G:H4'   | 1:1A:2238:C:C2     | 2.49                     | 0.48              |
| 1:1A:741:U:OP1    | 3:1D:59:LYS:NZ     | 2.44                     | 0.48              |
| 26:24:46:GLN:NE2  | 26:24:48:ARG:HH12  | 2.12                     | 0.48              |
| 26:24:1:MET:HB3   | 26:24:6:HIS:CD2    | 2.49                     | 0.48              |
| 1:2A:2134:A:N6    | 1:2A:2135:A:H62    | 2.12                     | 0.48              |
| 1:2A:479:A:N3     | 1:2A:481:G:H5''    | 2.29                     | 0.48              |
| 2:2B:95:C:H2'     | 2:2B:96:U:C6       | 2.48                     | 0.48              |
| 7:2H:3:ARG:NH1    | 7:2H:5:GLY:H       | 2.12                     | 0.48              |
| 8:2I:45:LYS:O     | 8:2I:49:ALA:N      | 2.38                     | 0.48              |
| 11:1P:50:ARG:HG3  | 30:18:61:LEU:HD11  | 1.94                     | 0.48              |
| 1:1A:1046:A:N6    | 1:1A:1211:U:O2     | 27.97                    | 0.48              |
| 1:1A:915:U:C4     | 1:1A:916:G:N7      | 2.82                     | 0.48              |
| 3:1D:69:ARG:C     | 3:1D:71:ASP:H      | 2.17                     | 0.48              |
| 12:1Q:108:GLY:HA3 | 21:1Z:116:VAL:HG13 | 1.96                     | 0.48              |
| 13:1R:72:ASP:O    | 13:1R:76:VAL:HG23  | 2.13                     | 0.48              |
| 28:26:25:LYS:HE3  | 28:26:27:LYS:HA    | 1.95                     | 0.48              |
| 1:2A:1079:C:C4    | 1:2A:1080:C:H1'    | 2.49                     | 0.48              |
| 1:2A:2573:C:OP1   | 1:2A:2574:G:H5''   | 2.13                     | 0.48              |
| 1:2A:2867:G:OP2   | 15:2T:119:LYS:NZ   | 2.36                     | 0.48              |
| 6:2G:16:ARG:O     | 6:2G:20:ILE:HG13   | 2.14                     | 0.48              |
| 1:1A:1309:U:C4    | 1:1A:1310:G:C6     | 3.02                     | 0.47              |
| 1:1A:2073:A:H4'   | 4:1E:141:ILE:HG12  | 1.95                     | 0.47              |
| 1:1A:2760:G:O6    | 1:1A:2768:C:H5''   | 2.14                     | 0.47              |
| 1:1A:2821:G:N2    | 1:1A:2900:G:H1'    | 2.29                     | 0.47              |
| 1:1A:211:A:H3'    | 1:1A:448:U:H5'     | 1.94                     | 0.47              |
| 1:1A:921:G:H1     | 1:1A:949:C:N4      | 2.10                     | 0.47              |
| 11:1P:88:LEU:HD21 | 11:1P:100:LEU:HD11 | 1.95                     | 0.47              |
| 1:1A:1040:C:OP1   | 16:1U:53:ARG:NH2   | 2.46                     | 0.47              |
| 24:22:63:VAL:O    | 24:22:67:LYS:HG2   | 2.13                     | 0.47              |
| 1:2A:687:C:H5''   | 29:27:2:LYS:HE2    | 1.94                     | 0.47              |
| 1:2A:1903:G:OP1   | 3:2D:241:PRO:HB2   | 2.13                     | 0.47              |
| 1:2A:2095:C:H2'   | 1:2A:2096:U:O4'    | 2.14                     | 0.47              |
| 1:2A:2102:U:H2'   | 1:2A:2103:C:O4'    | 2.14                     | 0.47              |
| 1:2A:2464:C:O2'   | 60:2A:4001:HOH:O   | 1.99                     | 0.47              |
| 1:2A:911:A:H2'    | 12:2Q:9:TYR:OH     | 2.14                     | 0.47              |
| 3:2D:112:GLN:O    | 3:2D:115:GLN:HG2   | 2.14                     | 0.47              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 12:2Q:5:ARG:O     | 21:2Z:194:PRO:HA   | 2.14                     | 0.47              |
| 21:2Z:31:ARG:HG3  | 21:2Z:32:HIS:CD2   | 2.49                     | 0.47              |
| 1:1A:2078:G:H1    | 27:15:3:LYS:HB3    | 1.78                     | 0.47              |
| 28:26:35:GLU:OE2  | 28:26:50:ARG:NH1   | 2.42                     | 0.47              |
| 1:2A:1062:G:O2'   | 1:2A:1063:G:H5'    | 2.14                     | 0.47              |
| 1:2A:1814:G:H2'   | 1:2A:1815:A:C8     | 2.48                     | 0.47              |
| 1:2A:586:A:N1     | 1:2A:809:G:O2'     | 2.40                     | 0.47              |
| 1:2A:605:C:H2'    | 1:2A:606:U:O4'     | 2.15                     | 0.47              |
| 1:1A:231:G:C8     | 30:18:5:LYS:HG2    | 2.49                     | 0.47              |
| 1:1A:1125:C:H41   | 1:1A:1134:A:P      | 2.37                     | 0.47              |
| 1:1A:2139:A:C2    | 1:1A:2141:A:H5'    | 2.50                     | 0.47              |
| 1:1A:2298:A:H4'   | 1:1A:2299:A:O4'    | 2.14                     | 0.47              |
| 1:1A:839:G:O2'    | 1:1A:2452:C:N3     | 2.43                     | 0.47              |
| 1:1A:818:G:OP1    | 29:17:10:ARG:NH1   | 2.47                     | 0.47              |
| 6:1G:28:VAL:O     | 6:1G:31:VAL:HG13   | 2.13                     | 0.47              |
| 11:1P:86:LYS:HB3  | 11:1P:118:GLY:HA3  | 1.95                     | 0.47              |
| 23:21:23:LYS:HB3  | 23:21:29:GLY:HA3   | 1.95                     | 0.47              |
| 1:2A:1186:G:C2    | 1:2A:1187:G:H1'    | 2.49                     | 0.47              |
| 1:2A:2023:G:H5'   | 1:2A:2617:C:H4'    | 1.95                     | 0.47              |
| 1:2A:2646:C:OP2   | 1:2A:2732:G:O2'    | 2.29                     | 0.47              |
| 1:2A:299:A:N3     | 1:2A:319:C:O2'     | 2.40                     | 0.47              |
| 1:2A:857:C:H2'    | 1:2A:858:U:C6      | 2.49                     | 0.47              |
| 6:2G:137:GLU:HG2  | 6:2G:152:LEU:HD22  | 1.95                     | 0.47              |
| 18:2W:71:VAL:HA   | 18:2W:107:LEU:HD12 | 1.96                     | 0.47              |
| 1:1A:1143:U:H3'   | 1:1A:1144:A:H8     | 1.79                     | 0.47              |
| 1:1A:1958:A:OP1   | 1:1A:1959:A:H5'    | 2.15                     | 0.47              |
| 1:1A:2099:A:H2'   | 1:1A:2100:C:H6     | 1.79                     | 0.47              |
| 6:1G:101:ILE:HG22 | 6:1G:105:LYS:HE2   | 1.96                     | 0.47              |
| 14:1S:39:ILE:HD11 | 14:1S:110:LEU:HD21 | 1.95                     | 0.47              |
| 30:28:56:GLU:HG2  | 30:28:57:ARG:N     | 2.30                     | 0.47              |
| 1:2A:1914:C:H2'   | 1:2A:1915:5MU:O4'  | 2.14                     | 0.47              |
| 1:2A:2319:G:C2    | 14:2S:3:ARG:HA     | 2.49                     | 0.47              |
| 1:2A:784:A:H5'    | 1:2A:785:G:OP1     | 2.14                     | 0.47              |
| 3:2D:108:PRO:HB3  | 3:2D:143:HIS:CE1   | 2.47                     | 0.47              |
| 21:2Z:99:TYR:HA   | 21:2Z:124:ILE:O    | 2.14                     | 0.47              |
| 1:1A:479:C:O2     | 1:1A:483:A:O2'     | 2.29                     | 0.47              |
| 5:1F:65:TRP:CZ2   | 5:1F:75:HIS:HD2    | 2.33                     | 0.47              |
| 12:1Q:6:ARG:C     | 12:1Q:7:MET:HG3    | 2.35                     | 0.47              |
| 21:1Z:145:GLU:O   | 21:1Z:148:ASP:N    | 2.24                     | 0.47              |
| 26:24:62:ARG:H    | 26:24:62:ARG:NH1   | 2.11                     | 0.47              |
| 1:2A:1084:A:H3'   | 1:2A:1085:A:H4'    | 1.95                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:2A:1688:U:O2     | 1:2A:1700:A:H5'    | 2.14                     | 0.47              |
| 5:2F:126:VAL:O     | 5:2F:196:LEU:HG    | 2.15                     | 0.47              |
| 19:2X:12:VAL:HG22  | 19:2X:29:TRP:CE2   | 2.50                     | 0.47              |
| 14:1S:20:ARG:NH2   | 22:10:47:PRO:HB2   | 2.30                     | 0.47              |
| 1:1A:2432:C:H5'    | 28:16:54:ILE:HD11  | 1.96                     | 0.47              |
| 1:1A:1102:G:H1'    | 1:1A:1149:A:H61    | 1.80                     | 0.47              |
| 1:1A:215:G:C2      | 1:1A:217:A:N6      | 2.82                     | 0.47              |
| 1:1A:2155:G:O2'    | 1:1A:2180:A:H2     | 1.97                     | 0.47              |
| 1:1A:776:G:OP2     | 3:1D:13:ARG:NH1    | 2.47                     | 0.47              |
| 6:1G:111:LEU:HA    | 6:1G:114:ILE:HD12  | 1.95                     | 0.47              |
| 1:2A:2869:G:H2'    | 1:2A:2870:C:O4'    | 2.14                     | 0.47              |
| 1:2A:323:G:H1'     | 1:2A:1205:U:O2     | 2.14                     | 0.47              |
| 1:2A:485:C:H2'     | 1:2A:486:C:C6      | 2.50                     | 0.47              |
| 3:2D:228:PRO:HD3   | 3:2D:235:GLY:HA3   | 1.96                     | 0.47              |
| 6:2G:11:TYR:CZ     | 6:2G:16:ARG:HD3    | 2.50                     | 0.47              |
| 10:2O:24:VAL:HB    | 10:2O:33:ALA:HB2   | 1.96                     | 0.47              |
| 12:2Q:141:GLN:HE22 | 21:2Z:74:VAL:HG13  | 1.79                     | 0.47              |
| 1:1A:69:G:H5''     | 1:1A:110:U:O2      | 2.14                     | 0.47              |
| 1:1A:1231:G:C2     | 1:1A:1232:G:H1'    | 2.49                     | 0.47              |
| 1:1A:1804:A:C5     | 1:1A:1860:A:H1'    | 2.49                     | 0.47              |
| 1:1A:1921:G:N3     | 1:1A:1921:G:H2'    | 2.29                     | 0.47              |
| 1:1A:346:A:OP2     | 5:1F:169:ASN:HB2   | 2.14                     | 0.47              |
| 13:1R:13:HIS:CE1   | 13:1R:16:HIS:HB2   | 2.49                     | 0.47              |
| 17:1V:14:VAL:HB    | 17:1V:96:ILE:HG13  | 1.96                     | 0.47              |
| 24:22:16:LEU:O     | 24:22:67:LYS:NZ    | 2.42                     | 0.47              |
| 30:28:23:VAL:HG11  | 30:28:47:LYS:HD3   | 1.95                     | 0.47              |
| 1:2A:1062:G:O6     | 1:2A:1088:A:H8     | 1.98                     | 0.47              |
| 1:2A:2561:A:H2     | 10:2O:23:ARG:NH2   | 2.12                     | 0.47              |
| 1:2A:882:G:H2'     | 1:2A:883:G:C8      | 2.49                     | 0.47              |
| 5:2F:21:ALA:CB     | 5:2F:22:ALA:HA     | 2.45                     | 0.47              |
| 6:2G:165:THR:OG1   | 6:2G:168:GLU:HG3   | 2.15                     | 0.47              |
| 7:2H:86:GLU:OE1    | 7:2H:130:ARG:HD2   | 2.15                     | 0.47              |
| 10:2O:102:VAL:HB   | 10:2O:106:LEU:HD12 | 1.95                     | 0.47              |
| 21:2Z:179:ASP:O    | 21:2Z:182:LYS:HG2  | 2.15                     | 0.47              |
| 24:12:3:LEU:HD22   | 24:12:7:ARG:HH21   | 1.80                     | 0.47              |
| 1:1A:1085:G:C6     | 1:1A:1162:C:N4     | 2.78                     | 0.47              |
| 1:1A:1113:A:H2'    | 1:1A:1113:A:N3     | 2.30                     | 0.47              |
| 1:1A:1688:A:H2'    | 1:1A:1689:G:O4'    | 2.13                     | 0.47              |
| 1:1A:1857:G:H4'    | 3:1D:242:ARG:NH1   | 2.30                     | 0.47              |
| 4:1E:51:PHE:CD2    | 4:1E:52:LEU:HG     | 2.49                     | 0.47              |
| 7:1H:20:ALA:HB1    | 7:1H:21:PRO:HD2    | 1.97                     | 0.47              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:2A:1296:G:OP1   | 1:2A:2709:G:O2'    | 2.22                     | 0.47              |
| 1:2A:1915:5MU:H3' | 1:2A:1916:A:C8     | 2.48                     | 0.47              |
| 1:2A:2111:C:H42   | 1:2A:2147:G:N2     | 2.03                     | 0.47              |
| 1:2A:2114:A:O2'   | 1:2A:2167:U:H5''   | 2.14                     | 0.47              |
| 1:2A:2206:G:C3'   | 1:2A:2207:G:H8     | 2.26                     | 0.47              |
| 1:2A:2331:G:O2'   | 1:2A:2336:A:N1     | 2.39                     | 0.47              |
| 1:2A:251:A:C5     | 1:2A:252:G:H1'     | 2.50                     | 0.47              |
| 1:2A:468:G:N7     | 29:27:39:ARG:NH2   | 2.57                     | 0.47              |
| 1:2A:493:G:H2'    | 1:2A:494:G:O4'     | 2.14                     | 0.47              |
| 9:2N:4:TYR:CD2    | 16:2U:100:VAL:HG11 | 2.49                     | 0.47              |
| 22:10:23:VAL:HG22 | 22:10:38:VAL:HG22  | 1.96                     | 0.47              |
| 28:16:18:ARG:HD3  | 28:16:42:TRP:CD1   | 2.49                     | 0.47              |
| 1:1A:1186:U:OP2   | 9:1N:63:THR:OG1    | 2.27                     | 0.47              |
| 1:1A:1287:A:H61   | 1:1A:1370:G:H21    | 74.08                    | 0.47              |
| 1:1A:664:U:H2'    | 1:1A:665:C:C6      | 2.49                     | 0.47              |
| 14:1S:61:ASN:O    | 14:1S:65:VAL:HG23  | 2.14                     | 0.47              |
| 15:1T:96:ARG:NH1  | 15:1T:96:ARG:HB2   | 2.29                     | 0.47              |
| 1:2A:875:G:H2'    | 1:2A:876:C:O4'     | 2.14                     | 0.47              |
| 6:2G:114:ILE:HG12 | 6:2G:140:ILE:HD13  | 1.97                     | 0.47              |
| 6:2G:28:VAL:O     | 6:2G:31:VAL:HG13   | 2.15                     | 0.47              |
| 1:1A:1617:A:H2'   | 1:1A:1618:A:C8     | 2.50                     | 0.47              |
| 1:1A:1925:G:OP1   | 3:1D:241:PRO:HB2   | 2.15                     | 0.47              |
| 1:1A:2346:G:H5'   | 14:1S:9:ARG:HG2    | 1.95                     | 0.47              |
| 2:1B:90:A:N7      | 2:1B:91:C:H1'      | 2.30                     | 0.47              |
| 4:1E:49:LEU:HD12  | 4:1E:49:LEU:HA     | 1.74                     | 0.47              |
| 6:1G:28:VAL:HG23  | 6:1G:29:TRP:CD1    | 2.49                     | 0.47              |
| 14:1S:82:ILE:HG22 | 14:1S:110:LEU:HD11 | 1.97                     | 0.47              |
| 15:1T:49:VAL:HG12 | 15:1T:63:VAL:HG22  | 1.96                     | 0.47              |
| 21:1Z:146:ILE:HA  | 21:1Z:147:GLY:HA2  | 1.71                     | 0.47              |
| 1:2A:2108:C:H2'   | 1:2A:2109:U:O4'    | 2.14                     | 0.47              |
| 1:2A:2115:G:N1    | 1:2A:2119:A:OP2    | 2.40                     | 0.47              |
| 1:2A:2870:C:H2'   | 1:2A:2871:C:O4'    | 2.14                     | 0.47              |
| 1:2A:923:C:H2'    | 1:2A:924:C:C6      | 2.50                     | 0.47              |
| 2:2B:52:A:N6      | 14:2S:33:LYS:HG2   | 2.29                     | 0.47              |
| 21:2Z:110:GLY:HA3 | 21:2Z:174:VAL:HG11 | 1.97                     | 0.47              |
| 1:1A:532:A:H5''   | 1:1A:533:G:H3'     | 1.97                     | 0.47              |
| 1:1A:629:U:H4'    | 1:1A:705:C:H4'     | 1.96                     | 0.47              |
| 19:2X:60:ARG:HH22 | 29:27:47:ARG:HH22  | 1.62                     | 0.47              |
| 1:2A:1906:G:H1    | 1:2A:1924:C:H42    | 1.63                     | 0.47              |
| 1:2A:2124:G:N1    | 1:2A:2174:C:O2     | 2.47                     | 0.47              |
| 5:2F:195:ASP:OD1  | 5:2F:196:LEU:N     | 2.47                     | 0.47              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 7:2H:72:ILE:O     | 7:2H:76:VAL:HG23   | 2.15                     | 0.47              |
| 17:2V:4:ILE:HD12  | 17:2V:39:LEU:HD22  | 1.97                     | 0.47              |
| 21:2Z:182:LYS:O   | 21:2Z:185:GLU:HG3  | 2.14                     | 0.47              |
| 1:1A:1287:A:N6    | 1:1A:1370:G:H21    | 73.36                    | 0.46              |
| 1:1A:97:G:P       | 24:12:2:LYS:HG2    | 2.55                     | 0.46              |
| 3:1D:148:GLU:HB2  | 3:1D:151:LYS:HD2   | 1.96                     | 0.46              |
| 4:1E:19:ARG:NH1   | 10:1O:72:PRO:HB3   | 2.29                     | 0.46              |
| 12:1Q:59:ARG:HA   | 21:1Z:180:VAL:HG23 | 1.96                     | 0.46              |
| 1:2A:1365:A:O2'   | 23:21:11:ARG:NH2   | 2.48                     | 0.46              |
| 26:24:15:ILE:HG23 | 26:24:21:VAL:HG22  | 1.96                     | 0.46              |
| 1:2A:1024:G:H2'   | 1:2A:1024:G:N3     | 3.44                     | 0.46              |
| 1:2A:1059:G:C6    | 1:2A:1060:U:N3     | 2.83                     | 0.46              |
| 1:2A:2321:G:N3    | 1:2A:2321:G:H2'    | 2.30                     | 0.46              |
| 1:2A:2698:U:H2'   | 1:2A:2699:C:C6     | 2.50                     | 0.46              |
| 1:2A:637:A:H8     | 11:2P:117:GLU:HG3  | 1.80                     | 0.46              |
| 1:1A:1541:A:H2'   | 1:1A:1542:A:C8     | 2.50                     | 0.46              |
| 1:1A:278:G:H2'    | 1:1A:279:G:H5''    | 1.96                     | 0.46              |
| 1:1A:597:C:N3     | 4:1E:145:LYS:NZ    | 2.62                     | 0.46              |
| 1:1A:875:U:H2'    | 1:1A:876:A:C8      | 2.49                     | 0.46              |
| 21:1Z:7:ALA:HB2   | 21:1Z:59:LEU:HD22  | 1.97                     | 0.46              |
| 1:2A:729:G:C5     | 3:2D:208:LYS:HB2   | 2.51                     | 0.46              |
| 6:2G:33:ARG:HH21  | 6:2G:162:THR:HG21  | 1.79                     | 0.46              |
| 13:2R:98:LEU:HB2  | 13:2R:113:LEU:HD11 | 1.96                     | 0.46              |
| 1:1A:1451:U:H2'   | 1:1A:1452:U:H6     | 1.78                     | 0.46              |
| 1:1A:1831:C:OP1   | 3:1D:260:ARG:NH2   | 2.48                     | 0.46              |
| 1:1A:1957:G:H1'   | 1:1A:1986:G:N2     | 2.30                     | 0.46              |
| 1:1A:2021:C:H4'   | 1:1A:2736:C:O2     | 2.16                     | 0.46              |
| 1:1A:337:C:H2'    | 1:1A:338:A:C8      | 2.97                     | 0.46              |
| 3:1D:111:LEU:HA   | 3:1D:111:LEU:HD23  | 1.81                     | 0.46              |
| 5:1F:102:PRO:HB2  | 5:1F:105:VAL:HG23  | 1.98                     | 0.46              |
| 1:2A:1783:A:H5'   | 1:2A:2608:G:H4'    | 1.97                     | 0.46              |
| 9:2N:30:ILE:HG23  | 9:2N:52:VAL:HG11   | 1.96                     | 0.46              |
| 21:2Z:67:LEU:HA   | 21:2Z:68:PRO:HD3   | 1.74                     | 0.46              |
| 22:10:43:THR:OG1  | 22:10:46:LYS:HG2   | 2.15                     | 0.46              |
| 1:1A:645:G:N3     | 1:1A:645:G:H5'     | 2.30                     | 0.46              |
| 1:1A:661:G:H1     | 1:1A:744:C:H42     | 107.45                   | 0.46              |
| 1:2A:1117:G:H2'   | 1:2A:1118:C:C6     | 2.50                     | 0.46              |
| 5:2F:192:LEU:HD13 | 5:2F:194:MET:HE2   | 1.97                     | 0.46              |
| 1:1A:1291:G:OP1   | 11:1P:13:ASN:ND2   | 2.42                     | 0.46              |
| 1:1A:1496:A:N3    | 1:1A:1576:G:H1'    | 2.31                     | 0.46              |
| 1:1A:1633:A:H2'   | 1:1A:1634:C:C6     | 2.51                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1A:1845:G:H4'   | 3:1D:51:VAL:HG21  | 1.98                     | 0.46              |
| 1:1A:2039:U:O2    | 27:15:10:LYS:HB2  | 2.16                     | 0.46              |
| 1:1A:2098:U:OP2   | 1:1A:2250:G:N2    | 2.43                     | 0.46              |
| 1:1A:632:A:H5'    | 1:1A:633:G:OP2    | 5.42                     | 0.46              |
| 1:1A:92:C:H2'     | 1:1A:93:G:C8      | 3.49                     | 0.46              |
| 1:2A:1111:A:O2'   | 1:2A:1112:G:H4'   | 2.16                     | 0.46              |
| 1:2A:322:A:OP1    | 5:2F:168:ARG:HD2  | 2.15                     | 0.46              |
| 5:2F:155:LEU:HD11 | 5:2F:176:LEU:HD12 | 1.98                     | 0.46              |
| 7:2H:11:VAL:HB    | 7:2H:48:GLY:HA2   | 1.97                     | 0.46              |
| 8:2I:57:ARG:O     | 8:2I:61:ARG:HG2   | 2.15                     | 0.46              |
| 11:2P:63:PRO:HG2  | 30:28:25:MET:HB2  | 1.97                     | 0.46              |
| 13:2R:29:LEU:HD11 | 13:2R:48:VAL:HG13 | 1.97                     | 0.46              |
| 19:2X:95:LEU:H    | 19:2X:95:LEU:HD12 | 1.80                     | 0.46              |
| 25:13:59:VAL:HG23 | 25:13:60:GLU:HG2  | 1.96                     | 0.46              |
| 1:1A:2108:U:H2'   | 1:1A:2109:G:H8    | 1.80                     | 0.46              |
| 1:1A:2156:A:O2'   | 1:1A:2181:G:N3    | 2.38                     | 0.46              |
| 1:1A:236:G:H4'    | 1:1A:413:G:C6     | 2.50                     | 0.46              |
| 1:1A:2859:U:H4'   | 1:1A:2878:A:C2    | 2.51                     | 0.46              |
| 2:1B:78:A:C2      | 2:1B:100:A:C4     | 3.03                     | 0.46              |
| 13:1R:54:LEU:HA   | 13:1R:54:LEU:HD12 | 1.75                     | 0.46              |
| 1:2A:264:C:O2'    | 1:2A:265:A:H2'    | 2.16                     | 0.46              |
| 6:2G:60:LEU:HA    | 6:2G:63:ILE:HD12  | 1.98                     | 0.46              |
| 18:2W:12:ILE:HD12 | 18:2W:42:ARG:HD3  | 1.98                     | 0.46              |
| 1:1A:2473:C:H2'   | 1:1A:2474:U:C6    | 2.51                     | 0.46              |
| 4:1E:119:ARG:HG2  | 4:1E:160:TYR:CG   | 2.51                     | 0.46              |
| 4:1E:35:GLN:OE1   | 4:1E:66:HIS:HE1   | 1.98                     | 0.46              |
| 6:1G:143:GLU:OE2  | 26:14:26:SER:OG   | 2.21                     | 0.46              |
| 16:1U:52:ARG:HB2  | 16:1U:52:ARG:HE   | 1.54                     | 0.46              |
| 2:1B:104:U:O2'    | 21:1Z:72:ARG:HG2  | 2.15                     | 0.46              |
| 1:2A:2102:U:H2'   | 1:2A:2103:C:C1'   | 2.45                     | 0.46              |
| 1:2A:2311:A:H5''  | 6:2G:77:ILE:HD11  | 1.97                     | 0.46              |
| 1:2A:2370:G:C6    | 1:2A:2371:G:C6    | 3.04                     | 0.46              |
| 1:2A:603:A:O4'    | 1:2A:655:A:N6     | 2.48                     | 0.46              |
| 1:2A:879:G:H2'    | 1:2A:880:G:O4'    | 2.15                     | 0.46              |
| 13:2R:56:LYS:NZ   | 13:2R:90:ARG:O    | 2.47                     | 0.46              |
| 18:2W:70:TYR:OH   | 18:2W:72:LYS:HG3  | 2.14                     | 0.46              |
| 30:18:17:THR:OG1  | 30:18:21:LYS:HB2  | 2.16                     | 0.46              |
| 1:1A:442:A:H2'    | 1:1A:443:C:C6     | 2.51                     | 0.46              |
| 2:1B:73:A:C4      | 2:1B:105:A:C2     | 3.04                     | 0.46              |
| 2:1B:90:A:C5      | 2:1B:91:C:H1'     | 2.50                     | 0.46              |
| 23:21:64:ALA:HA   | 23:21:67:ILE:HG13 | 1.96                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:21:85:LEU:HB3  | 23:21:89:GLU:HB2  | 1.98                     | 0.46              |
| 1:2A:1914:C:P     | 1:2A:1914:C:H6    | 2.38                     | 0.46              |
| 1:2A:2454:G:P     | 20:2Y:2:ARG:HH22  | 99.35                    | 0.46              |
| 1:2A:2615:U:H2'   | 1:2A:2616:C:H6    | 1.81                     | 0.46              |
| 1:2A:2734:A:H2'   | 1:2A:2735:G:O4'   | 2.16                     | 0.46              |
| 1:2A:588:U:H1'    | 5:2F:90:PHE:HB3   | 1.97                     | 0.46              |
| 2:2B:4:C:H42      | 2:2B:117:G:H1     | 1.62                     | 0.46              |
| 2:2B:78:A:H2'     | 2:2B:79:C:O4'     | 2.16                     | 0.46              |
| 8:2I:9:LEU:HD11   | 8:2I:35:LEU:HB3   | 1.98                     | 0.46              |
| 1:1A:2650:G:OP2   | 4:1E:82:ARG:NH1   | 2.43                     | 0.46              |
| 6:1G:148:MET:H    | 6:1G:148:MET:HG2  | 1.62                     | 0.46              |
| 6:1G:72:ARG:HG3   | 6:1G:72:ARG:HH11  | 4.47                     | 0.46              |
| 7:1H:164:TYR:HB2  | 7:1H:167:GLU:HB2  | 1.98                     | 0.46              |
| 13:1R:103:ARG:NH1 | 13:1R:108:GLY:O   | 2.48                     | 0.46              |
| 1:2A:1441:G:H5''  | 1:2A:1442:G:H5'   | 5.63                     | 0.46              |
| 1:2A:2138:C:C2    | 1:2A:2153:G:N2    | 2.84                     | 0.46              |
| 1:2A:2314:C:H2'   | 1:2A:2315:G:C8    | 2.50                     | 0.46              |
| 1:2A:2314:C:H2'   | 1:2A:2315:G:H8    | 1.81                     | 0.46              |
| 1:2A:2410:G:H2'   | 1:2A:2411:A:O4'   | 2.16                     | 0.46              |
| 1:2A:824:A:H1'    | 1:2A:2358:G:N7    | 2.31                     | 0.46              |
| 2:2B:82:G:H5''    | 60:2B:3118:HOH:O  | 2.16                     | 0.46              |
| 7:2H:144:VAL:O    | 7:2H:148:ILE:HG12 | 2.16                     | 0.46              |
| 7:2H:46:GLU:HB2   | 7:2H:49:VAL:HG12  | 1.97                     | 0.46              |
| 19:2X:36:LYS:HG2  | 19:2X:56:THR:HG23 | 1.98                     | 0.46              |
| 1:1A:1091:A:H1'   | 1:1A:1093:G:C2    | 2.49                     | 0.46              |
| 1:1A:1314:A:C2    | 1:1A:2035:A:C4    | 3.04                     | 0.46              |
| 1:1A:2390:A:H8    | 1:1A:2390:A:O5'   | 1.98                     | 0.46              |
| 23:21:83:GLU:HA   | 23:21:84:GLY:HA2  | 1.65                     | 0.46              |
| 1:2A:224:G:N7     | 1:2A:420:C:H4'    | 2.31                     | 0.46              |
| 1:2A:668:G:H5'    | 1:2A:669:G:OP2    | 2.15                     | 0.46              |
| 1:1A:1821:C:H5''  | 1:1A:1822:A:OP1   | 2.16                     | 0.45              |
| 1:1A:1954:A:H2'   | 1:1A:1955:G:O4'   | 2.16                     | 0.45              |
| 1:1A:2136:A:N3    | 1:1A:2137:G:H1'   | 2.31                     | 0.45              |
| 4:1E:18:ASP:HA    | 15:1T:82:LEU:HD11 | 1.98                     | 0.45              |
| 4:1E:51:PHE:H     | 4:1E:75:VAL:CG1   | 2.29                     | 0.45              |
| 6:1G:161:THR:HG22 | 6:1G:162:THR:N    | 2.31                     | 0.45              |
| 29:27:24:THR:O    | 29:27:28:ARG:HG3  | 2.17                     | 0.45              |
| 1:2A:1430:C:H2'   | 1:2A:1431:U:C6    | 2.51                     | 0.45              |
| 1:2A:1575:C:H2'   | 1:2A:1576:U:O4'   | 2.15                     | 0.45              |
| 1:2A:1681:G:O5'   | 1:2A:1681:G:H8    | 1.99                     | 0.45              |
| 1:2A:1930:G:N2    | 1:2A:1968:G:H2'   | 2.31                     | 0.45              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:2A:2157:G:C8    | 1:2A:2157:G:H3'    | 2.51                     | 0.45              |
| 1:2A:2889:C:H2'   | 1:2A:2891:G:O4'    | 2.16                     | 0.45              |
| 1:1A:1171:G:H5'   | 31:19:37:GLY:HA2   | 1.98                     | 0.45              |
| 1:1A:303:C:N3     | 1:1A:385:G:N2      | 2.45                     | 0.45              |
| 1:1A:354:A:H2     | 1:1A:1255:A:O2'    | 1.78                     | 0.45              |
| 1:1A:641:G:OP2    | 5:1F:43:LYS:NZ     | 2.42                     | 0.45              |
| 6:1G:150:ASP:OD1  | 6:1G:151:ALA:N     | 2.49                     | 0.45              |
| 8:1I:72:LEU:HD12  | 8:1I:138:ILE:HG21  | 1.97                     | 0.45              |
| 1:1A:872:C:O2     | 11:1P:55:ARG:NH1   | 2.48                     | 0.45              |
| 19:1X:11:PRO:HB3  | 19:1X:92:LEU:HD11  | 1.99                     | 0.45              |
| 1:2A:1180:C:H2'   | 1:2A:1181:C:C6     | 2.51                     | 0.45              |
| 1:2A:1218:C:H42   | 1:2A:1231:G:H1     | 1.63                     | 0.45              |
| 1:2A:272(B):G:H2' | 1:2A:272(C):G:C8   | 2.50                     | 0.45              |
| 1:2A:608:A:C6     | 1:2A:609:A:C6      | 3.04                     | 0.45              |
| 1:2A:656:G:H2'    | 1:2A:657:U:O4'     | 2.16                     | 0.45              |
| 1:2A:828:U:H4'    | 1:2A:831:G:N1      | 2.30                     | 0.45              |
| 6:2G:72:ARG:HG3   | 6:2G:72:ARG:HH11   | 4.45                     | 0.45              |
| 7:2H:6:ARG:HE     | 7:2H:6:ARG:HB2     | 1.28                     | 0.45              |
| 1:2A:811:U:H2'    | 11:2P:21:ARG:HA    | 1.97                     | 0.45              |
| 21:2Z:10:ARG:HB2  | 21:2Z:36:LYS:HB3   | 1.97                     | 0.45              |
| 1:1A:1093:G:H2'   | 1:1A:1156:G:H1     | 1.81                     | 0.45              |
| 1:1A:2156:A:C5    | 1:1A:2179:G:H4'    | 2.51                     | 0.45              |
| 1:1A:416:G:H8     | 1:1A:416:G:O5'     | 1.99                     | 0.45              |
| 18:1W:71:VAL:HA   | 18:1W:107:LEU:HD12 | 1.99                     | 0.45              |
| 19:1X:27:THR:HG23 | 19:1X:80:ILE:HG12  | 1.98                     | 0.45              |
| 1:2A:2395:C:O2'   | 23:21:30:VAL:HG23  | 2.17                     | 0.45              |
| 1:2A:1517:G:H1'   | 1:2A:1919:A:O3'    | 103.05                   | 0.45              |
| 1:2A:1667:G:O2'   | 1:2A:1991:U:O4     | 2.26                     | 0.45              |
| 1:2A:2809:A:OP2   | 1:2A:2891:G:N1     | 2.47                     | 0.45              |
| 1:2A:603:A:N1     | 1:2A:625:G:O2'     | 2.40                     | 0.45              |
| 1:2A:752:A:H4'    | 1:2A:753:C:H5'     | 1.97                     | 0.45              |
| 2:2B:59:A:H2'     | 2:2B:60:C:O4'      | 2.17                     | 0.45              |
| 5:2F:129:PHE:CD2  | 5:2F:163:VAL:HG21  | 2.50                     | 0.45              |
| 21:2Z:70:LEU:HD11 | 21:2Z:98:MET:SD    | 2.56                     | 0.45              |
| 1:1A:2119:C:H2'   | 1:1A:2120:U:O4'    | 2.17                     | 0.45              |
| 1:1A:517:A:H2'    | 1:1A:518:G:O4'     | 2.16                     | 0.45              |
| 6:1G:11:TYR:HA    | 6:1G:15:VAL:HB     | 1.98                     | 0.45              |
| 11:1P:96:THR:H    | 11:1P:99:LEU:HD12  | 1.81                     | 0.45              |
| 18:1W:37:ARG:HG2  | 18:1W:38:TYR:CE2   | 2.51                     | 0.45              |
| 1:2A:1450:G:H2'   | 1:2A:1450(A):C:H6  | 1.81                     | 0.45              |
| 1:2A:2615:U:H2'   | 1:2A:2616:C:C6     | 2.51                     | 0.45              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:2A:918:A:OP2     | 1:2A:2268:A:N6    | 2.45                     | 0.45              |
| 6:2G:77:ILE:HG22   | 6:2G:80:PHE:H     | 1.81                     | 0.45              |
| 21:2Z:150:LEU:HD12 | 21:2Z:150:LEU:HA  | 1.84                     | 0.45              |
| 1:1A:1732:C:H2'    | 1:1A:1733:C:H6    | 1.81                     | 0.45              |
| 1:1A:2208:G:C2     | 1:1A:2209:G:C8    | 3.04                     | 0.45              |
| 1:1A:1709:C:O2'    | 1:1A:2699:U:OP1   | 2.33                     | 0.45              |
| 1:1A:276:C:H2'     | 1:1A:277:G:O4'    | 2.17                     | 0.45              |
| 3:1D:168:ARG:HA    | 3:1D:168:ARG:HD3  | 4.05                     | 0.45              |
| 4:1E:51:PHE:HB3    | 4:1E:77:ILE:HD12  | 1.98                     | 0.45              |
| 31:29:10:ILE:HD12  | 31:29:32:HIS:HA   | 1.97                     | 0.45              |
| 1:2A:1167:U:H2'    | 1:2A:1168:G:H8    | 1.82                     | 0.45              |
| 1:2A:1889:A:C6     | 1:2A:1890:A:C6    | 3.04                     | 0.45              |
| 1:2A:2273:A:H2'    | 1:2A:2274:A:C8    | 2.52                     | 0.45              |
| 5:2F:34:TRP:NE1    | 11:2P:8:PRO:HD3   | 2.31                     | 0.45              |
| 8:2I:92:VAL:HG23   | 8:2I:120:ILE:HB   | 1.99                     | 0.45              |
| 23:11:3:LYS:HB3    | 23:11:61:ARG:HH22 | 1.82                     | 0.45              |
| 1:1A:2167:C:H6     | 1:1A:2167:C:OP1   | 1.99                     | 0.45              |
| 1:1A:518:G:H2'     | 1:1A:519:G:O4'    | 2.16                     | 0.45              |
| 3:1D:61:LEU:O      | 3:1D:63:ARG:NH1   | 2.45                     | 0.45              |
| 1:1A:2797:C:H1'    | 4:1E:37:ARG:HH12  | 1.82                     | 0.45              |
| 6:1G:7:LEU:HA      | 6:1G:7:LEU:HD23   | 1.75                     | 0.45              |
| 21:1Z:30:ASN:HD22  | 21:1Z:90:VAL:HB   | 1.81                     | 0.45              |
| 25:23:57:GLU:HG2   | 25:23:59:VAL:HG13 | 1.99                     | 0.45              |
| 1:2A:1077:A:C6     | 1:2A:1078:U:O4    | 2.70                     | 0.45              |
| 19:2X:60:ARG:HH22  | 29:27:47:ARG:HH12 | 1.64                     | 0.45              |
| 20:2Y:81:LYS:HB3   | 20:2Y:81:LYS:HE3  | 1.85                     | 0.45              |
| 28:16:10:LEU:HD23  | 28:16:22:ALA:HB2  | 1.98                     | 0.45              |
| 1:1A:1188:A:C4     | 1:1A:1190:G:N7    | 2.85                     | 0.45              |
| 1:1A:1239:A:H62    | 1:1A:1299:A:N6    | 20.77                    | 0.45              |
| 1:1A:1435:G:H2'    | 1:1A:1436:U:H6    | 2.54                     | 0.45              |
| 1:1A:1529:G:H4'    | 1:1A:1530:G:OP2   | 4.56                     | 0.45              |
| 15:1T:120:ARG:HA   | 15:1T:123:GLN:HB3 | 1.98                     | 0.45              |
| 1:2A:1472:A:H61    | 1:2A:1519:G:H1'   | 1.81                     | 0.45              |
| 1:2A:1799:G:O3'    | 3:2D:183:ARG:NH1  | 2.48                     | 0.45              |
| 1:2A:1935:G:H1'    | 1:2A:1964:G:N2    | 2.31                     | 0.45              |
| 4:2E:50:GLY:O      | 4:2E:51:PHE:HB2   | 2.15                     | 0.45              |
| 7:2H:124:GLU:HB2   | 7:2H:132:ARG:HB3  | 1.97                     | 0.45              |
| 9:2N:20:GLY:O      | 9:2N:61:ARG:NE    | 2.48                     | 0.45              |
| 20:2Y:20:TYR:HB3   | 20:2Y:23:ARG:HG3  | 1.99                     | 0.45              |
| 26:14:62:ARG:O     | 26:14:64:GLY:HA2  | 2.17                     | 0.45              |
| 1:1A:1405:A:N1     | 1:1A:1418:U:C4    | 2.81                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1A:2157:A:N6    | 1:1A:2178:G:O2'   | 2.49                     | 0.45              |
| 1:1A:27:G:H22     | 1:1A:537:G:H1'    | 1.82                     | 0.45              |
| 9:1N:108:PRO:O    | 9:1N:113:GLY:HA3  | 2.16                     | 0.45              |
| 21:1Z:200:GLY:C   | 21:1Z:202:GLU:H   | 2.20                     | 0.45              |
| 1:2A:1784:A:H4'   | 1:2A:1785:A:O5'   | 2.17                     | 0.45              |
| 1:2A:1914:C:H2'   | 1:2A:1915:5MU:O2  | 2.17                     | 0.45              |
| 1:2A:272(E):G:C2  | 1:2A:364:C:C2     | 3.05                     | 0.45              |
| 1:2A:361:G:O2'    | 1:2A:362:U:H5'    | 2.17                     | 0.45              |
| 7:2H:118:PRO:HD2  | 7:2H:121:ILE:HG13 | 1.98                     | 0.45              |
| 22:10:27:GLU:HB2  | 22:10:69:PHE:HD1  | 1.82                     | 0.45              |
| 1:1A:1968:U:H2'   | 1:1A:1969:C:C6    | 2.51                     | 0.45              |
| 1:1A:2648:U:H2'   | 1:1A:2649:U:C6    | 2.52                     | 0.45              |
| 2:1B:41:U:C4      | 6:1G:70:VAL:HB    | 2.52                     | 0.45              |
| 6:1G:45:GLU:H     | 6:1G:45:GLU:HG2   | 1.44                     | 0.45              |
| 16:1U:16:LYS:HB3  | 16:1U:16:LYS:HE2  | 1.63                     | 0.45              |
| 26:24:46:GLN:HE21 | 26:24:48:ARG:HH12 | 1.64                     | 0.45              |
| 1:2A:1418:G:H8    | 1:2A:1418:G:O5'   | 2.00                     | 0.45              |
| 1:2A:1857:G:C6    | 1:2A:1858:G:C6    | 3.04                     | 0.45              |
| 1:2A:2139:C:N4    | 1:2A:2152:G:H1    | 2.15                     | 0.45              |
| 11:2P:70:GLN:O    | 11:2P:73:GLY:N    | 2.42                     | 0.45              |
| 18:2W:59:VAL:HG12 | 18:2W:60:ASN:ND2  | 2.32                     | 0.45              |
| 1:1A:2148:A:H1'   | 1:1A:2184:G:N2    | 2.32                     | 0.45              |
| 1:1A:2023:A:H4'   | 1:1A:2701:U:H2'   | 1.99                     | 0.45              |
| 1:1A:722:A:C8     | 1:1A:851:A:C6     | 3.05                     | 0.45              |
| 9:1N:26:LEU:HG    | 9:1N:30:ILE:HD11  | 2.00                     | 0.45              |
| 25:23:10:LYS:NZ   | 25:23:15:TYR:OH   | 2.50                     | 0.45              |
| 31:29:22:ARG:HD3  | 31:29:35:ARG:HD2  | 1.97                     | 0.45              |
| 1:2A:1246:A:OP1   | 5:2F:38:ARG:NH1   | 2.46                     | 0.45              |
| 1:2A:1721:G:O6    | 1:2A:1739:U:H5''  | 2.17                     | 0.45              |
| 1:2A:236:C:H2'    | 1:2A:237:C:C6     | 2.52                     | 0.45              |
| 1:2A:2462:U:H1'   | 1:2A:2491:U:O4    | 2.16                     | 0.45              |
| 1:2A:2585:U:O2'   | 60:2A:4007:HOH:O  | 2.21                     | 0.45              |
| 1:2A:2711:A:OP1   | 1:2A:2712:U:H3'   | 2.17                     | 0.45              |
| 5:2F:107:LYS:NZ   | 5:2F:205:ARG:O    | 2.29                     | 0.45              |
| 7:2H:149:ARG:HD3  | 7:2H:164:TYR:CE2  | 2.52                     | 0.45              |
| 8:2I:104:GLN:HG2  | 8:2I:105:HIS:CD2  | 2.52                     | 0.45              |
| 1:1A:154:G:C6     | 1:1A:155:C:N4     | 2.85                     | 0.44              |
| 1:1A:1750:G:H2'   | 1:1A:1751:G:C8    | 2.52                     | 0.44              |
| 1:1A:1849:U:H4'   | 1:1A:1852:A:H1'   | 1.99                     | 0.44              |
| 1:1A:2319:G:H4'   | 1:1A:2320:G:O5'   | 2.17                     | 0.44              |
| 1:1A:2531:U:C6    | 1:1A:2554:A:N6    | 2.85                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:1A:718:C:N4      | 60:1A:9031:HOH:O   | 2.50                     | 0.44              |
| 1:2A:1068:G:H3'    | 1:2A:1096:A:OP2    | 2.17                     | 0.44              |
| 1:2A:340:A:H2'     | 1:2A:341:G:O4'     | 2.17                     | 0.44              |
| 1:2A:35:G:H1'      | 1:2A:454:A:C4      | 2.53                     | 0.44              |
| 1:2A:98:G:C6       | 1:2A:99:U:C4       | 9.85                     | 0.44              |
| 9:2N:130:HIS:O     | 9:2N:133:GLN:HG2   | 2.16                     | 0.44              |
| 1:2A:1012:U:C5     | 9:2N:28:THR:HG21   | 2.52                     | 0.44              |
| 10:2O:115:VAL:HG13 | 10:2O:121:VAL:HG21 | 1.98                     | 0.44              |
| 1:1A:1952:G:O2'    | 1:1A:1990:G:O6     | 2.29                     | 0.44              |
| 1:1A:2713:C:H2'    | 1:1A:2714:U:H2'    | 1.99                     | 0.44              |
| 1:1A:2639:G:N2     | 1:1A:2790:G:OP2    | 2.47                     | 0.44              |
| 1:1A:337:C:H2'     | 1:1A:338:A:H8      | 2.27                     | 0.44              |
| 1:1A:385:G:N1      | 1:1A:386:U:C4      | 2.85                     | 0.44              |
| 1:1A:590:A:OP2     | 11:1P:29:LYS:NZ    | 2.40                     | 0.44              |
| 1:1A:673:G:N2      | 1:1A:674:G:C2      | 4.31                     | 0.44              |
| 6:1G:131:TYR:HB3   | 6:1G:159:VAL:HG13  | 1.99                     | 0.44              |
| 7:1H:3:ARG:HH21    | 7:1H:65:HIS:HB3    | 1.82                     | 0.44              |
| 23:21:50:ARG:NH1   | 23:21:57:GLU:OE2   | 2.50                     | 0.44              |
| 1:2A:1050:A:H2'    | 1:2A:1051:G:O4'    | 2.16                     | 0.44              |
| 1:2A:1085:A:H2'    | 1:2A:1086:A:C2     | 2.53                     | 0.44              |
| 1:2A:212:G:H2'     | 1:2A:213:A:O4'     | 2.17                     | 0.44              |
| 2:2B:42:C:C4       | 2:2B:43:C:C4       | 3.05                     | 0.44              |
| 1:2A:1007:C:H5''   | 9:2N:35:ARG:HH11   | 1.82                     | 0.44              |
| 12:2Q:36:ALA:HB2   | 12:2Q:103:MET:SD   | 2.57                     | 0.44              |
| 19:2X:35:THR:HG22  | 19:2X:38:GLU:H     | 1.82                     | 0.44              |
| 1:1A:1530:G:OP1    | 1:1A:1530:G:H4'    | 4.86                     | 0.44              |
| 1:1A:1809:U:H2'    | 1:1A:1815:A:N6     | 2.33                     | 0.44              |
| 1:1A:2073:A:H8     | 1:1A:2073:A:OP2    | 2.00                     | 0.44              |
| 1:1A:2137:G:N2     | 1:1A:2141:A:C8     | 2.85                     | 0.44              |
| 1:1A:2612:A:N6     | 60:1A:9038:HOH:O   | 2.50                     | 0.44              |
| 1:2A:1067:A:N3     | 1:2A:1068:G:H1'    | 9.30                     | 0.44              |
| 1:2A:1115:G:H2'    | 1:2A:1116:C:H6     | 1.82                     | 0.44              |
| 1:2A:1131:G:C2     | 1:2A:1132:A:C4     | 3.05                     | 0.44              |
| 1:2A:2022:U:O2'    | 1:2A:2617:C:H5'    | 2.17                     | 0.44              |
| 1:2A:2489:G:C6     | 1:2A:2490:G:C6     | 3.06                     | 0.44              |
| 1:2A:2602:A:H4'    | 1:2A:2603:G:C5'    | 2.47                     | 0.44              |
| 1:2A:1297:C:OP1    | 1:2A:2710:C:H4'    | 2.17                     | 0.44              |
| 3:2D:155:LEU:HD23  | 3:2D:177:LEU:HD21  | 1.99                     | 0.44              |
| 21:2Z:14:LYS:HE3   | 21:2Z:16:SER:OG    | 2.17                     | 0.44              |
| 1:1A:1822:A:H3'    | 1:1A:1823:G:H8     | 1.81                     | 0.44              |
| 1:1A:2053:A:C6     | 1:1A:2510:C:H1'    | 2.51                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1A:2784:C:H2'   | 1:1A:2785:C:C6    | 2.53                     | 0.44              |
| 1:1A:564:G:H2'    | 1:1A:565:C:H6     | 1.81                     | 0.44              |
| 14:1S:58:LEU:HD23 | 14:1S:58:LEU:HA   | 1.74                     | 0.44              |
| 17:1V:76:LYS:HD2  | 17:1V:81:TYR:CD2  | 2.51                     | 0.44              |
| 30:28:29:LYS:NZ   | 30:28:45:GLY:HA2  | 2.32                     | 0.44              |
| 1:2A:1178:C:H2'   | 1:2A:1179:C:C6    | 2.52                     | 0.44              |
| 1:2A:1359:A:N3    | 1:2A:1359:A:H5'   | 2.33                     | 0.44              |
| 1:2A:1778:U:H2'   | 1:2A:1784:A:N6    | 2.32                     | 0.44              |
| 1:2A:708:C:H2'    | 1:2A:709:U:C6     | 2.52                     | 0.44              |
| 1:2A:833:U:H2'    | 1:2A:834:C:H6     | 2.12                     | 0.44              |
| 3:2D:175:LEU:HD12 | 3:2D:185:VAL:HG21 | 1.98                     | 0.44              |
| 16:2U:17:ILE:HG23 | 16:2U:39:LEU:HD12 | 2.00                     | 0.44              |
| 16:2U:49:HIS:HA   | 16:2U:52:ARG:HB3  | 2.00                     | 0.44              |
| 20:2Y:76:CYS:SG   | 20:2Y:78:ALA:HB3  | 2.56                     | 0.44              |
| 1:1A:2211:U:H2'   | 1:1A:2212:G:H8    | 1.82                     | 0.44              |
| 1:1A:2255:U:H2'   | 1:1A:2256:U:C6    | 2.52                     | 0.44              |
| 1:1A:2368:C:H2'   | 1:1A:2369:U:O4'   | 2.17                     | 0.44              |
| 1:1A:801:C:H2'    | 1:1A:802:C:C6     | 2.52                     | 0.44              |
| 2:1B:77:U:OP1     | 21:1Z:19:ARG:NH2  | 2.51                     | 0.44              |
| 21:1Z:77:ASP:OD2  | 21:1Z:80:ARG:NH1  | 2.46                     | 0.44              |
| 26:24:40:HIS:O    | 26:24:44:THR:HG22 | 2.17                     | 0.44              |
| 1:2A:1790:C:H5''  | 1:2A:1791:A:OP1   | 2.17                     | 0.44              |
| 1:2A:2328:A:H2'   | 1:2A:2329:G:C8    | 2.52                     | 0.44              |
| 1:2A:2649:U:H2'   | 1:2A:2650:U:C6    | 2.53                     | 0.44              |
| 1:2A:2660:A:H2'   | 1:2A:2661:G:O4'   | 2.18                     | 0.44              |
| 1:2A:861:A:C6     | 1:2A:917:A:C8     | 3.06                     | 0.44              |
| 3:2D:73:VAL:HG13  | 3:2D:120:GLY:HA3  | 1.99                     | 0.44              |
| 1:2A:2305:A:H5''  | 6:2G:134:GLY:HA3  | 1.99                     | 0.44              |
| 10:2O:53:LYS:HE3  | 10:2O:56:ASP:OD2  | 2.18                     | 0.44              |
| 12:2Q:2:LEU:HD12  | 12:2Q:2:LEU:HA    | 1.72                     | 0.44              |
| 14:2S:64:GLU:HG3  | 14:2S:64:GLU:H    | 1.97                     | 0.44              |
| 1:1A:1102:G:H21   | 1:1A:1149:A:H62   | 1.65                     | 0.44              |
| 1:1A:1314:A:H2'   | 1:1A:1315:A:O4'   | 2.18                     | 0.44              |
| 1:1A:142:G:H2'    | 1:1A:143:C:C6     | 2.53                     | 0.44              |
| 1:1A:1732:C:H2'   | 1:1A:1733:C:C6    | 2.53                     | 0.44              |
| 1:1A:233:A:H2'    | 1:1A:234:G:O4'    | 2.17                     | 0.44              |
| 1:1A:253:C:O2'    | 1:1A:254:A:H2'    | 2.17                     | 0.44              |
| 1:1A:302:A:H2'    | 1:1A:303:C:H6     | 1.80                     | 0.44              |
| 1:1A:865:G:H4'    | 1:1A:885:C:O3'    | 2.17                     | 0.44              |
| 6:1G:114:ILE:HG12 | 6:1G:140:ILE:HD13 | 1.98                     | 0.44              |
| 14:1S:34:HIS:ND1  | 14:1S:53:SER:OG   | 2.42                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 16:1U:107:ALA:O    | 16:1U:110:VAL:HB   | 2.18                     | 0.44              |
| 1:2A:1633:G:C6     | 1:2A:1635:G:C4     | 3.06                     | 0.44              |
| 1:2A:1800:C:P      | 3:2D:183:ARG:HH12  | 2.40                     | 0.44              |
| 1:2A:2113:U:H2'    | 1:2A:2114:A:O4'    | 2.17                     | 0.44              |
| 18:2W:18:ARG:HG2   | 18:2W:76:VAL:HB    | 1.98                     | 0.44              |
| 23:11:10:LYS:NZ    | 23:11:65:SER:OG    | 2.49                     | 0.44              |
| 1:1A:1397:C:H2'    | 1:1A:1397:C:O2     | 2.94                     | 0.44              |
| 1:1A:207:A:C2      | 1:1A:224:U:H4'     | 2.52                     | 0.44              |
| 1:1A:2418:U:C2     | 11:1P:72:PRO:HG2   | 2.52                     | 0.44              |
| 1:1A:572:A:O2'     | 1:1A:573:G:OP1     | 2.33                     | 0.44              |
| 2:1B:2:C:H2'       | 2:1B:3:C:C6        | 2.52                     | 0.44              |
| 31:29:32:HIS:O     | 31:29:34:GLN:HG3   | 2.17                     | 0.44              |
| 1:2A:2186:G:C2     | 1:2A:2187:G:C5     | 3.06                     | 0.44              |
| 1:2A:298:G:H5''    | 1:2A:299:A:OP1     | 2.18                     | 0.44              |
| 1:2A:622:G:H2'     | 1:2A:623:G:C8      | 2.51                     | 0.44              |
| 1:2A:897:C:H2'     | 1:2A:898:C:C6      | 2.52                     | 0.44              |
| 3:2D:37:LEU:HB2    | 3:2D:62:TYR:HB2    | 2.00                     | 0.44              |
| 4:2E:7:VAL:HG12    | 4:2E:27:LEU:HB3    | 2.00                     | 0.44              |
| 7:2H:98:LEU:HD13   | 7:2H:103:LEU:HD13  | 2.00                     | 0.44              |
| 11:2P:27:HIS:O     | 11:2P:31:ALA:HA    | 2.18                     | 0.44              |
| 1:1A:1140:U:H2'    | 1:1A:1142:A:OP2    | 2.18                     | 0.44              |
| 1:1A:1223:C:H2'    | 1:1A:1224:C:H6     | 1.82                     | 0.44              |
| 1:1A:2357:G:N3     | 1:1A:2393:C:H2'    | 2.33                     | 0.44              |
| 4:1E:14:ILE:HG13   | 4:1E:21:VAL:HG23   | 1.99                     | 0.44              |
| 1:2A:1405:U:H2'    | 1:2A:1406:U:C6     | 2.51                     | 0.44              |
| 1:2A:1637:A:H5'    | 1:2A:1760:A:O2'    | 2.18                     | 0.44              |
| 1:2A:2057:A:H2'    | 1:2A:2058:A:C8     | 2.53                     | 0.44              |
| 1:2A:322:A:OP1     | 5:2F:168:ARG:NH1   | 2.45                     | 0.44              |
| 7:2H:164:TYR:HB2   | 7:2H:167:GLU:HB2   | 1.99                     | 0.44              |
| 13:2R:72:ASP:O     | 13:2R:76:VAL:HG23  | 2.18                     | 0.44              |
| 21:2Z:144:LEU:HD11 | 21:2Z:150:LEU:HD22 | 2.00                     | 0.44              |
| 1:1A:1067:A:H3'    | 1:1A:1067:A:N3     | 2.33                     | 0.44              |
| 1:1A:1476:C:H2'    | 1:1A:1477:U:C6     | 2.53                     | 0.44              |
| 1:1A:2156:A:N7     | 1:1A:2179:G:H4'    | 2.33                     | 0.44              |
| 1:1A:2728:C:H2'    | 1:1A:2729:U:H6     | 1.83                     | 0.44              |
| 1:1A:2863:C:H2'    | 1:1A:2864:G:C8     | 2.53                     | 0.44              |
| 1:1A:2240:G:P      | 3:1D:263:ARG:HH12  | 2.41                     | 0.44              |
| 7:1H:98:LEU:HD13   | 7:1H:125:VAL:HG23  | 2.00                     | 0.44              |
| 11:1P:88:LEU:HD11  | 11:1P:114:ILE:HD12 | 1.99                     | 0.44              |
| 12:1Q:29:PHE:O     | 21:1Z:122:ARG:NH2  | 2.50                     | 0.44              |
| 19:1X:49:VAL:HG11  | 19:1X:89:ILE:HG12  | 2.00                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:23:7:LYS:HE3    | 25:23:32:GLN:HE21  | 1.83                     | 0.44              |
| 1:2A:1064:C:OP2    | 1:2A:1065:U:H5'    | 2.17                     | 0.44              |
| 1:2A:1092:C:O2     | 1:2A:1092:C:H2'    | 2.18                     | 0.44              |
| 1:2A:571:A:N6      | 1:2A:2499:C:O3'    | 2.51                     | 0.44              |
| 3:2D:275:LYS:HD2   | 3:2D:275:LYS:HA    | 1.77                     | 0.44              |
| 8:2I:12:LEU:HD22   | 8:2I:19:VAL:HG21   | 2.00                     | 0.44              |
| 25:13:3:ARG:HD3    | 25:13:60:GLU:OE2   | 2.17                     | 0.43              |
| 6:1G:5:VAL:HG12    | 26:14:25:TYR:CE2   | 2.53                     | 0.43              |
| 1:1A:2812:A:N3     | 1:1A:2904:U:H1'    | 2.32                     | 0.43              |
| 1:1A:776:G:C6      | 3:1D:208:LYS:HB2   | 2.53                     | 0.43              |
| 2:1B:45:A:OP2      | 6:1G:96:ARG:NH2    | 2.39                     | 0.43              |
| 7:1H:4:ILE:O       | 7:1H:69:ARG:HD2    | 2.18                     | 0.43              |
| 9:1N:102:ALA:O     | 9:1N:106:MET:HG3   | 2.18                     | 0.43              |
| 1:2A:1069:A:O2'    | 1:2A:1073:A:N7     | 2.34                     | 0.43              |
| 1:2A:1566:A:OP1    | 3:2D:211:ARG:NH1   | 2.51                     | 0.43              |
| 1:2A:323:G:O2'     | 1:2A:1205:U:N3     | 2.48                     | 0.43              |
| 4:2E:11:MET:HG2    | 4:2E:24:THR:HB     | 1.99                     | 0.43              |
| 19:2X:31:HIS:HA    | 19:2X:32:PRO:HD3   | 1.84                     | 0.43              |
| 1:1A:1310:G:H2'    | 1:1A:2036:A:N6     | 2.33                     | 0.43              |
| 1:1A:800:C:O2'     | 1:1A:801:C:H5'     | 2.18                     | 0.43              |
| 1:2A:1062:G:C8     | 1:2A:1070:A:H1'    | 2.53                     | 0.43              |
| 1:2A:1203:G:C6     | 1:2A:1204:A:N6     | 2.86                     | 0.43              |
| 1:2A:1430:C:N3     | 1:2A:1563:G:N2     | 2.58                     | 0.43              |
| 1:2A:2130:U:H3'    | 1:2A:2130:U:C6     | 2.52                     | 0.43              |
| 1:2A:1843:C:H5'    | 3:2D:253:GLN:NE2   | 2.32                     | 0.43              |
| 7:2H:126:PRO:HB2   | 7:2H:127:GLU:HG3   | 2.00                     | 0.43              |
| 7:2H:55:PRO:HG2    | 7:2H:61:HIS:ND1    | 2.32                     | 0.43              |
| 12:2Q:10:ARG:HB2   | 21:2Z:196:VAL:HG21 | 2.00                     | 0.43              |
| 15:2T:29:ARG:HB3   | 15:2T:87:ASP:HB2   | 2.00                     | 0.43              |
| 1:1A:1374:G:O2'    | 1:1A:1375:U:H2'    | 2.18                     | 0.43              |
| 1:1A:1634:C:H2'    | 1:1A:1635:C:C6     | 2.52                     | 0.43              |
| 1:1A:2045:G:H5'    | 1:1A:2629:C:H4'    | 1.99                     | 0.43              |
| 1:1A:2623:U:H5'    | 1:1A:2623:U:H6     | 1.83                     | 0.43              |
| 1:1A:2724:U:O2'    | 1:1A:2726:A:H5'    | 2.19                     | 0.43              |
| 1:1A:2735:G:H2'    | 1:1A:2736:C:C6     | 2.53                     | 0.43              |
| 1:1A:402:C:H2'     | 1:1A:403:C:H6      | 1.80                     | 0.43              |
| 4:1E:144:ARG:HB3   | 4:1E:145:LYS:H     | 1.49                     | 0.43              |
| 6:1G:11:TYR:CE2    | 6:1G:16:ARG:HD3    | 2.54                     | 0.43              |
| 7:1H:118:PRO:HG2   | 7:1H:121:ILE:HG13  | 2.01                     | 0.43              |
| 20:1Y:38:ILE:HD11  | 20:1Y:66:PRO:HG3   | 2.00                     | 0.43              |
| 21:1Z:144:LEU:HD21 | 21:1Z:150:LEU:HD13 | 2.00                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 26:24:57:GLU:HA    | 26:24:58:ARG:HA    | 1.82                     | 0.43              |
| 1:2A:1102:C:H2'    | 1:2A:1103:A:H8     | 1.82                     | 0.43              |
| 1:2A:839:U:H2'     | 1:2A:840:C:C6      | 2.52                     | 0.43              |
| 6:2G:161:THR:HG22  | 6:2G:163:ALA:H     | 1.83                     | 0.43              |
| 21:2Z:123:ASP:N    | 21:2Z:123:ASP:OD1  | 2.51                     | 0.43              |
| 21:2Z:40:ASP:OD2   | 21:2Z:42:VAL:HG13  | 2.18                     | 0.43              |
| 26:14:49:PHE:HB3   | 26:14:50:VAL:H     | 1.37                     | 0.43              |
| 29:17:24:THR:HG23  | 29:17:26:GLY:H     | 1.84                     | 0.43              |
| 1:1A:1501:U:O2'    | 1:1A:1502:G:N7     | 2.46                     | 0.43              |
| 1:1A:2136:A:H2     | 1:1A:2189:U:O2'    | 1.99                     | 0.43              |
| 1:1A:2432:C:O5'    | 1:1A:2432:C:H6     | 2.02                     | 0.43              |
| 1:1A:469:A:H5''    | 1:1A:470:C:O5'     | 2.18                     | 0.43              |
| 1:1A:503:A:H2'     | 1:1A:504:A:C8      | 2.53                     | 0.43              |
| 6:1G:118:ARG:O     | 6:1G:181:ARG:HB3   | 2.17                     | 0.43              |
| 6:1G:50:ALA:O      | 6:1G:52:ILE:N      | 2.46                     | 0.43              |
| 15:1T:108:ARG:HA   | 15:1T:111:ARG:NH1  | 2.33                     | 0.43              |
| 1:2A:1028:A:H61    | 1:2A:1125:G:H2'    | 1.80                     | 0.43              |
| 1:2A:1509(B):A:H2' | 1:2A:1510:G:C8     | 2.54                     | 0.43              |
| 1:2A:2186:G:N1     | 1:2A:2187:G:C6     | 2.86                     | 0.43              |
| 1:2A:300:A:N3      | 1:2A:319:C:H1'     | 2.33                     | 0.43              |
| 6:2G:4:ASP:OD2     | 6:2G:9:ARG:NH2     | 2.48                     | 0.43              |
| 8:2I:130:TYR:HD2   | 8:2I:138:ILE:HD12  | 1.83                     | 0.43              |
| 8:2I:95:LYS:O      | 8:2I:99:GLU:HG3    | 2.18                     | 0.43              |
| 12:2Q:42:ILE:HD13  | 12:2Q:97:VAL:HG21  | 2.00                     | 0.43              |
| 1:2A:1248:G:C2     | 16:2U:3:ARG:HD2    | 2.54                     | 0.43              |
| 28:16:2:ALA:HB2    | 30:18:34:TRP:CZ2   | 2.54                     | 0.43              |
| 1:1A:1124:U:C5     | 1:1A:1134:A:H5''   | 2.54                     | 0.43              |
| 1:1A:600:G:O2'     | 1:1A:1300:A:OP1    | 2.30                     | 0.43              |
| 1:1A:1613:A:OP1    | 3:1D:211:ARG:NH1   | 2.51                     | 0.43              |
| 1:1A:2182:G:H2'    | 1:1A:2183:C:H6     | 1.82                     | 0.43              |
| 1:1A:559:U:H2'     | 1:1A:560:C:C6      | 2.53                     | 0.43              |
| 12:1Q:111:GLU:O    | 12:1Q:115:MET:HG2  | 2.19                     | 0.43              |
| 18:1W:16:LYS:O     | 18:1W:19:LEU:HB2   | 2.18                     | 0.43              |
| 1:2A:1214:A:H61    | 1:2A:1235:G:H1'    | 1.83                     | 0.43              |
| 1:2A:2469:A:H4'    | 12:2Q:56:ARG:HG2   | 2.00                     | 0.43              |
| 1:2A:539:G:H2'     | 1:2A:540:C:C6      | 2.54                     | 0.43              |
| 6:2G:55:LYS:NZ     | 6:2G:153:ARG:HH22  | 2.15                     | 0.43              |
| 7:2H:61:HIS:O      | 7:2H:65:HIS:HB2    | 2.19                     | 0.43              |
| 11:2P:97:PRO:HG3   | 11:2P:112:LEU:HD12 | 2.00                     | 0.43              |
| 12:2Q:52:VAL:HA    | 12:2Q:55:VAL:HG12  | 1.99                     | 0.43              |
| 14:2S:69:VAL:HA    | 14:2S:72:ALA:HB3   | 2.00                     | 0.43              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 29:17:31:LEU:O    | 29:17:35:ARG:HB2   | 2.18                     | 0.43              |
| 1:1A:1750:G:H2'   | 1:1A:1751:G:H8     | 1.82                     | 0.43              |
| 1:1A:1836:U:O2    | 3:1D:50:THR:HB     | 2.19                     | 0.43              |
| 1:1A:861:C:H2'    | 1:1A:862:C:H6      | 1.83                     | 0.43              |
| 4:1E:181:LEU:HA   | 4:1E:181:LEU:HD12  | 1.77                     | 0.43              |
| 7:1H:3:ARG:HH22   | 7:1H:66:GLY:N      | 2.17                     | 0.43              |
| 14:1S:10:ARG:O    | 14:1S:14:VAL:HG13  | 2.18                     | 0.43              |
| 1:1A:1785:C:OP1   | 15:1T:96:ARG:NH1   | 2.52                     | 0.43              |
| 21:1Z:10:ARG:HG3  | 21:1Z:36:LYS:HB3   | 2.00                     | 0.43              |
| 21:1Z:193:GLU:HA  | 21:1Z:194:PRO:HD3  | 1.74                     | 0.43              |
| 1:2A:1180:C:H2'   | 1:2A:1181:C:H6     | 1.84                     | 0.43              |
| 1:2A:1991:U:C2'   | 1:2A:1992:G:H5''   | 2.47                     | 0.43              |
| 1:2A:2122:U:H2'   | 1:2A:2123:G:O4'    | 2.18                     | 0.43              |
| 1:2A:2704:C:H2'   | 1:2A:2705:A:O4'    | 2.17                     | 0.43              |
| 1:2A:459:U:OP2    | 29:27:39:ARG:NH1   | 2.50                     | 0.43              |
| 1:2A:81:G:C2      | 1:2A:106:C:N3      | 2.87                     | 0.43              |
| 1:2A:924:C:H2'    | 1:2A:925:C:C6      | 2.54                     | 0.43              |
| 6:2G:171:ALA:O    | 6:2G:175:LEU:HD22  | 2.18                     | 0.43              |
| 12:2Q:17:LEU:HD13 | 12:2Q:39:PRO:HB2   | 2.01                     | 0.43              |
| 13:2R:65:LEU:HD12 | 13:2R:65:LEU:HA    | 1.85                     | 0.43              |
| 17:2V:60:GLU:HB2  | 17:2V:97:LYS:HG2   | 2.01                     | 0.43              |
| 21:2Z:30:ASN:HD22 | 21:2Z:90:VAL:HB    | 1.83                     | 0.43              |
| 1:1A:2813:G:H2'   | 1:1A:2814:C:C6     | 2.53                     | 0.43              |
| 1:1A:549:U:H2'    | 1:1A:550:U:C6      | 2.53                     | 0.43              |
| 1:1A:865:G:H5'    | 1:1A:886:U:OP1     | 2.18                     | 0.43              |
| 20:1Y:56:PRO:C    | 20:1Y:58:GLY:H     | 2.20                     | 0.43              |
| 1:2A:2519:U:C6    | 1:2A:2542:A:N6     | 2.87                     | 0.43              |
| 1:2A:2650:U:H2'   | 1:2A:2651:C:C6     | 2.54                     | 0.43              |
| 1:2A:700:G:H2'    | 1:2A:701:G:O4'     | 2.19                     | 0.43              |
| 1:2A:782:A:H5''   | 60:2A:4830:HOH:O   | 2.17                     | 0.43              |
| 1:2A:889:C:O2'    | 1:2A:890:A:O5'     | 2.36                     | 0.43              |
| 4:2E:144:ARG:HB3  | 4:2E:145:LYS:H     | 1.48                     | 0.43              |
| 13:2R:87:TYR:OH   | 13:2R:117:VAL:O    | 2.25                     | 0.43              |
| 28:16:9:LEU:HD13  | 28:16:51:GLU:HG3   | 2.00                     | 0.43              |
| 1:1A:123:G:H1'    | 29:17:48:LYS:HE3   | 1.99                     | 0.43              |
| 1:1A:1159:U:H2'   | 1:1A:1160:G:C8     | 2.53                     | 0.43              |
| 1:1A:1232:G:H5''  | 17:1V:81:TYR:CE1   | 2.54                     | 0.43              |
| 1:1A:2697:G:H5'   | 10:1O:68:GLU:OE2   | 2.18                     | 0.43              |
| 7:1H:121:ILE:HD11 | 7:1H:140:LYS:HG2   | 1.99                     | 0.43              |
| 9:1N:72:TYR:CE2   | 9:1N:87:LEU:HD23   | 2.52                     | 0.43              |
| 14:1S:110:LEU:HA  | 14:1S:110:LEU:HD12 | 1.86                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 19:1X:95:LEU:H    | 19:1X:95:LEU:HD12 | 1.84                     | 0.43              |
| 1:2A:387:U:P      | 23:21:20:ARG:HH12 | 2.41                     | 0.43              |
| 31:29:29:ASN:HA   | 31:29:30:PRO:HD3  | 1.89                     | 0.43              |
| 1:2A:1359:A:H2'   | 1:2A:1360:A:H5'   | 1.99                     | 0.43              |
| 1:2A:476:G:H4'    | 1:2A:502:A:N1     | 2.34                     | 0.43              |
| 1:2A:866:A:N6     | 1:2A:914:C:C4     | 2.87                     | 0.43              |
| 1:2A:996:A:H4'    | 16:2U:91:ASP:OD2  | 2.19                     | 0.43              |
| 1:2A:1798:U:H5'   | 3:2D:259:THR:HG22 | 2.01                     | 0.43              |
| 5:2F:24:LEU:HD21  | 5:2F:114:VAL:HG12 | 2.01                     | 0.43              |
| 6:2G:77:ILE:HG21  | 6:2G:80:PHE:CD2   | 2.53                     | 0.43              |
| 12:2Q:55:VAL:HG23 | 21:2Z:178:GLU:HB3 | 2.01                     | 0.43              |
| 21:2Z:97:GLU:HA   | 21:2Z:126:VAL:O   | 2.19                     | 0.43              |
| 24:12:8:LYS:HD2   | 24:12:8:LYS:HA    | 1.90                     | 0.43              |
| 1:1A:1116:A:N7    | 1:1A:1143:U:H4'   | 2.34                     | 0.43              |
| 1:1A:1431:G:O2'   | 1:1A:1442:U:O2    | 2.35                     | 0.43              |
| 1:1A:564:G:H2'    | 1:1A:565:C:C6     | 2.54                     | 0.43              |
| 1:1A:923:C:H2'    | 1:1A:924:U:O4'    | 2.18                     | 0.43              |
| 26:24:42:PHE:HD2  | 26:24:43:TYR:CD1  | 2.37                     | 0.43              |
| 26:24:62:ARG:HD3  | 26:24:62:ARG:HA   | 1.77                     | 0.43              |
| 28:26:6:ARG:HH12  | 28:26:26:ASN:HB2  | 1.82                     | 0.43              |
| 1:2A:1641:A:H2'   | 1:2A:1642:G:O4'   | 2.19                     | 0.43              |
| 1:2A:1833:U:O2'   | 1:2A:1969:A:N1    | 2.42                     | 0.43              |
| 1:2A:2125:G:H1'   | 1:2A:2173:A:H61   | 1.82                     | 0.43              |
| 1:2A:518:G:H2'    | 1:2A:519:U:C6     | 2.53                     | 0.43              |
| 1:2A:601:C:OP1    | 5:2F:108:LYS:NZ   | 2.44                     | 0.43              |
| 1:2A:783:A:N3     | 1:2A:783:A:H2'    | 2.33                     | 0.43              |
| 1:2A:616:G:H5'    | 5:2F:205:ARG:HD3  | 2.00                     | 0.43              |
| 6:2G:18:GLU:CD    | 6:2G:21:ARG:HH21  | 2.21                     | 0.43              |
| 6:2G:86:MET:HA    | 6:2G:87:PRO:HD3   | 1.85                     | 0.43              |
| 15:2T:28:VAL:HG13 | 15:2T:86:ILE:HG23 | 2.01                     | 0.43              |
| 20:2Y:86:ARG:HB2  | 20:2Y:98:VAL:CG2  | 2.48                     | 0.43              |
| 1:1A:1131:A:H1'   | 1:1A:1151:U:H1'   | 2.00                     | 0.43              |
| 1:1A:1594:C:H2'   | 1:1A:1595:C:C6    | 2.54                     | 0.43              |
| 1:1A:1821:C:H2'   | 1:1A:1822:A:C5    | 2.53                     | 0.43              |
| 1:1A:2303:U:H2'   | 1:1A:2304:C:H6    | 1.81                     | 0.43              |
| 1:1A:2899:C:H2'   | 1:1A:2900:G:O4'   | 2.19                     | 0.43              |
| 1:1A:302:A:O2'    | 1:1A:303:C:O5'    | 2.30                     | 0.43              |
| 3:1D:166:GLN:HB2  | 3:1D:174:ILE:HG22 | 2.00                     | 0.43              |
| 5:1F:184:TYR:O    | 5:1F:188:ARG:HG3  | 2.19                     | 0.43              |
| 6:1G:143:GLU:O    | 6:1G:144:ILE:HD13 | 2.19                     | 0.43              |
| 9:1N:42:TRP:CH2   | 9:1N:44:PRO:HB3   | 2.54                     | 0.43              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 21:1Z:200:GLY:C   | 21:1Z:202:GLU:N    | 2.72                     | 0.43              |
| 1:2A:1286:A:H8    | 1:2A:1287:A:H4'    | 8.35                     | 0.43              |
| 1:2A:1607:C:H4'   | 1:2A:1608:A:O5'    | 2.18                     | 0.43              |
| 1:2A:2001:A:H4'   | 1:2A:2689:U:H2'    | 2.01                     | 0.43              |
| 1:2A:674:G:N2     | 1:2A:2444:G:O3'    | 2.52                     | 0.43              |
| 1:2A:968:G:H2'    | 1:2A:969:U:C6      | 2.54                     | 0.43              |
| 5:2F:158:THR:HB   | 5:2F:195:ASP:HB2   | 2.01                     | 0.43              |
| 9:2N:67:LEU:O     | 9:2N:88:GLU:HG3    | 2.19                     | 0.43              |
| 1:1A:2342:G:O2'   | 22:10:41:ARG:O     | 2.30                     | 0.42              |
| 1:1A:1124:U:H4'   | 1:1A:1125:C:H5'    | 2.00                     | 0.42              |
| 1:1A:1640:G:H2'   | 1:1A:1641:G:O4'    | 2.19                     | 0.42              |
| 1:1A:1715:A:O2'   | 1:1A:1721:G:N7     | 2.41                     | 0.42              |
| 3:1D:206:LEU:HD23 | 3:1D:206:LEU:HA    | 1.90                     | 0.42              |
| 11:1P:107:LYS:O   | 11:1P:110:TYR:HB2  | 2.18                     | 0.42              |
| 1:2A:1782:C:O2'   | 1:2A:2609:U:H5''   | 2.19                     | 0.42              |
| 1:2A:424:G:H2'    | 1:2A:425:G:H8      | 2.61                     | 0.42              |
| 1:2A:873:G:H1     | 1:2A:904:C:H42     | 1.67                     | 0.42              |
| 6:2G:145:THR:HG22 | 6:2G:148:MET:HG2   | 2.01                     | 0.42              |
| 1:2A:1007:C:P     | 9:2N:37:LYS:HZ3    | 2.42                     | 0.42              |
| 10:2O:120:GLU:OE2 | 10:2O:122:LEU:HD21 | 2.19                     | 0.42              |
| 1:1A:1347:A:H2    | 1:1A:1672:G:N3     | 2.16                     | 0.42              |
| 1:1A:2258:G:H2'   | 1:1A:2259:A:C8     | 2.54                     | 0.42              |
| 1:1A:36:G:N3      | 1:1A:476:G:O2'     | 2.51                     | 0.42              |
| 7:1H:13:LYS:HG2   | 7:1H:13:LYS:H      | 1.64                     | 0.42              |
| 25:23:48:GLU:HA   | 25:23:51:ALA:HB2   | 2.00                     | 0.42              |
| 1:2A:1202:C:N3    | 1:2A:1243:G:N2     | 2.59                     | 0.42              |
| 1:2A:184:C:H2'    | 1:2A:185:U:C6      | 2.54                     | 0.42              |
| 1:2A:2115:G:H4'   | 1:2A:2166:G:O2'    | 2.20                     | 0.42              |
| 1:2A:954:G:O2'    | 1:2A:2274:A:N1     | 2.48                     | 0.42              |
| 8:2I:123:LEU:HD12 | 8:2I:144:VAL:HB    | 2.01                     | 0.42              |
| 13:2R:90:ARG:CZ   | 13:2R:117:VAL:HG11 | 2.49                     | 0.42              |
| 21:2Z:17:ALA:O    | 21:2Z:21:ALA:N     | 2.47                     | 0.42              |
| 1:1A:1675:U:H2'   | 1:1A:1676:G:C8     | 2.54                     | 0.42              |
| 1:1A:1879:A:H2'   | 1:1A:1880:G:C8     | 2.52                     | 0.42              |
| 1:1A:2205:C:H2'   | 1:1A:2206:G:C8     | 2.54                     | 0.42              |
| 1:1A:2479:C:H4'   | 12:1Q:123:HIS:CD2  | 2.54                     | 0.42              |
| 1:1A:2679:C:H2'   | 1:1A:2680:G:O4'    | 2.19                     | 0.42              |
| 1:1A:293:C:H42    | 1:1A:391:G:H1      | 1.67                     | 0.42              |
| 3:1D:8:PRO:HB3    | 3:1D:14:ARG:HG3    | 2.02                     | 0.42              |
| 15:1T:45:PHE:CE2  | 15:1T:74:ARG:HB2   | 2.54                     | 0.42              |
| 26:24:40:HIS:CG   | 26:24:41:PRO:HD2   | 2.54                     | 0.42              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:2A:1288:U:C2   | 1:2A:1327:C:O2    | 2.72                     | 0.42              |
| 1:2A:1503:U:H2'  | 1:2A:1504:C:C6    | 2.54                     | 0.42              |
| 1:2A:2506:U:H5'  | 60:2A:4356:HOH:O  | 2.19                     | 0.42              |
| 1:2A:321:G:OP2   | 5:2F:135:LYS:HG3  | 2.19                     | 0.42              |
| 9:2N:42:TRP:CH2  | 9:2N:44:PRO:HB3   | 2.55                     | 0.42              |
| 1:2A:2684:U:O2'  | 10:2O:68:GLU:OE2  | 2.34                     | 0.42              |
| 11:2P:82:GLY:HA2 | 11:2P:113:LYS:O   | 2.19                     | 0.42              |
| 1:2A:2376:A:N3   | 14:2S:106:ARG:NH2 | 2.67                     | 0.42              |
| 16:2U:16:LYS:HB3 | 16:2U:16:LYS:HE2  | 1.84                     | 0.42              |
| 1:2A:1248:G:C5   | 16:2U:3:ARG:HB2   | 2.54                     | 0.42              |
| 21:2Z:63:ASP:OD1 | 21:2Z:65:GLN:HG3  | 2.20                     | 0.42              |
| 30:18:52:LYS:HB3 | 30:18:53:PRO:HD3  | 2.00                     | 0.42              |
| 1:1A:1053:C:OP1  | 9:1N:37:LYS:NZ    | 2.50                     | 0.42              |
| 1:1A:1054:C:H4'  | 1:1A:1055:A:O5'   | 3.09                     | 0.42              |
| 1:1A:1556:A:H2'  | 1:1A:1557:A:C8    | 2.54                     | 0.42              |
| 1:1A:1645:C:OP1  | 19:1X:36:LYS:HG3  | 2.19                     | 0.42              |
| 1:1A:1805:C:O5'  | 1:1A:1805:C:H6    | 2.02                     | 0.42              |
| 1:1A:1814:A:H5'  | 1:1A:2620:G:H4'   | 2.01                     | 0.42              |
| 1:1A:602:G:H2'   | 1:1A:603:C:H6     | 1.83                     | 0.42              |
| 6:1G:72:ARG:HD3  | 6:1G:85:GLY:O     | 2.19                     | 0.42              |
| 7:1H:124:GLU:OE2 | 7:1H:132:ARG:HD2  | 2.20                     | 0.42              |
| 1:2A:1359:A:N1   | 1:2A:1372:U:O4    | 2.52                     | 0.42              |
| 1:2A:13:A:N1     | 1:2A:525:U:H2'    | 2.35                     | 0.42              |
| 1:2A:36:G:N3     | 1:2A:450:G:O2'    | 2.52                     | 0.42              |
| 1:2A:264:C:H4'   | 1:2A:428:A:C2     | 2.54                     | 0.42              |
| 2:2B:17:C:H2'    | 2:2B:18:G:O4'     | 2.20                     | 0.42              |
| 6:2G:33:ARG:NH2  | 6:2G:162:THR:HG21 | 2.34                     | 0.42              |
| 8:2I:69:LYS:HE3  | 8:2I:69:LYS:HB2   | 1.86                     | 0.42              |
| 17:2V:37:VAL:O   | 17:2V:52:VAL:HG22 | 2.19                     | 0.42              |
| 23:11:3:LYS:HG3  | 23:11:4:VAL:H     | 1.85                     | 0.42              |
| 28:16:11:LEU:HB3 | 28:16:49:HIS:HB3  | 2.02                     | 0.42              |
| 1:1A:1114:G:O2'  | 1:1A:1142:A:O2'   | 2.27                     | 0.42              |
| 1:1A:1463:C:OP1  | 15:1T:111:ARG:NE  | 106.94                   | 0.42              |
| 1:1A:2205:C:H2'  | 1:1A:2206:G:H8    | 1.84                     | 0.42              |
| 1:1A:2450:U:O2'  | 1:1A:2452:C:OP1   | 2.24                     | 0.42              |
| 1:1A:2589:A:H5'  | 27:15:3:LYS:HD3   | 2.01                     | 0.42              |
| 1:1A:676:G:OP2   | 30:18:21:LYS:NZ   | 2.48                     | 0.42              |
| 1:1A:821:A:H2'   | 1:1A:821:A:N3     | 2.35                     | 0.42              |
| 1:1A:973:G:H2'   | 1:1A:974:G:O4'    | 2.19                     | 0.42              |
| 4:1E:174:ASP:OD1 | 4:1E:175:VAL:N    | 2.53                     | 0.42              |
| 5:1F:10:PRO:HB3  | 5:1F:17:ARG:CZ    | 2.50                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:1P:125:VAL:HG13 | 11:1P:138:LEU:HD21 | 2.01                     | 0.42              |
| 1:2A:116:C:H2'     | 1:2A:117:G:O4'     | 2.19                     | 0.42              |
| 1:2A:1493:C:H5     | 1:2A:2206:G:HO2'   | 1.62                     | 0.42              |
| 1:2A:2461:C:H2'    | 1:2A:2462:U:H6     | 1.85                     | 0.42              |
| 1:2A:774:A:OP1     | 3:2D:48:ARG:NH2    | 2.46                     | 0.42              |
| 1:2A:954:G:C5      | 1:2A:955:C:C5      | 3.07                     | 0.42              |
| 6:2G:11:TYR:OH     | 6:2G:33:ARG:HG2    | 2.19                     | 0.42              |
| 6:2G:55:LYS:O      | 6:2G:58:GLN:HB3    | 2.20                     | 0.42              |
| 7:2H:105:LEU:HD12  | 7:2H:105:LEU:HA    | 1.84                     | 0.42              |
| 12:2Q:130:LYS:HB3  | 12:2Q:130:LYS:HE3  | 1.88                     | 0.42              |
| 17:2V:100:ARG:HH11 | 17:2V:100:ARG:CB   | 2.27                     | 0.42              |
| 1:1A:2161:C:H6     | 1:1A:2161:C:O5'    | 2.01                     | 0.42              |
| 1:1A:2484:G:C5     | 1:1A:2487:C:C4     | 3.07                     | 0.42              |
| 1:1A:2849:G:H5'    | 13:1R:46:GLY:HA2   | 2.00                     | 0.42              |
| 1:1A:310:C:H2'     | 1:1A:311:C:H6      | 1.85                     | 0.42              |
| 1:1A:632:A:H3'     | 1:1A:633:G:H8      | 2.45                     | 0.42              |
| 9:1N:34:LEU:HD12   | 9:1N:34:LEU:HA     | 1.86                     | 0.42              |
| 6:2G:113:ARG:HG3   | 26:24:34:GLU:OE2   | 2.20                     | 0.42              |
| 6:2G:67:LYS:HE3    | 26:24:5:ILE:HD12   | 2.01                     | 0.42              |
| 1:2A:1421:G:C2     | 1:2A:1422:G:C8     | 3.07                     | 0.42              |
| 1:2A:143:G:H2'     | 1:2A:143(A):C:C6   | 2.55                     | 0.42              |
| 1:2A:2186:G:N1     | 1:2A:2187:G:C5     | 2.88                     | 0.42              |
| 1:2A:2406:U:OP2    | 1:2A:2406:U:H2'    | 2.20                     | 0.42              |
| 1:2A:817:C:N3      | 1:2A:1529:G:N2     | 117.29                   | 0.42              |
| 2:2B:11:C:OP2      | 2:2B:12:C:N4       | 2.38                     | 0.42              |
| 9:2N:26:LEU:HG     | 9:2N:30:ILE:HD11   | 2.01                     | 0.42              |
| 16:2U:89:GLU:HG3   | 17:2V:50:PRO:HB3   | 2.01                     | 0.42              |
| 21:2Z:24:LEU:HA    | 21:2Z:25:PRO:HD3   | 1.86                     | 0.42              |
| 21:2Z:5:LEU:HD21   | 21:2Z:39:VAL:HG11  | 2.02                     | 0.42              |
| 24:12:22:GLU:OE2   | 24:12:68:ARG:NH2   | 2.53                     | 0.42              |
| 26:14:40:HIS:HA    | 26:14:41:PRO:HD3   | 1.94                     | 0.42              |
| 1:1A:1056:A:N3     | 1:1A:1199:C:H1'    | 2.34                     | 0.42              |
| 1:1A:1110:C:OP2    | 1:1A:1111:U:H5'    | 2.20                     | 0.42              |
| 1:1A:1275:G:C6     | 1:1A:1276:C:C4     | 3.08                     | 0.42              |
| 1:1A:1490:G:H2'    | 1:1A:1492:C:C5     | 2.55                     | 0.42              |
| 1:1A:1547:C:O4'    | 3:1D:100:GLY:HA2   | 2.20                     | 0.42              |
| 1:1A:2156:A:H2'    | 1:1A:2181:G:H1'    | 2.02                     | 0.42              |
| 1:1A:439:A:N1      | 1:1A:496:A:H1'     | 75.86                    | 0.42              |
| 3:1D:13:ARG:HA     | 3:1D:13:ARG:HD2    | 1.40                     | 0.42              |
| 3:1D:17:THR:HG23   | 3:1D:205:VAL:HB    | 2.02                     | 0.42              |
| 3:1D:85:ASP:HA     | 3:1D:86:PRO:HD2    | 1.92                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:1E:21:VAL:HG12  | 4:1E:185:LYS:HD2  | 2.00                     | 0.42              |
| 12:1Q:51:ARG:HD3  | 12:1Q:66:ILE:HD11 | 2.01                     | 0.42              |
| 20:1Y:9:LYS:HA    | 20:1Y:10:GLY:HA2  | 1.73                     | 0.42              |
| 1:2A:1059:G:C2    | 1:2A:1060:U:O4    | 2.73                     | 0.42              |
| 1:2A:2845:G:H5''  | 15:2T:54:ARG:O    | 2.19                     | 0.42              |
| 1:2A:335:C:H4'    | 20:2Y:73:ARG:HD2  | 2.02                     | 0.42              |
| 5:2F:74:ARG:HG3   | 5:2F:74:ARG:H     | 1.48                     | 0.42              |
| 22:10:12:ASN:O    | 22:10:14:ARG:NH2  | 2.53                     | 0.42              |
| 28:16:6:ARG:NE    | 28:16:24:GLU:OE2  | 2.32                     | 0.42              |
| 1:1A:1005:A:H4'   | 1:1A:1037:C:O2'   | 45.26                    | 0.42              |
| 1:1A:1093:G:HO2'  | 1:1A:1094:A:H8    | 1.68                     | 0.42              |
| 1:1A:1110:C:C4    | 1:1A:1120:G:O6    | 2.73                     | 0.42              |
| 1:1A:1386:U:OP1   | 19:1X:16:LYS:NZ   | 2.46                     | 0.42              |
| 1:1A:1405:A:H2'   | 1:1A:1406:A:H5'   | 2.01                     | 0.42              |
| 1:1A:1817:A:H1'   | 1:1A:1960:A:N6    | 2.35                     | 0.42              |
| 1:1A:2342:G:H2'   | 1:1A:2343:G:O4'   | 2.20                     | 0.42              |
| 1:1A:474:U:H5'    | 60:1A:9159:HOH:O  | 2.19                     | 0.42              |
| 1:1A:691:G:N2     | 1:1A:700:A:H1'    | 2.34                     | 0.42              |
| 5:1F:125:LEU:HD21 | 5:1F:199:TRP:CD2  | 2.55                     | 0.42              |
| 7:1H:94:TYR:N     | 7:1H:94:TYR:CD1   | 2.87                     | 0.42              |
| 11:1P:82:GLY:HA2  | 11:1P:113:LYS:O   | 2.19                     | 0.42              |
| 21:1Z:35:ARG:HA   | 21:1Z:35:ARG:HD2  | 1.89                     | 0.42              |
| 29:27:34:ARG:NH1  | 29:27:41:ARG:O    | 2.52                     | 0.42              |
| 1:2A:1116:C:H2'   | 1:2A:1117:G:O4'   | 2.19                     | 0.42              |
| 1:2A:1588:C:H2'   | 1:2A:1589:C:C6    | 2.55                     | 0.42              |
| 1:2A:1686:C:H2'   | 1:2A:1687:G:O4'   | 2.20                     | 0.42              |
| 1:2A:1794:U:H2'   | 1:2A:1795:C:H6    | 1.84                     | 0.42              |
| 1:2A:2348:U:H5'   | 28:26:21:TYR:OH   | 2.19                     | 0.42              |
| 1:2A:2464:C:H1'   | 60:2A:4675:HOH:O  | 2.20                     | 0.42              |
| 1:2A:455:C:N3     | 1:2A:473:G:H5'    | 2.35                     | 0.42              |
| 1:2A:779:U:OP1    | 3:2D:49:ILE:HG13  | 2.19                     | 0.42              |
| 1:2A:2319:G:N1    | 14:2S:3:ARG:HA    | 2.35                     | 0.42              |
| 18:2W:27:LYS:O    | 18:2W:71:VAL:HG23 | 2.20                     | 0.42              |
| 19:2X:61:GLY:HA3  | 19:2X:73:ARG:O    | 2.20                     | 0.42              |
| 21:2Z:118:GLN:N   | 21:2Z:173:ALA:O   | 2.48                     | 0.42              |
| 26:14:62:ARG:C    | 26:14:64:GLY:HA2  | 2.40                     | 0.42              |
| 1:1A:1686:U:O2'   | 1:1A:1687:C:H5'   | 2.20                     | 0.42              |
| 1:1A:2136:A:C2    | 1:1A:2137:G:H1'   | 2.55                     | 0.42              |
| 1:1A:2131:U:H1'   | 1:1A:2203:G:N2    | 2.35                     | 0.42              |
| 1:1A:2333:G:N3    | 1:1A:2333:G:H2'   | 2.35                     | 0.42              |
| 1:1A:2899:C:H3'   | 1:1A:2900:G:H8    | 1.84                     | 0.42              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 6:1G:117:PHE:HZ   | 6:1G:179:PRO:HG2   | 1.84                     | 0.42              |
| 1:2A:1099:G:H8    | 1:2A:1099:G:O5'    | 2.03                     | 0.42              |
| 1:2A:1805:U:C2    | 1:2A:1813:G:N2     | 2.88                     | 0.42              |
| 1:2A:443:A:H1'    | 1:2A:1201:C:O4'    | 2.19                     | 0.42              |
| 15:2T:46:GLU:O    | 15:2T:65:LYS:HD2   | 2.20                     | 0.42              |
| 15:2T:92:GLY:O    | 15:2T:120:ARG:NH2  | 2.53                     | 0.42              |
| 1:1A:1362:U:H2'   | 1:1A:1363:A:H8     | 1.85                     | 0.42              |
| 1:1A:1756:U:H2'   | 1:1A:1757:C:C6     | 2.54                     | 0.42              |
| 1:1A:2564:OMU:C6  | 1:1A:2564:OMU:C4   | 2.47                     | 0.42              |
| 1:1A:2797:C:H1'   | 4:1E:37:ARG:NH1    | 2.35                     | 0.42              |
| 1:1A:540:A:H1'    | 1:1A:604:C:H1'     | 2.02                     | 0.42              |
| 1:1A:637:U:H4'    | 1:1A:640:A:C6      | 2.55                     | 0.42              |
| 1:1A:800:C:H2'    | 1:1A:801:C:C6      | 2.55                     | 0.42              |
| 1:1A:964:A:N3     | 2:1B:80:U:O2'      | 2.43                     | 0.42              |
| 2:1B:29:A:C2      | 2:1B:30:C:C2       | 3.08                     | 0.42              |
| 3:1D:4:LYS:HB3    | 3:1D:18:VAL:CG2    | 2.45                     | 0.42              |
| 6:1G:181:ARG:HG3  | 6:1G:182:LYS:N     | 2.35                     | 0.42              |
| 8:1I:78:THR:HA    | 8:1I:143:SER:HG    | 1.85                     | 0.42              |
| 19:1X:66:LEU:HD23 | 19:1X:66:LEU:HA    | 1.72                     | 0.42              |
| 20:1Y:107:ASP:OD1 | 20:1Y:107:ASP:N    | 2.53                     | 0.42              |
| 1:2A:2065:C:H4'   | 1:2A:2251:OMG:HM22 | 2.01                     | 0.42              |
| 1:2A:2511:U:O4    | 1:2A:2575:C:N3     | 2.53                     | 0.42              |
| 1:2A:2809:A:H2'   | 1:2A:2810:A:C8     | 2.55                     | 0.42              |
| 1:2A:729:G:H2'    | 1:2A:1775:U:H1'    | 2.02                     | 0.42              |
| 1:2A:389:G:H1     | 11:2P:70:GLN:HB3   | 1.85                     | 0.42              |
| 12:2Q:39:PRO:HA   | 12:2Q:97:VAL:O     | 2.20                     | 0.42              |
| 16:2U:112:ARG:HE  | 16:2U:112:ARG:HB3  | 1.37                     | 0.42              |
| 21:2Z:53:ILE:H    | 21:2Z:53:ILE:HG13  | 1.72                     | 0.42              |
| 31:19:2:LYS:HD3   | 31:19:4:ARG:NH2    | 2.35                     | 0.41              |
| 1:1A:1147:U:H2'   | 1:1A:1148:C:H6     | 1.80                     | 0.41              |
| 1:1A:1270:C:H2'   | 1:1A:1271:G:O4'    | 2.20                     | 0.41              |
| 1:1A:2538:G:H5'   | 1:1A:2755:C:O2'    | 2.20                     | 0.41              |
| 20:1Y:13:VAL:HG12 | 20:1Y:74:PRO:HA    | 2.02                     | 0.41              |
| 25:23:16:PRO:HB2  | 25:23:18:ASP:OD1   | 2.19                     | 0.41              |
| 1:2A:1075:C:H2'   | 1:2A:1076:C:H5'    | 2.02                     | 0.41              |
| 1:2A:1159:U:H2'   | 1:2A:1160:G:H8     | 1.84                     | 0.41              |
| 1:2A:1366:A:H2'   | 1:2A:1367:A:O4'    | 2.20                     | 0.41              |
| 1:2A:2611:U:C4    | 27:25:3:LYS:HG2    | 2.55                     | 0.41              |
| 1:2A:2881:C:H2'   | 1:2A:2882:A:O4'    | 2.20                     | 0.41              |
| 1:2A:952:G:C6     | 1:2A:966:G:C6      | 3.08                     | 0.41              |
| 2:2B:18:G:H2'     | 2:2B:19:G:C8       | 2.55                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:2B:2:C:H2'      | 2:2B:3:C:H6       | 1.84                     | 0.41              |
| 7:2H:125:VAL:HG22 | 7:2H:131:VAL:HG22 | 2.02                     | 0.41              |
| 14:2S:15:ARG:O    | 14:2S:19:LYS:HG2  | 2.20                     | 0.41              |
| 28:16:40:CYS:HA   | 28:16:41:PRO:HD3  | 1.76                     | 0.41              |
| 31:19:11:CYS:SG   | 31:19:13:LYS:HB2  | 2.60                     | 0.41              |
| 1:1A:1101:G:O2'   | 1:1A:1131:A:N1    | 2.40                     | 0.41              |
| 1:1A:1554:A:H4'   | 1:1A:1556:A:C6    | 2.55                     | 0.41              |
| 1:1A:2125:C:N4    | 1:1A:2126:G:O6    | 2.53                     | 0.41              |
| 1:1A:2151:C:C4    | 1:1A:2152:U:C4    | 3.07                     | 0.41              |
| 1:1A:2672:A:H2'   | 1:1A:2673:G:O4'   | 2.19                     | 0.41              |
| 1:1A:272:U:H5'    | 8:1I:50:ARG:NH1   | 2.35                     | 0.41              |
| 1:1A:287:G:N7     | 1:1A:448:U:H2'    | 2.36                     | 0.41              |
| 1:1A:934:A:O2'    | 1:1A:935:C:H5''   | 2.20                     | 0.41              |
| 2:1B:78:A:H2'     | 2:1B:79:C:O4'     | 2.19                     | 0.41              |
| 5:1F:9:ILE:HA     | 5:1F:10:PRO:HD2   | 1.91                     | 0.41              |
| 9:1N:33:LEU:HD12  | 9:1N:33:LEU:HA    | 1.91                     | 0.41              |
| 21:1Z:14:LYS:HA   | 21:1Z:15:PRO:HD3  | 1.95                     | 0.41              |
| 22:20:23:VAL:HA   | 22:20:38:VAL:HG22 | 2.00                     | 0.41              |
| 23:21:3:LYS:HB2   | 23:21:61:ARG:HH22 | 1.85                     | 0.41              |
| 30:28:23:VAL:HG23 | 30:28:49:VAL:HG22 | 2.02                     | 0.41              |
| 1:2A:1469:A:H2'   | 1:2A:1470:G:O4'   | 2.20                     | 0.41              |
| 3:2D:70:TRP:CE2   | 3:2D:150:LYS:HD3  | 2.55                     | 0.41              |
| 3:2D:70:TRP:CZ2   | 3:2D:150:LYS:HA   | 2.55                     | 0.41              |
| 4:2E:16:ARG:NH1   | 4:2E:173:VAL:HG13 | 2.35                     | 0.41              |
| 6:2G:112:PRO:HB2  | 26:24:35:VAL:HG13 | 2.02                     | 0.41              |
| 1:1A:1102:G:N2    | 1:1A:1149:A:H62   | 2.18                     | 0.41              |
| 1:1A:1653:C:H4'   | 1:1A:1654:A:O5'   | 2.20                     | 0.41              |
| 1:1A:2466:G:H1'   | 60:1A:9637:HOH:O  | 2.19                     | 0.41              |
| 1:1A:385:G:C2     | 1:1A:386:U:N3     | 2.88                     | 0.41              |
| 1:1A:800:C:H2'    | 1:1A:801:C:H6     | 1.85                     | 0.41              |
| 6:1G:60:LEU:HA    | 6:1G:60:LEU:HD23  | 1.92                     | 0.41              |
| 9:1N:70:LYS:HE3   | 9:1N:72:TYR:CE1   | 2.55                     | 0.41              |
| 20:1Y:14:LEU:HD11 | 20:1Y:22:GLY:HA2  | 2.01                     | 0.41              |
| 20:1Y:90:LEU:HD21 | 20:1Y:96:ILE:HG23 | 2.00                     | 0.41              |
| 1:2A:10:G:H2'     | 1:2A:11:G:C8      | 2.55                     | 0.41              |
| 1:2A:1510:G:H2'   | 1:2A:1511:C:C6    | 2.55                     | 0.41              |
| 1:2A:2207:G:H2'   | 1:2A:2208:A:C2    | 2.54                     | 0.41              |
| 1:2A:2377:A:H2'   | 1:2A:2378:A:C8    | 2.55                     | 0.41              |
| 1:2A:2687:U:H2'   | 1:2A:2688:U:O4'   | 2.21                     | 0.41              |
| 1:2A:2802:G:H2'   | 1:2A:2803:C:O4'   | 2.20                     | 0.41              |
| 1:2A:2748:A:H5'   | 7:2H:4:ILE:CD1    | 2.49                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:1A:2169:G:H2'    | 1:1A:2170:G:O4'    | 2.20                     | 0.41              |
| 1:1A:251:A:H2'     | 1:1A:252:C:O4'     | 2.20                     | 0.41              |
| 1:1A:310:C:H2'     | 1:1A:311:C:C6      | 2.55                     | 0.41              |
| 7:1H:94:TYR:N      | 7:1H:94:TYR:HD1    | 2.18                     | 0.41              |
| 8:1I:52:ARG:HB2    | 8:1I:52:ARG:NH2    | 2.36                     | 0.41              |
| 9:1N:99:LEU:O      | 9:1N:103:VAL:HG23  | 2.20                     | 0.41              |
| 23:21:73:LEU:HD23  | 23:21:73:LEU:HA    | 1.87                     | 0.41              |
| 27:25:8:LYS:O      | 27:25:9:LYS:HD2    | 2.20                     | 0.41              |
| 1:2A:1297:C:H5''   | 60:2A:4143:HOH:O   | 2.20                     | 0.41              |
| 1:2A:1657:C:H2'    | 1:2A:1658:C:C6     | 2.55                     | 0.41              |
| 1:2A:2089:U:H2'    | 1:2A:2090:G:C8     | 2.55                     | 0.41              |
| 1:2A:2206:G:C3'    | 1:2A:2207:G:C8     | 3.00                     | 0.41              |
| 1:2A:2674:G:H2'    | 1:2A:2675:A:C8     | 2.56                     | 0.41              |
| 7:2H:104:GLU:HA    | 7:2H:113:VAL:O     | 2.20                     | 0.41              |
| 11:2P:47:ASP:HA    | 11:2P:48:PRO:HD3   | 1.92                     | 0.41              |
| 1:1A:1532:A:H2'    | 1:1A:1533:G:H8     | 1.85                     | 0.41              |
| 1:1A:2327:G:H2'    | 1:1A:2328:C:C6     | 2.55                     | 0.41              |
| 7:1H:3:ARG:NH2     | 7:1H:65:HIS:HB3    | 2.36                     | 0.41              |
| 9:1N:62:VAL:CG2    | 9:1N:66:LYS:HD2    | 2.50                     | 0.41              |
| 14:1S:59:LYS:HB2   | 14:1S:60:GLY:H     | 1.46                     | 0.41              |
| 1:1A:1270:C:O2'    | 17:1V:85:LYS:HA    | 2.20                     | 0.41              |
| 20:1Y:92:ASN:CB    | 20:1Y:94:LYS:HG2   | 2.51                     | 0.41              |
| 28:26:14:THR:OG1   | 28:26:48:VAL:HG13  | 2.20                     | 0.41              |
| 1:2A:1359:A:C6     | 1:2A:1372:U:O4     | 2.73                     | 0.41              |
| 1:2A:2128:C:O2'    | 1:2A:2174:C:H4'    | 2.20                     | 0.41              |
| 1:2A:828:U:H2'     | 1:2A:829:A:C8      | 2.56                     | 0.41              |
| 5:2F:80:ALA:HB3    | 5:2F:83:PHE:HD2    | 1.85                     | 0.41              |
| 6:2G:43:LEU:HD11   | 6:2G:153:ARG:HB3   | 2.02                     | 0.41              |
| 6:2G:46:ALA:O      | 6:2G:51:ARG:HG3    | 2.20                     | 0.41              |
| 11:2P:125:VAL:HG13 | 11:2P:138:LEU:HD21 | 2.02                     | 0.41              |
| 18:2W:35:ILE:O     | 18:2W:39:THR:OG1   | 2.35                     | 0.41              |
| 20:2Y:56:PRO:O     | 20:2Y:57:GLN:HB2   | 2.19                     | 0.41              |
| 1:1A:1159:U:H2'    | 1:1A:1160:G:H8     | 1.86                     | 0.41              |
| 1:1A:210:A:C4      | 1:1A:255:G:N7      | 2.88                     | 0.41              |
| 1:1A:2207:C:C4     | 1:1A:2208:G:N7     | 2.89                     | 0.41              |
| 1:1A:2398:C:H2'    | 1:1A:2399:U:C6     | 2.56                     | 0.41              |
| 1:1A:925:A:H2'     | 1:1A:926:G:H5'     | 2.03                     | 0.41              |
| 2:1B:12:C:H2'      | 22:10:73:GLY:HA3   | 2.03                     | 0.41              |
| 5:1F:178:PRO:HB2   | 5:1F:201:VAL:CG2   | 2.50                     | 0.41              |
| 5:1F:74:ARG:H      | 5:1F:74:ARG:HG3    | 1.64                     | 0.41              |
| 6:1G:16:ARG:HB2    | 6:1G:17:PRO:HD3    | 2.01                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 11:1P:98:GLU:O    | 11:1P:101:VAL:HB   | 2.21                     | 0.41              |
| 1:1A:509:A:O4'    | 20:1Y:48:ALA:HB1   | 2.20                     | 0.41              |
| 1:2A:1683:C:H2'   | 1:2A:1684:C:C6     | 2.56                     | 0.41              |
| 1:2A:1946:U:H2'   | 1:2A:1947:C:H6     | 1.83                     | 0.41              |
| 1:2A:2472:G:H2'   | 1:2A:2475:C:H42    | 1.86                     | 0.41              |
| 1:2A:625:G:H2'    | 1:2A:626:U:H6      | 2.86                     | 0.41              |
| 1:2A:885:C:H2'    | 1:2A:886:C:O4'     | 2.21                     | 0.41              |
| 9:2N:75:TYR:HA    | 9:2N:81:GLY:O      | 2.21                     | 0.41              |
| 1:2A:1422:G:H5''  | 10:2O:48:PRO:HB3   | 100.32                   | 0.41              |
| 1:2A:626:U:O2     | 11:2P:105:LEU:HD23 | 2.20                     | 0.41              |
| 15:2T:13:ARG:HG2  | 15:2T:14:TYR:CE2   | 2.55                     | 0.41              |
| 16:2U:107:ALA:O   | 16:2U:111:GLU:HG2  | 2.20                     | 0.41              |
| 20:2Y:73:ARG:HG2  | 20:2Y:73:ARG:HH11  | 1.85                     | 0.41              |
| 24:12:3:LEU:HD22  | 24:12:7:ARG:NH2    | 2.36                     | 0.41              |
| 1:1A:1230:C:H5''  | 1:1A:1231:G:OP1    | 2.21                     | 0.41              |
| 1:1A:1896:G:N2    | 1:1A:1898:A:H3'    | 2.35                     | 0.41              |
| 1:1A:1948:U:O2'   | 1:1A:1950:A:N7     | 2.47                     | 0.41              |
| 1:1A:2156:A:C2    | 1:1A:2180:A:H4'    | 2.56                     | 0.41              |
| 1:1A:2216:G:H2'   | 1:1A:2217:C:O4'    | 2.19                     | 0.41              |
| 1:1A:870:G:C2     | 1:1A:882:A:C2      | 3.09                     | 0.41              |
| 4:1E:9:VAL:HG13   | 4:1E:25:VAL:O      | 2.21                     | 0.41              |
| 1:1A:1303:C:H4'   | 5:1F:83:PHE:CD1    | 2.56                     | 0.41              |
| 6:1G:18:GLU:O     | 6:1G:21:ARG:HB3    | 2.20                     | 0.41              |
| 12:1Q:137:TYR:O   | 12:1Q:141:GLN:HG2  | 2.20                     | 0.41              |
| 17:1V:97:LYS:HD3  | 17:1V:97:LYS:HA    | 1.72                     | 0.41              |
| 19:1X:35:THR:O    | 19:1X:38:GLU:HB3   | 2.20                     | 0.41              |
| 21:1Z:145:GLU:N   | 21:1Z:148:ASP:HB2  | 2.35                     | 0.41              |
| 1:2A:2577:A:O4'   | 27:25:3:LYS:HB2    | 2.21                     | 0.41              |
| 28:26:11:LEU:HB3  | 28:26:49:HIS:HB3   | 2.03                     | 0.41              |
| 1:2A:2126:A:H4'   | 1:2A:2127:G:C4'    | 2.51                     | 0.41              |
| 1:2A:2134:A:N1    | 1:2A:2135:A:N6     | 2.69                     | 0.41              |
| 1:2A:2298:A:N6    | 1:2A:2318:G:C8     | 2.88                     | 0.41              |
| 1:2A:2819:G:H1    | 1:2A:2827:C:N4     | 2.18                     | 0.41              |
| 3:2D:16:MET:HB2   | 3:2D:207:GLY:HA3   | 2.03                     | 0.41              |
| 3:2D:218:ARG:HB3  | 3:2D:219:PRO:HD2   | 2.03                     | 0.41              |
| 3:2D:264:LYS:HA   | 3:2D:265:PRO:HD3   | 1.91                     | 0.41              |
| 6:2G:145:THR:HG23 | 6:2G:147:ASP:H     | 1.86                     | 0.41              |
| 10:2O:121:VAL:O   | 15:2T:43:GLN:NE2   | 2.51                     | 0.41              |
| 13:2R:82:GLU:O    | 13:2R:85:PRO:HD2   | 2.20                     | 0.41              |
| 16:2U:5:LYS:HG2   | 16:2U:5:LYS:H      | 1.67                     | 0.41              |
| 19:2X:35:THR:HG22 | 19:2X:37:THR:N     | 2.35                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:13:7:LYS:HE3   | 25:13:32:GLN:NE2   | 2.36                     | 0.41              |
| 30:18:63:PRO:HG2  | 30:18:64:TYR:CE2   | 2.56                     | 0.41              |
| 1:1A:1854:G:OP1   | 3:1D:54:ARG:NH1    | 2.53                     | 0.41              |
| 1:1A:2418:U:OP1   | 1:1A:2423:A:N6     | 2.54                     | 0.41              |
| 1:1A:2545:A:H2'   | 1:1A:2546:A:O4'    | 2.21                     | 0.41              |
| 1:1A:2820:A:H61   | 1:1A:2900:G:C2'    | 2.34                     | 0.41              |
| 1:1A:831:A:C5     | 3:1D:229:VAL:HG21  | 2.56                     | 0.41              |
| 1:1A:848:G:O6     | 5:1F:53:THR:OG1    | 2.36                     | 0.41              |
| 5:1F:200:GLU:O    | 5:1F:203:GLN:HB2   | 2.20                     | 0.41              |
| 1:1A:1302:G:O2'   | 5:1F:75:HIS:HE1    | 2.04                     | 0.41              |
| 19:1X:29:TRP:CE3  | 19:1X:78:LYS:HB3   | 2.56                     | 0.41              |
| 1:2A:1021:A:H3'   | 1:2A:1021:A:N3     | 2.36                     | 0.41              |
| 1:2A:1847:A:H3'   | 1:2A:1848:A:H5'    | 2.02                     | 0.41              |
| 1:2A:1899:G:N3    | 1:2A:1899:G:H2'    | 2.36                     | 0.41              |
| 1:2A:2130:U:O2'   | 1:2A:2133:G:H4'    | 2.21                     | 0.41              |
| 1:2A:2157:G:H8    | 1:2A:2157:G:H3'    | 1.84                     | 0.41              |
| 1:2A:2360:A:C2    | 1:2A:2361:A:H1'    | 2.56                     | 0.41              |
| 1:2A:2439:A:H1'   | 1:2A:2587:A:OP1    | 2.21                     | 0.41              |
| 1:2A:874:G:C6     | 1:2A:875:G:C5      | 3.08                     | 0.41              |
| 3:2D:43:ARG:HA    | 3:2D:48:ARG:O      | 2.20                     | 0.41              |
| 4:2E:101:ARG:HA   | 4:2E:101:ARG:HD3   | 1.69                     | 0.41              |
| 6:2G:16:ARG:NH1   | 6:2G:31:VAL:HG22   | 2.36                     | 0.41              |
| 7:2H:124:GLU:OE1  | 7:2H:132:ARG:HD2   | 2.20                     | 0.41              |
| 10:2O:61:VAL:HG11 | 10:2O:114:ILE:CD1  | 2.51                     | 0.41              |
| 21:2Z:193:GLU:HA  | 21:2Z:194:PRO:HD3  | 1.88                     | 0.41              |
| 21:2Z:35:ARG:HA   | 21:2Z:35:ARG:HD2   | 1.89                     | 0.41              |
| 22:10:24:LYS:HA   | 22:10:24:LYS:HD3   | 1.82                     | 0.41              |
| 30:18:62:LEU:HB3  | 30:18:65:GLU:CG    | 2.50                     | 0.41              |
| 1:1A:1136:U:C2    | 1:1A:1148:C:O2     | 2.74                     | 0.41              |
| 1:1A:1404:G:O2'   | 1:1A:1405:A:H5''   | 2.21                     | 0.41              |
| 1:1A:1497:G:H2'   | 1:1A:1498:C:H6     | 1.85                     | 0.41              |
| 1:1A:1588:G:H3'   | 1:1A:1589:A:H2'    | 2.03                     | 0.41              |
| 1:1A:2125:C:C2    | 1:1A:2126:G:N7     | 2.88                     | 0.41              |
| 1:1A:2476:C:H1'   | 60:1A:9872:HOH:O   | 2.20                     | 0.41              |
| 3:1D:206:LEU:HD22 | 3:1D:211:ARG:HG2   | 2.02                     | 0.41              |
| 9:1N:75:TYR:CE2   | 9:1N:77:GLY:HA2    | 2.56                     | 0.41              |
| 15:1T:53:ARG:CZ   | 15:1T:53:ARG:HB3   | 2.51                     | 0.41              |
| 16:1U:34:LYS:HD3  | 16:1U:34:LYS:HA    | 1.91                     | 0.41              |
| 21:1Z:158:PRO:O   | 21:1Z:161:VAL:HG12 | 2.20                     | 0.41              |
| 24:22:32:LEU:HD22 | 24:22:36:ARG:NH1   | 2.35                     | 0.41              |
| 1:2A:2784:C:H1'   | 4:2E:37:ARG:HH12   | 1.86                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1A:1324:A:OP1   | 13:1R:36:THR:HG23 | 2.21                     | 0.41              |
| 1:1A:1961:5MU:OP1 | 1:1A:2616:U:O2'   | 2.35                     | 0.41              |
| 1:1A:2167:C:C6    | 1:1A:2167:C:OP1   | 2.74                     | 0.41              |
| 1:1A:2156:A:N3    | 1:1A:2180:A:H4'   | 2.36                     | 0.41              |
| 1:1A:2573:A:H2    | 10:1O:23:ARG:HH21 | 1.67                     | 0.41              |
| 1:1A:2734:A:H2'   | 1:1A:2735:G:O4'   | 2.21                     | 0.41              |
| 1:1A:424:G:H1'    | 1:1A:2243:C:O2'   | 2.20                     | 0.41              |
| 1:1A:789:G:H4'    | 1:1A:1723:A:H5'   | 2.03                     | 0.41              |
| 3:1D:108:PRO:HD2  | 3:1D:111:LEU:HG   | 2.03                     | 0.41              |
| 6:1G:121:ASN:O    | 6:1G:131:TYR:OH   | 2.30                     | 0.41              |
| 7:1H:126:PRO:HD2  | 7:1H:130:ARG:O    | 2.21                     | 0.41              |
| 8:1I:81:VAL:O     | 8:1I:146:ALA:HA   | 2.20                     | 0.41              |
| 1:1A:276:C:OP1    | 8:1I:45:LYS:HD3   | 2.21                     | 0.41              |
| 16:1U:81:HIS:O    | 16:1U:85:LYS:HG3  | 2.21                     | 0.41              |
| 25:23:26:LEU:HD21 | 25:23:46:ASN:HB2  | 2.03                     | 0.41              |
| 26:24:58:ARG:HD2  | 26:24:58:ARG:HA   | 1.91                     | 0.41              |
| 26:24:62:ARG:HH11 | 26:24:62:ARG:H    | 1.68                     | 0.41              |
| 1:2A:2650:U:H2'   | 1:2A:2651:C:H6    | 1.85                     | 0.41              |
| 6:2G:135:LEU:O    | 6:2G:154:GLY:HA3  | 2.21                     | 0.41              |
| 7:2H:3:ARG:NH1    | 7:2H:4:ILE:H      | 2.19                     | 0.41              |
| 5:2F:184:TYR:CE1  | 11:2P:3:LEU:HD21  | 2.55                     | 0.41              |
| 1:2A:2392:A:N3    | 11:2P:61:ARG:HG2  | 2.35                     | 0.41              |
| 1:2A:583:G:OP2    | 16:2U:10:ARG:NH1  | 2.54                     | 0.41              |
| 1:1A:1005:A:H5'   | 1:1A:1038:C:H1'   | 50.66                    | 0.41              |
| 1:1A:1117:G:C6    | 1:1A:1118:C:C4    | 3.09                     | 0.41              |
| 1:1A:593:G:C6     | 1:1A:2052:A:C2    | 3.09                     | 0.41              |
| 1:1A:1911:A:N1    | 1:1A:2246:G:H1'   | 2.36                     | 0.41              |
| 1:1A:662:A:H4'    | 1:1A:663:G:O5'    | 2.21                     | 0.41              |
| 1:1A:802:C:H2'    | 1:1A:803:C:C6     | 2.56                     | 0.41              |
| 1:1A:1874:C:H5'   | 3:1D:253:GLN:NE2  | 2.36                     | 0.41              |
| 7:1H:19:VAL:HA    | 7:1H:24:VAL:HG12  | 2.02                     | 0.41              |
| 9:1N:33:LEU:HD12  | 9:1N:38:HIS:CE1   | 2.56                     | 0.41              |
| 11:1P:2:LYS:HD2   | 11:1P:4:SER:H     | 1.86                     | 0.41              |
| 24:22:9:GLN:HE22  | 24:22:56:GLN:HB3  | 1.86                     | 0.41              |
| 25:23:52:HIS:CD2  | 25:23:53:LEU:HG   | 2.56                     | 0.41              |
| 19:2X:60:ARG:NH2  | 29:27:47:ARG:HH22 | 2.18                     | 0.41              |
| 1:2A:1024:G:C6    | 1:2A:1025:G:C6    | 3.09                     | 0.41              |
| 1:2A:2342:C:O2'   | 1:2A:2374:C:OP1   | 2.29                     | 0.41              |
| 1:2A:266:G:H2'    | 1:2A:266:G:N3     | 3.22                     | 0.41              |
| 1:2A:271(O):C:H2' | 1:2A:271(P):C:C6  | 2.56                     | 0.41              |
| 1:2A:2740:A:C6    | 1:2A:2764:A:C8    | 3.09                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:2A:601:C:O2'    | 1:2A:605:C:OP1     | 2.32                     | 0.41              |
| 1:2A:999:U:O2'    | 1:2A:1000:A:H5'    | 2.21                     | 0.41              |
| 2:2B:29:A:C6      | 2:2B:30:C:C4       | 3.09                     | 0.41              |
| 4:2E:167:VAL:CG1  | 4:2E:189:PRO:HD3   | 2.51                     | 0.41              |
| 6:2G:52:ILE:O     | 6:2G:53:LEU:HD23   | 2.21                     | 0.41              |
| 7:2H:126:PRO:HD2  | 7:2H:130:ARG:O     | 2.21                     | 0.41              |
| 8:2I:116:LEU:HD11 | 8:2I:119:PRO:HA    | 2.03                     | 0.41              |
| 21:2Z:52:SER:HB3  | 21:2Z:53:ILE:H     | 1.62                     | 0.41              |
| 23:11:60:PHE:HZ   | 23:11:94:LEU:HD12  | 1.86                     | 0.40              |
| 24:12:35:LEU:HA   | 24:12:35:LEU:HD23  | 1.92                     | 0.40              |
| 27:15:8:LYS:O     | 27:15:9:LYS:HD2    | 2.21                     | 0.40              |
| 1:1A:2054:G:H1'   | 4:1E:145:LYS:HD3   | 2.03                     | 0.40              |
| 1:1A:2150:C:H2'   | 1:1A:2151:C:C6     | 2.56                     | 0.40              |
| 1:1A:234:G:O6     | 30:18:8:LYS:NZ     | 2.37                     | 0.40              |
| 1:1A:2856:G:H2'   | 1:1A:2857:U:O4'    | 2.21                     | 0.40              |
| 1:1A:304:C:C2     | 1:1A:385:G:C2      | 3.09                     | 0.40              |
| 1:1A:116:A:N6     | 1:1A:313:A:N3      | 38.72                    | 0.40              |
| 4:1E:36:ARG:NH1   | 4:1E:85:ASN:OD1    | 2.54                     | 0.40              |
| 7:1H:3:ARG:HG2    | 7:1H:6:ARG:NE      | 2.36                     | 0.40              |
| 8:1I:130:TYR:HB3  | 8:1I:138:ILE:HB    | 2.01                     | 0.40              |
| 11:1P:90:ARG:NH1  | 11:1P:105:LEU:HD11 | 2.35                     | 0.40              |
| 13:1R:17:ARG:O    | 13:1R:20:LEU:HB3   | 2.21                     | 0.40              |
| 1:1A:2331:G:H1    | 14:1S:3:ARG:HA     | 1.86                     | 0.40              |
| 18:1W:107:LEU:HA  | 18:1W:107:LEU:HD12 | 1.91                     | 0.40              |
| 22:20:52:GLY:O    | 22:20:59:LEU:HA    | 2.21                     | 0.40              |
| 26:24:46:GLN:C    | 26:24:48:ARG:H     | 2.23                     | 0.40              |
| 1:2A:1065:U:HO2'  | 1:2A:1066:U:P      | 2.41                     | 0.40              |
| 1:2A:1141:U:O2    | 1:2A:1142(A):A:N6  | 2.54                     | 0.40              |
| 1:2A:1364:G:P     | 23:21:3:LYS:HG3    | 2.62                     | 0.40              |
| 1:2A:171:G:H2'    | 1:2A:172:C:C6      | 2.56                     | 0.40              |
| 1:2A:2100:G:C6    | 1:2A:2101:G:C8     | 3.09                     | 0.40              |
| 1:2A:2138:C:N3    | 1:2A:2153:G:N2     | 2.69                     | 0.40              |
| 1:2A:2259:G:C2    | 1:2A:2282:G:C6     | 3.09                     | 0.40              |
| 3:2D:70:TRP:HB3   | 3:2D:190:TYR:CE2   | 2.57                     | 0.40              |
| 4:2E:51:PHE:CE1   | 4:2E:52:LEU:HD23   | 2.56                     | 0.40              |
| 10:2O:120:GLU:HB2 | 15:2T:68:TYR:HE2   | 1.86                     | 0.40              |
| 29:17:8:ASN:HB3   | 29:17:11:LYS:HB3   | 2.02                     | 0.40              |
| 1:1A:1005:A:C8    | 1:1A:1007:G:C8     | 3.10                     | 0.40              |
| 1:1A:1524:A:C2    | 1:1A:1563:G:C2     | 3.09                     | 0.40              |
| 1:1A:1785:C:H2'   | 1:1A:1786:A:O4'    | 2.21                     | 0.40              |
| 1:1A:2302:G:H2'   | 1:1A:2303:U:O4'    | 2.21                     | 0.40              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:1A:26:G:C6       | 1:1A:27:G:N1      | 2.89                     | 0.40              |
| 1:1A:721:G:H4'     | 1:1A:722:A:O4'    | 6.12                     | 0.40              |
| 1:1A:908:A:C2      | 1:1A:963:A:C4     | 3.09                     | 0.40              |
| 11:1P:79:ARG:HD3   | 11:1P:79:ARG:HA   | 1.94                     | 0.40              |
| 26:24:2:LYS:O      | 26:24:6:HIS:HD2   | 2.04                     | 0.40              |
| 1:2A:1528(A):A:H2' | 1:2A:1529:G:O4'   | 2.21                     | 0.40              |
| 1:2A:2133:G:N2     | 1:2A:2158:A:OP2   | 2.54                     | 0.40              |
| 1:2A:2134:A:C4     | 1:2A:2157:G:H4'   | 2.56                     | 0.40              |
| 1:2A:539:G:H2'     | 1:2A:540:C:H6     | 1.87                     | 0.40              |
| 1:2A:581:C:H2'     | 1:2A:582:G:H8     | 1.85                     | 0.40              |
| 1:2A:820:A:H2'     | 1:2A:821:A:O4'    | 2.21                     | 0.40              |
| 8:2I:53:ALA:O      | 8:2I:57:ARG:HG2   | 2.21                     | 0.40              |
| 9:2N:108:PRO:O     | 9:2N:113:GLY:HA3  | 2.21                     | 0.40              |
| 1:2A:557:U:O2      | 9:2N:45:ASN:HB2   | 2.22                     | 0.40              |
| 11:2P:95:VAL:HA    | 11:2P:99:LEU:HD22 | 2.02                     | 0.40              |
| 21:2Z:145:GLU:HB2  | 21:2Z:148:ASP:OD2 | 2.21                     | 0.40              |
| 1:1A:1550:C:H2'    | 1:1A:1551:C:C6    | 2.57                     | 0.40              |
| 1:1A:170:A:H1'     | 1:1A:462:C:H5'    | 2.02                     | 0.40              |
| 1:1A:2196:C:H2'    | 1:1A:2197:C:H6    | 1.85                     | 0.40              |
| 1:1A:2054:G:N2     | 1:1A:2584:A:OP2   | 2.54                     | 0.40              |
| 1:1A:264:G:H1      | 1:1A:280:C:H42    | 1.69                     | 0.40              |
| 1:1A:481:C:N3      | 1:1A:498:A:H2'    | 2.36                     | 0.40              |
| 6:1G:6:ALA:HB3     | 6:1G:104:GLU:OE2  | 2.22                     | 0.40              |
| 9:1N:1:MET:O       | 9:1N:1:MET:HG3    | 2.22                     | 0.40              |
| 14:1S:25:ARG:O     | 14:1S:39:ILE:HA   | 2.20                     | 0.40              |
| 25:23:12:PRO:HB2   | 25:23:20:LYS:HG2  | 2.04                     | 0.40              |
| 1:2A:1059:G:C5     | 1:2A:1060:U:N3    | 2.90                     | 0.40              |
| 1:2A:1721:G:H5'    | 1:2A:1722:A:OP2   | 2.21                     | 0.40              |
| 1:2A:2127:G:N2     | 1:2A:2173:A:H1'   | 2.37                     | 0.40              |
| 1:2A:2302:G:C6     | 1:2A:2315:G:C6    | 3.10                     | 0.40              |
| 1:2A:2432:A:C6     | 1:2A:2433:A:C6    | 3.10                     | 0.40              |
| 1:2A:2031:A:C6     | 1:2A:2498:C:H1'   | 2.55                     | 0.40              |
| 1:2A:2810:A:H2'    | 1:2A:2811:G:O4'   | 2.22                     | 0.40              |
| 1:2A:660:G:C6      | 1:2A:661:C:C4     | 3.09                     | 0.40              |
| 1:2A:723:G:H2'     | 1:2A:724:U:O4'    | 2.22                     | 0.40              |
| 4:2E:14:ILE:HD11   | 4:2E:173:VAL:HG11 | 2.03                     | 0.40              |
| 5:2F:150:GLY:HA2   | 5:2F:172:TRP:CE3  | 2.56                     | 0.40              |
| 6:2G:36:LYS:O      | 6:2G:159:VAL:HA   | 2.21                     | 0.40              |
| 9:2N:110:GLY:O     | 9:2N:114:ARG:HG3  | 2.21                     | 0.40              |
| 4:2E:15:PHE:CD2    | 15:2T:81:PRO:HD3  | 2.56                     | 0.40              |
| 21:2Z:28:MET:HA    | 21:2Z:88:PHE:O    | 2.21                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1A:1018:A:H8    | 1:1A:1018:A:OP1   | 2.04                     | 0.40              |
| 1:1A:2382:G:C6    | 1:1A:2383:G:C6    | 3.09                     | 0.40              |
| 1:1A:2401:G:H5''  | 1:1A:2402:U:O4'   | 2.22                     | 0.40              |
| 1:1A:2451:A:C8    | 1:1A:2451:A:H5'   | 2.56                     | 0.40              |
| 1:1A:2658:C:H2'   | 1:1A:2659:U:O4'   | 2.21                     | 0.40              |
| 1:1A:2669:A:O3'   | 7:1H:160:LYS:NZ   | 2.55                     | 0.40              |
| 1:1A:910:A:H8     | 1:1A:910:A:O5'    | 2.04                     | 0.40              |
| 1:1A:969:C:H2'    | 1:1A:970:C:C6     | 2.57                     | 0.40              |
| 4:1E:4:ILE:HD13   | 4:1E:28:ALA:HB1   | 2.02                     | 0.40              |
| 6:1G:37:VAL:HG22  | 6:1G:159:VAL:HB   | 2.04                     | 0.40              |
| 6:1G:43:LEU:C     | 6:1G:45:GLU:H     | 2.25                     | 0.40              |
| 1:2A:1268:A:H2'   | 1:2A:1269:A:O4'   | 2.22                     | 0.40              |
| 1:2A:1494:A:H2'   | 1:2A:1495:A:C8    | 2.57                     | 0.40              |
| 1:2A:1636:C:H2'   | 1:2A:1637:A:C8    | 2.56                     | 0.40              |
| 1:2A:919:G:N2     | 1:2A:2269:A:OP2   | 2.54                     | 0.40              |
| 1:2A:2489:G:C6    | 1:2A:2490:G:N1    | 2.90                     | 0.40              |
| 1:2A:271(K):U:O2  | 8:2I:50:ARG:HD2   | 2.21                     | 0.40              |
| 1:2A:629:G:H2'    | 1:2A:630:G:O4'    | 2.52                     | 0.40              |
| 10:2O:68:GLU:HB3  | 10:2O:78:ARG:HD3  | 2.03                     | 0.40              |
| 21:2Z:28:MET:O    | 21:2Z:34:ASN:HA   | 2.22                     | 0.40              |
| 28:16:16:CYS:SG   | 28:16:18:ARG:HD2  | 2.61                     | 0.40              |
| 1:1A:1259:A:H2'   | 1:1A:1260:G:O4'   | 2.22                     | 0.40              |
| 1:1A:142:G:H1'    | 19:1X:37:THR:CG2  | 2.51                     | 0.40              |
| 1:1A:1513:G:H2'   | 1:1A:1594:C:N4    | 2.36                     | 0.40              |
| 1:1A:178:G:O6     | 1:1A:194:G:O2'    | 2.37                     | 0.40              |
| 1:1A:2163:G:C6    | 1:1A:2173:G:C6    | 3.09                     | 0.40              |
| 1:1A:18:C:O2'     | 1:1A:577:U:OP1    | 2.34                     | 0.40              |
| 1:1A:829:A:C2     | 3:1D:226:MET:HG2  | 2.56                     | 0.40              |
| 6:1G:110:ALA:HB1  | 6:1G:140:ILE:HG22 | 2.04                     | 0.40              |
| 7:1H:117:PRO:HG3  | 7:1H:123:PHE:CD2  | 2.56                     | 0.40              |
| 7:1H:11:VAL:HA    | 7:1H:12:PRO:HD2   | 1.98                     | 0.40              |
| 11:1P:141:ALA:HA  | 25:23:38:GLU:CG   | 2.51                     | 0.40              |
| 16:1U:81:HIS:CE1  | 16:1U:85:LYS:HD2  | 2.57                     | 0.40              |
| 21:1Z:92:SER:O    | 21:1Z:130:PRO:HG2 | 2.22                     | 0.40              |
| 23:21:8:SER:HB3   | 23:21:66:HIS:CD2  | 2.56                     | 0.40              |
| 1:2A:2364:C:H2'   | 1:2A:2365:G:O4'   | 2.21                     | 0.40              |
| 1:2A:271(D):G:H2' | 1:2A:271(E):U:C6  | 2.56                     | 0.40              |
| 1:2A:414:C:H1'    | 1:2A:1864:U:H1'   | 2.04                     | 0.40              |
| 1:2A:265:A:N6     | 1:2A:428:A:H1'    | 2.37                     | 0.40              |
| 1:2A:757:U:H2'    | 1:2A:758:C:O4'    | 2.21                     | 0.40              |
| 6:2G:43:LEU:HA    | 6:2G:43:LEU:HD12  | 1.77                     | 0.40              |

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| Atom-1          | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-------------------|--------------------------|-------------------|
| 7:2H:103:LEU:HG | 7:2H:105:LEU:HD13 | 2.03                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 3   | 1D    | 273/275 (99%) | 259 (95%) | 13 (5%) | 1 (0%)   | 39          | 74  |
| 3   | 2D    | 273/275 (99%) | 261 (96%) | 12 (4%) | 0        | 100         | 100 |
| 4   | 1E    | 202/204 (99%) | 193 (96%) | 8 (4%)  | 1 (0%)   | 34          | 69  |
| 4   | 2E    | 202/204 (99%) | 192 (95%) | 9 (4%)  | 1 (0%)   | 34          | 69  |
| 5   | 1F    | 201/203 (99%) | 196 (98%) | 5 (2%)  | 0        | 100         | 100 |
| 5   | 2F    | 201/203 (99%) | 192 (96%) | 8 (4%)  | 1 (0%)   | 34          | 69  |
| 6   | 1G    | 179/181 (99%) | 161 (90%) | 16 (9%) | 2 (1%)   | 17          | 50  |
| 6   | 2G    | 179/181 (99%) | 164 (92%) | 14 (8%) | 1 (1%)   | 30          | 65  |
| 7   | 1H    | 172/174 (99%) | 161 (94%) | 11 (6%) | 0        | 100         | 100 |
| 7   | 2H    | 171/174 (98%) | 161 (94%) | 10 (6%) | 0        | 100         | 100 |
| 8   | 1I    | 145/147 (99%) | 130 (90%) | 12 (8%) | 3 (2%)   | 9           | 29  |
| 8   | 2I    | 144/147 (98%) | 131 (91%) | 13 (9%) | 0        | 100         | 100 |
| 9   | 1N    | 138/140 (99%) | 135 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 9   | 2N    | 138/140 (99%) | 136 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 10  | 1O    | 120/122 (98%) | 113 (94%) | 6 (5%)  | 1 (1%)   | 24          | 58  |
| 10  | 2O    | 120/122 (98%) | 113 (94%) | 6 (5%)  | 1 (1%)   | 24          | 58  |
| 11  | 1P    | 147/149 (99%) | 137 (93%) | 10 (7%) | 0        | 100         | 100 |
| 11  | 2P    | 147/149 (99%) | 138 (94%) | 9 (6%)  | 0        | 100         | 100 |
| 12  | 1Q    | 139/141 (99%) | 133 (96%) | 6 (4%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 12  | 2Q    | 139/141 (99%) | 133 (96%) | 6 (4%)   | 0        | 100         | 100 |
| 13  | 1R    | 116/118 (98%) | 110 (95%) | 6 (5%)   | 0        | 100         | 100 |
| 13  | 2R    | 116/118 (98%) | 109 (94%) | 7 (6%)   | 0        | 100         | 100 |
| 14  | 1S    | 108/110 (98%) | 102 (94%) | 5 (5%)   | 1 (1%)   | 21          | 55  |
| 14  | 2S    | 108/110 (98%) | 103 (95%) | 5 (5%)   | 0        | 100         | 100 |
| 15  | 1T    | 129/131 (98%) | 122 (95%) | 7 (5%)   | 0        | 100         | 100 |
| 15  | 2T    | 129/131 (98%) | 123 (95%) | 6 (5%)   | 0        | 100         | 100 |
| 16  | 1U    | 114/116 (98%) | 112 (98%) | 2 (2%)   | 0        | 100         | 100 |
| 16  | 2U    | 114/116 (98%) | 112 (98%) | 2 (2%)   | 0        | 100         | 100 |
| 17  | 1V    | 99/101 (98%)  | 95 (96%)  | 3 (3%)   | 1 (1%)   | 19          | 52  |
| 17  | 2V    | 99/101 (98%)  | 95 (96%)  | 3 (3%)   | 1 (1%)   | 19          | 52  |
| 18  | 1W    | 110/112 (98%) | 106 (96%) | 4 (4%)   | 0        | 100         | 100 |
| 18  | 2W    | 110/112 (98%) | 108 (98%) | 2 (2%)   | 0        | 100         | 100 |
| 19  | 1X    | 93/95 (98%)   | 90 (97%)  | 2 (2%)   | 1 (1%)   | 17          | 50  |
| 19  | 2X    | 93/95 (98%)   | 88 (95%)  | 4 (4%)   | 1 (1%)   | 17          | 50  |
| 20  | 1Y    | 105/107 (98%) | 98 (93%)  | 7 (7%)   | 0        | 100         | 100 |
| 20  | 2Y    | 105/107 (98%) | 100 (95%) | 5 (5%)   | 0        | 100         | 100 |
| 21  | 1Z    | 201/203 (99%) | 186 (92%) | 15 (8%)  | 0        | 100         | 100 |
| 21  | 2Z    | 199/203 (98%) | 184 (92%) | 15 (8%)  | 0        | 100         | 100 |
| 22  | 10    | 75/77 (97%)   | 70 (93%)  | 5 (7%)   | 0        | 100         | 100 |
| 22  | 20    | 75/77 (97%)   | 70 (93%)  | 5 (7%)   | 0        | 100         | 100 |
| 23  | 11    | 95/97 (98%)   | 94 (99%)  | 1 (1%)   | 0        | 100         | 100 |
| 23  | 21    | 95/97 (98%)   | 93 (98%)  | 1 (1%)   | 1 (1%)   | 17          | 50  |
| 24  | 12    | 68/70 (97%)   | 66 (97%)  | 2 (3%)   | 0        | 100         | 100 |
| 24  | 22    | 68/70 (97%)   | 66 (97%)  | 2 (3%)   | 0        | 100         | 100 |
| 25  | 13    | 57/59 (97%)   | 55 (96%)  | 2 (4%)   | 0        | 100         | 100 |
| 25  | 23    | 57/59 (97%)   | 54 (95%)  | 3 (5%)   | 0        | 100         | 100 |
| 26  | 14    | 67/69 (97%)   | 55 (82%)  | 8 (12%)  | 4 (6%)   | 2           | 5   |
| 26  | 24    | 67/69 (97%)   | 52 (78%)  | 14 (21%) | 1 (2%)   | 13          | 40  |
| 27  | 15    | 57/59 (97%)   | 54 (95%)  | 3 (5%)   | 0        | 100         | 100 |
| 27  | 25    | 57/59 (97%)   | 54 (95%)  | 3 (5%)   | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 28  | 16    | 51/53 (96%)   | 49 (96%)  | 2 (4%)   | 0        | 100         | 100 |
| 28  | 26    | 51/53 (96%)   | 49 (96%)  | 2 (4%)   | 0        | 100         | 100 |
| 29  | 17    | 46/48 (96%)   | 44 (96%)  | 2 (4%)   | 0        | 100         | 100 |
| 29  | 27    | 46/48 (96%)   | 44 (96%)  | 2 (4%)   | 0        | 100         | 100 |
| 30  | 18    | 62/64 (97%)   | 60 (97%)  | 2 (3%)   | 0        | 100         | 100 |
| 30  | 28    | 62/64 (97%)   | 59 (95%)  | 3 (5%)   | 0        | 100         | 100 |
| 31  | 19    | 35/37 (95%)   | 35 (100%) | 0        | 0        | 100         | 100 |
| 31  | 29    | 35/37 (95%)   | 35 (100%) | 0        | 0        | 100         | 100 |
| 33  | 1b    | 229/231 (99%) | 201 (88%) | 20 (9%)  | 8 (4%)   | 4           | 15  |
| 33  | 2b    | 229/231 (99%) | 198 (86%) | 24 (10%) | 7 (3%)   | 5           | 17  |
| 34  | 1c    | 204/206 (99%) | 185 (91%) | 17 (8%)  | 2 (1%)   | 19          | 52  |
| 34  | 2c    | 204/206 (99%) | 186 (91%) | 16 (8%)  | 2 (1%)   | 19          | 52  |
| 35  | 1d    | 206/208 (99%) | 188 (91%) | 18 (9%)  | 0        | 100         | 100 |
| 35  | 2d    | 206/208 (99%) | 188 (91%) | 18 (9%)  | 0        | 100         | 100 |
| 36  | 1e    | 146/148 (99%) | 138 (94%) | 6 (4%)   | 2 (1%)   | 14          | 42  |
| 36  | 2e    | 146/148 (99%) | 139 (95%) | 7 (5%)   | 0        | 100         | 100 |
| 37  | 1f    | 98/100 (98%)  | 92 (94%)  | 6 (6%)   | 0        | 100         | 100 |
| 37  | 2f    | 98/100 (98%)  | 92 (94%)  | 6 (6%)   | 0        | 100         | 100 |
| 38  | 1g    | 153/155 (99%) | 148 (97%) | 5 (3%)   | 0        | 100         | 100 |
| 38  | 2g    | 153/155 (99%) | 145 (95%) | 7 (5%)   | 1 (1%)   | 26          | 62  |
| 39  | 1h    | 135/137 (98%) | 130 (96%) | 5 (4%)   | 0        | 100         | 100 |
| 39  | 2h    | 135/137 (98%) | 129 (96%) | 6 (4%)   | 0        | 100         | 100 |
| 40  | 1i    | 125/127 (98%) | 112 (90%) | 12 (10%) | 1 (1%)   | 24          | 58  |
| 40  | 2i    | 124/127 (98%) | 109 (88%) | 13 (10%) | 2 (2%)   | 12          | 38  |
| 41  | 1j    | 95/97 (98%)   | 82 (86%)  | 10 (10%) | 3 (3%)   | 5           | 17  |
| 41  | 2j    | 94/97 (97%)   | 83 (88%)  | 9 (10%)  | 2 (2%)   | 9           | 29  |
| 42  | 1k    | 112/114 (98%) | 100 (89%) | 12 (11%) | 0        | 100         | 100 |
| 42  | 2k    | 112/114 (98%) | 100 (89%) | 12 (11%) | 0        | 100         | 100 |
| 43  | 1l    | 119/122 (98%) | 114 (96%) | 5 (4%)   | 0        | 100         | 100 |
| 43  | 2l    | 119/122 (98%) | 115 (97%) | 4 (3%)   | 0        | 100         | 100 |
| 44  | 1m    | 114/116 (98%) | 102 (90%) | 9 (8%)   | 3 (3%)   | 7           | 22  |

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| Mol | Chain | Analysed          | Favoured    | Allowed  | Outliers | Percentiles |     |
|-----|-------|-------------------|-------------|----------|----------|-------------|-----|
| 44  | 2m    | 112/116 (97%)     | 96 (86%)    | 13 (12%) | 3 (3%)   | 6           | 21  |
| 45  | 1n    | 58/60 (97%)       | 54 (93%)    | 4 (7%)   | 0        | 100         | 100 |
| 45  | 2n    | 58/60 (97%)       | 54 (93%)    | 4 (7%)   | 0        | 100         | 100 |
| 46  | 1o    | 86/88 (98%)       | 84 (98%)    | 2 (2%)   | 0        | 100         | 100 |
| 46  | 2o    | 86/88 (98%)       | 81 (94%)    | 3 (4%)   | 2 (2%)   | 8           | 26  |
| 47  | 1p    | 80/82 (98%)       | 77 (96%)    | 3 (4%)   | 0        | 100         | 100 |
| 47  | 2p    | 80/82 (98%)       | 76 (95%)    | 4 (5%)   | 0        | 100         | 100 |
| 48  | 1q    | 97/99 (98%)       | 89 (92%)    | 7 (7%)   | 1 (1%)   | 19          | 52  |
| 48  | 2q    | 97/99 (98%)       | 90 (93%)    | 6 (6%)   | 1 (1%)   | 19          | 52  |
| 49  | 1r    | 66/68 (97%)       | 60 (91%)    | 5 (8%)   | 1 (2%)   | 13          | 40  |
| 49  | 2r    | 66/68 (97%)       | 61 (92%)    | 4 (6%)   | 1 (2%)   | 13          | 40  |
| 50  | 1s    | 81/83 (98%)       | 72 (89%)    | 8 (10%)  | 1 (1%)   | 16          | 47  |
| 50  | 2s    | 81/83 (98%)       | 73 (90%)    | 7 (9%)   | 1 (1%)   | 16          | 47  |
| 51  | 1t    | 94/98 (96%)       | 85 (90%)    | 6 (6%)   | 3 (3%)   | 5           | 17  |
| 51  | 2t    | 96/98 (98%)       | 87 (91%)    | 5 (5%)   | 4 (4%)   | 3           | 11  |
| 52  | 1u    | 21/23 (91%)       | 19 (90%)    | 2 (10%)  | 0        | 100         | 100 |
| 52  | 2u    | 21/23 (91%)       | 19 (90%)    | 2 (10%)  | 0        | 100         | 100 |
| 55  | 1y    | 14/16 (88%)       | 13 (93%)    | 0        | 1 (7%)   | 1           | 3   |
| 55  | 2y    | 14/16 (88%)       | 13 (93%)    | 0        | 1 (7%)   | 1           | 3   |
| All | All   | 11468/11680 (98%) | 10719 (94%) | 673 (6%) | 76 (1%)  | 26          | 62  |

All (76) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8   | 1I    | 11  | ASN  |
| 14  | 1S    | 59  | LYS  |
| 33  | 1b    | 17  | PHE  |
| 33  | 1b    | 21  | ARG  |
| 33  | 1b    | 37  | ASN  |
| 34  | 1c    | 108 | ASN  |
| 36  | 1e    | 96  | PRO  |
| 40  | 1i    | 127 | LYS  |
| 41  | 1j    | 79  | ARG  |
| 44  | 1m    | 67  | GLU  |
| 48  | 1q    | 49  | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 51  | 1t    | 95  | ALA  |
| 4   | 2E    | 51  | PHE  |
| 5   | 2F    | 21  | ALA  |
| 6   | 2G    | 43  | LEU  |
| 23  | 2I    | 3   | LYS  |
| 33  | 2b    | 8   | LYS  |
| 33  | 2b    | 17  | PHE  |
| 33  | 2b    | 124 | SER  |
| 34  | 2c    | 98  | ASN  |
| 40  | 2i    | 44  | VAL  |
| 40  | 2i    | 54  | ASP  |
| 51  | 2t    | 95  | ALA  |
| 3   | 1D    | 274 | ARG  |
| 6   | 1G    | 43  | LEU  |
| 8   | 1I    | 72  | LEU  |
| 8   | 1I    | 73  | GLU  |
| 19  | 1X    | 94  | GLY  |
| 26  | 14    | 45  | GLY  |
| 26  | 14    | 47  | GLN  |
| 26  | 14    | 49  | PHE  |
| 26  | 14    | 55  | ARG  |
| 33  | 1b    | 95  | GLN  |
| 33  | 1b    | 127 | ILE  |
| 44  | 1m    | 12  | ASN  |
| 49  | 1r    | 25  | THR  |
| 55  | 1y    | 15  | PRO  |
| 17  | 2V    | 79  | VAL  |
| 19  | 2X    | 94  | GLY  |
| 26  | 24    | 55  | ARG  |
| 33  | 2b    | 10  | LEU  |
| 33  | 2b    | 125 | PRO  |
| 34  | 2c    | 61  | ALA  |
| 41  | 2j    | 79  | ARG  |
| 44  | 2m    | 67  | GLU  |
| 49  | 2r    | 25  | THR  |
| 55  | 2y    | 15  | PRO  |
| 4   | 1E    | 52  | LEU  |
| 6   | 1G    | 51  | ARG  |
| 17  | 1V    | 79  | VAL  |
| 33  | 1b    | 125 | PRO  |
| 44  | 1m    | 106 | ASN  |
| 50  | 1s    | 7   | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10  | 2O    | 5   | GLN  |
| 44  | 2m    | 106 | ASN  |
| 51  | 2t    | 7   | LYS  |
| 10  | 1O    | 5   | GLN  |
| 33  | 1b    | 11  | LEU  |
| 34  | 1c    | 98  | ASN  |
| 51  | 1t    | 10  | LEU  |
| 33  | 2b    | 20  | GLU  |
| 33  | 2b    | 95  | GLN  |
| 48  | 2q    | 49  | GLU  |
| 50  | 2s    | 7   | LYS  |
| 38  | 2g    | 6   | ARG  |
| 44  | 2m    | 5   | ALA  |
| 46  | 2o    | 88  | ARG  |
| 51  | 2t    | 100 | ILE  |
| 41  | 1j    | 77  | PRO  |
| 51  | 1t    | 100 | ILE  |
| 36  | 1e    | 97  | GLY  |
| 46  | 2o    | 23  | GLY  |
| 33  | 1b    | 124 | SER  |
| 41  | 1j    | 31  | GLY  |
| 51  | 2t    | 102 | GLY  |
| 41  | 2j    | 37  | 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    | 214/217 (99%) | 193 (90%) | 21 (10%) | 10          | 28 |
| 3   | 2D    | 215/217 (99%) | 197 (92%) | 18 (8%)  | 14          | 37 |
| 4   | 1E    | 164/165 (99%) | 146 (89%) | 18 (11%) | 8           | 23 |
| 4   | 2E    | 164/165 (99%) | 148 (90%) | 16 (10%) | 10          | 28 |
| 5   | 1F    | 160/161 (99%) | 149 (93%) | 11 (7%)  | 19          | 48 |
| 5   | 2F    | 159/161 (99%) | 151 (95%) | 8 (5%)   | 30          | 64 |

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| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 6   | 1G    | 144/155 (93%)  | 134 (93%) | 10 (7%)  | 19          | 48 |
| 6   | 2G    | 142/155 (92%)  | 129 (91%) | 13 (9%)  | 11          | 32 |
| 7   | 1H    | 144/145 (99%)  | 133 (92%) | 11 (8%)  | 16          | 42 |
| 7   | 2H    | 143/145 (99%)  | 131 (92%) | 12 (8%)  | 14          | 37 |
| 8   | 1I    | 111/123 (90%)  | 101 (91%) | 10 (9%)  | 12          | 34 |
| 8   | 2I    | 108/123 (88%)  | 93 (86%)  | 15 (14%) | 4           | 13 |
| 9   | 1N    | 119/119 (100%) | 110 (92%) | 9 (8%)   | 16          | 42 |
| 9   | 2N    | 118/119 (99%)  | 104 (88%) | 14 (12%) | 6           | 19 |
| 10  | 1O    | 100/100 (100%) | 94 (94%)  | 6 (6%)   | 24          | 56 |
| 10  | 2O    | 100/100 (100%) | 97 (97%)  | 3 (3%)   | 48          | 82 |
| 11  | 1P    | 115/116 (99%)  | 107 (93%) | 8 (7%)   | 19          | 47 |
| 11  | 2P    | 115/116 (99%)  | 108 (94%) | 7 (6%)   | 23          | 55 |
| 12  | 1Q    | 111/111 (100%) | 102 (92%) | 9 (8%)   | 15          | 39 |
| 12  | 2Q    | 111/111 (100%) | 104 (94%) | 7 (6%)   | 22          | 53 |
| 13  | 1R    | 101/101 (100%) | 91 (90%)  | 10 (10%) | 10          | 28 |
| 13  | 2R    | 101/101 (100%) | 93 (92%)  | 8 (8%)   | 15          | 40 |
| 14  | 1S    | 87/87 (100%)   | 83 (95%)  | 4 (5%)   | 33          | 67 |
| 14  | 2S    | 85/87 (98%)    | 79 (93%)  | 6 (7%)   | 18          | 46 |
| 15  | 1T    | 115/115 (100%) | 110 (96%) | 5 (4%)   | 35          | 70 |
| 15  | 2T    | 113/115 (98%)  | 104 (92%) | 9 (8%)   | 15          | 40 |
| 16  | 1U    | 93/93 (100%)   | 86 (92%)  | 7 (8%)   | 17          | 43 |
| 16  | 2U    | 93/93 (100%)   | 89 (96%)  | 4 (4%)   | 35          | 70 |
| 17  | 1V    | 81/82 (99%)    | 70 (86%)  | 11 (14%) | 5           | 14 |
| 17  | 2V    | 80/82 (98%)    | 73 (91%)  | 7 (9%)   | 12          | 35 |
| 18  | 1W    | 90/91 (99%)    | 85 (94%)  | 5 (6%)   | 26          | 59 |
| 18  | 2W    | 90/91 (99%)    | 85 (94%)  | 5 (6%)   | 26          | 59 |
| 19  | 1X    | 77/77 (100%)   | 75 (97%)  | 2 (3%)   | 54          | 86 |
| 19  | 2X    | 77/77 (100%)   | 73 (95%)  | 4 (5%)   | 29          | 62 |
| 20  | 1Y    | 86/88 (98%)    | 81 (94%)  | 5 (6%)   | 25          | 57 |
| 20  | 2Y    | 86/88 (98%)    | 83 (96%)  | 3 (4%)   | 43          | 77 |
| 21  | 1Z    | 169/176 (96%)  | 149 (88%) | 20 (12%) | 6           | 19 |

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| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |     |
|-----|-------|----------------|-----------|----------|-------------|-----|
| 21  | 2Z    | 165/176 (94%)  | 152 (92%) | 13 (8%)  | 15          | 40  |
| 22  | 10    | 61/62 (98%)    | 56 (92%)  | 5 (8%)   | 14          | 38  |
| 22  | 20    | 61/62 (98%)    | 59 (97%)  | 2 (3%)   | 45          | 79  |
| 23  | 11    | 79/82 (96%)    | 74 (94%)  | 5 (6%)   | 22          | 53  |
| 23  | 21    | 81/82 (99%)    | 75 (93%)  | 6 (7%)   | 17          | 43  |
| 24  | 12    | 65/66 (98%)    | 61 (94%)  | 4 (6%)   | 23          | 54  |
| 24  | 22    | 66/66 (100%)   | 61 (92%)  | 5 (8%)   | 16          | 42  |
| 25  | 13    | 51/51 (100%)   | 48 (94%)  | 3 (6%)   | 24          | 57  |
| 25  | 23    | 50/51 (98%)    | 47 (94%)  | 3 (6%)   | 24          | 56  |
| 26  | 14    | 58/62 (94%)    | 52 (90%)  | 6 (10%)  | 9           | 26  |
| 26  | 24    | 54/62 (87%)    | 48 (89%)  | 6 (11%)  | 8           | 23  |
| 27  | 15    | 51/51 (100%)   | 48 (94%)  | 3 (6%)   | 24          | 57  |
| 27  | 25    | 50/51 (98%)    | 49 (98%)  | 1 (2%)   | 63          | 90  |
| 28  | 16    | 51/51 (100%)   | 50 (98%)  | 1 (2%)   | 63          | 90  |
| 28  | 26    | 50/51 (98%)    | 45 (90%)  | 5 (10%)  | 9           | 27  |
| 29  | 17    | 41/41 (100%)   | 39 (95%)  | 2 (5%)   | 31          | 65  |
| 29  | 27    | 41/41 (100%)   | 40 (98%)  | 1 (2%)   | 57          | 87  |
| 30  | 18    | 54/54 (100%)   | 49 (91%)  | 5 (9%)   | 11          | 32  |
| 30  | 28    | 54/54 (100%)   | 48 (89%)  | 6 (11%)  | 8           | 23  |
| 31  | 19    | 34/34 (100%)   | 33 (97%)  | 1 (3%)   | 50          | 83  |
| 31  | 29    | 34/34 (100%)   | 34 (100%) | 0        | 100         | 100 |
| 33  | 1b    | 191/199 (96%)  | 169 (88%) | 22 (12%) | 7           | 21  |
| 33  | 2b    | 187/199 (94%)  | 167 (89%) | 20 (11%) | 8           | 24  |
| 34  | 1c    | 144/160 (90%)  | 135 (94%) | 9 (6%)   | 22          | 53  |
| 34  | 2c    | 140/160 (88%)  | 131 (94%) | 9 (6%)   | 22          | 52  |
| 35  | 1d    | 171/180 (95%)  | 161 (94%) | 10 (6%)  | 25          | 57  |
| 35  | 2d    | 172/180 (96%)  | 159 (92%) | 13 (8%)  | 16          | 42  |
| 36  | 1e    | 114/114 (100%) | 106 (93%) | 8 (7%)   | 19          | 47  |
| 36  | 2e    | 114/114 (100%) | 105 (92%) | 9 (8%)   | 15          | 40  |
| 37  | 1f    | 85/90 (94%)    | 82 (96%)  | 3 (4%)   | 43          | 77  |
| 37  | 2f    | 85/90 (94%)    | 75 (88%)  | 10 (12%) | 6           | 19  |

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| Mol | Chain | Analysed      | Rotameric | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|-------------|-----|
| 38  | 1g    | 120/126 (95%) | 108 (90%) | 12 (10%) | 9           | 27  |
| 38  | 2g    | 119/126 (94%) | 111 (93%) | 8 (7%)   | 20          | 50  |
| 39  | 1h    | 116/118 (98%) | 112 (97%) | 4 (3%)   | 44          | 78  |
| 39  | 2h    | 114/118 (97%) | 108 (95%) | 6 (5%)   | 28          | 61  |
| 40  | 1i    | 91/98 (93%)   | 80 (88%)  | 11 (12%) | 6           | 18  |
| 40  | 2i    | 88/98 (90%)   | 75 (85%)  | 13 (15%) | 4           | 11  |
| 41  | 1j    | 68/87 (78%)   | 61 (90%)  | 7 (10%)  | 9           | 26  |
| 41  | 2j    | 68/87 (78%)   | 62 (91%)  | 6 (9%)   | 12          | 35  |
| 42  | 1k    | 83/86 (96%)   | 78 (94%)  | 5 (6%)   | 24          | 56  |
| 42  | 2k    | 83/86 (96%)   | 78 (94%)  | 5 (6%)   | 24          | 56  |
| 43  | 1l    | 96/102 (94%)  | 92 (96%)  | 4 (4%)   | 36          | 71  |
| 43  | 2l    | 96/102 (94%)  | 90 (94%)  | 6 (6%)   | 22          | 53  |
| 44  | 1m    | 90/94 (96%)   | 84 (93%)  | 6 (7%)   | 20          | 50  |
| 44  | 2m    | 87/94 (93%)   | 80 (92%)  | 7 (8%)   | 15          | 40  |
| 45  | 1n    | 49/49 (100%)  | 43 (88%)  | 6 (12%)  | 6           | 18  |
| 45  | 2n    | 49/49 (100%)  | 46 (94%)  | 3 (6%)   | 23          | 55  |
| 46  | 1o    | 78/79 (99%)   | 74 (95%)  | 4 (5%)   | 29          | 63  |
| 46  | 2o    | 78/79 (99%)   | 72 (92%)  | 6 (8%)   | 16          | 41  |
| 47  | 1p    | 69/71 (97%)   | 58 (84%)  | 11 (16%) | 3           | 9   |
| 47  | 2p    | 68/71 (96%)   | 56 (82%)  | 12 (18%) | 2           | 7   |
| 48  | 1q    | 94/94 (100%)  | 92 (98%)  | 2 (2%)   | 61          | 90  |
| 48  | 2q    | 94/94 (100%)  | 91 (97%)  | 3 (3%)   | 46          | 80  |
| 49  | 1r    | 59/59 (100%)  | 57 (97%)  | 2 (3%)   | 44          | 78  |
| 49  | 2r    | 59/59 (100%)  | 56 (95%)  | 3 (5%)   | 29          | 63  |
| 50  | 1s    | 68/72 (94%)   | 61 (90%)  | 7 (10%)  | 9           | 26  |
| 50  | 2s    | 67/72 (93%)   | 63 (94%)  | 4 (6%)   | 24          | 56  |
| 51  | 1t    | 71/76 (93%)   | 64 (90%)  | 7 (10%)  | 10          | 28  |
| 51  | 2t    | 70/76 (92%)   | 65 (93%)  | 5 (7%)   | 18          | 46  |
| 52  | 1u    | 18/18 (100%)  | 17 (94%)  | 1 (6%)   | 26          | 59  |
| 52  | 2u    | 18/18 (100%)  | 18 (100%) | 0        | 100         | 100 |
| 55  | 1y    | 16/16 (100%)  | 13 (81%)  | 3 (19%)  | 2           | 6   |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 55  | 2y    | 16/16 (100%)    | 14 (88%)   | 2 (12%)  | 6           | 17 |
| All | All   | 9395/9728 (97%) | 8677 (92%) | 718 (8%) | 16          | 42 |

All (718) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | 1D    | 3   | VAL  |
| 3   | 1D    | 13  | ARG  |
| 3   | 1D    | 37  | LEU  |
| 3   | 1D    | 61  | LEU  |
| 3   | 1D    | 88  | ARG  |
| 3   | 1D    | 94  | LEU  |
| 3   | 1D    | 103 | ARG  |
| 3   | 1D    | 111 | LEU  |
| 3   | 1D    | 113 | VAL  |
| 3   | 1D    | 138 | VAL  |
| 3   | 1D    | 155 | LEU  |
| 3   | 1D    | 162 | SER  |
| 3   | 1D    | 173 | VAL  |
| 3   | 1D    | 193 | VAL  |
| 3   | 1D    | 200 | ASP  |
| 3   | 1D    | 211 | ARG  |
| 3   | 1D    | 217 | ARG  |
| 3   | 1D    | 221 | VAL  |
| 3   | 1D    | 229 | VAL  |
| 3   | 1D    | 242 | ARG  |
| 3   | 1D    | 253 | GLN  |
| 4   | 1E    | 21  | VAL  |
| 4   | 1E    | 33  | VAL  |
| 4   | 1E    | 45  | THR  |
| 4   | 1E    | 47  | VAL  |
| 4   | 1E    | 49  | LEU  |
| 4   | 1E    | 75  | VAL  |
| 4   | 1E    | 77  | ILE  |
| 4   | 1E    | 78  | LEU  |
| 4   | 1E    | 89  | ASP  |
| 4   | 1E    | 101 | ARG  |
| 4   | 1E    | 116 | VAL  |
| 4   | 1E    | 119 | ARG  |
| 4   | 1E    | 127 | ASP  |
| 4   | 1E    | 144 | ARG  |
| 4   | 1E    | 154 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | 1E    | 175 | VAL  |
| 4   | 1E    | 178 | GLU  |
| 4   | 1E    | 181 | LEU  |
| 5   | 1F    | 18  | ARG  |
| 5   | 1F    | 33  | LEU  |
| 5   | 1F    | 53  | THR  |
| 5   | 1F    | 60  | SER  |
| 5   | 1F    | 74  | ARG  |
| 5   | 1F    | 88  | VAL  |
| 5   | 1F    | 110 | LEU  |
| 5   | 1F    | 170 | LEU  |
| 5   | 1F    | 175 | THR  |
| 5   | 1F    | 191 | ARG  |
| 5   | 1F    | 192 | LEU  |
| 6   | 1G    | 28  | VAL  |
| 6   | 1G    | 43  | LEU  |
| 6   | 1G    | 45  | GLU  |
| 6   | 1G    | 53  | LEU  |
| 6   | 1G    | 79  | ASN  |
| 6   | 1G    | 82  | LEU  |
| 6   | 1G    | 136 | ARG  |
| 6   | 1G    | 153 | ARG  |
| 6   | 1G    | 167 | GLU  |
| 6   | 1G    | 175 | LEU  |
| 7   | 1H    | 2   | SER  |
| 7   | 1H    | 13  | LYS  |
| 7   | 1H    | 23  | ARG  |
| 7   | 1H    | 32  | GLU  |
| 7   | 1H    | 45  | VAL  |
| 7   | 1H    | 47  | GLU  |
| 7   | 1H    | 98  | LEU  |
| 7   | 1H    | 104 | GLU  |
| 7   | 1H    | 105 | LEU  |
| 7   | 1H    | 107 | VAL  |
| 7   | 1H    | 172 | LYS  |
| 8   | 1I    | 9   | LEU  |
| 8   | 1I    | 12  | LEU  |
| 8   | 1I    | 38  | LEU  |
| 8   | 1I    | 44  | LEU  |
| 8   | 1I    | 75  | LEU  |
| 8   | 1I    | 101 | LEU  |
| 8   | 1I    | 103 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8   | 1I    | 109 | ILE  |
| 8   | 1I    | 140 | LEU  |
| 8   | 1I    | 144 | VAL  |
| 9   | 1N    | 5   | VAL  |
| 9   | 1N    | 8   | GLN  |
| 9   | 1N    | 33  | LEU  |
| 9   | 1N    | 34  | LEU  |
| 9   | 1N    | 48  | MET  |
| 9   | 1N    | 83  | LYS  |
| 9   | 1N    | 99  | LEU  |
| 9   | 1N    | 133 | GLN  |
| 9   | 1N    | 140 | VAL  |
| 10  | 1O    | 8   | LEU  |
| 10  | 1O    | 24  | VAL  |
| 10  | 1O    | 26  | LYS  |
| 10  | 1O    | 69  | ILE  |
| 10  | 1O    | 80  | ASP  |
| 10  | 1O    | 94  | ARG  |
| 11  | 1P    | 2   | LYS  |
| 11  | 1P    | 59  | LEU  |
| 11  | 1P    | 76  | LYS  |
| 11  | 1P    | 83  | VAL  |
| 11  | 1P    | 125 | VAL  |
| 11  | 1P    | 147 | LEU  |
| 11  | 1P    | 148 | LEU  |
| 11  | 1P    | 149 | GLU  |
| 12  | 1Q    | 2   | LEU  |
| 12  | 1Q    | 7   | MET  |
| 12  | 1Q    | 22  | LYS  |
| 12  | 1Q    | 35  | VAL  |
| 12  | 1Q    | 60  | ARG  |
| 12  | 1Q    | 75  | THR  |
| 12  | 1Q    | 98  | LYS  |
| 12  | 1Q    | 109 | VAL  |
| 12  | 1Q    | 110 | THR  |
| 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    | 75  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 13  | 1R    | 96  | ARG  |
| 13  | 1R    | 100 | LEU  |
| 13  | 1R    | 111 | LEU  |
| 14  | 1S    | 14  | VAL  |
| 14  | 1S    | 17  | ARG  |
| 14  | 1S    | 59  | LYS  |
| 14  | 1S    | 75  | GLU  |
| 15  | 1T    | 6   | LEU  |
| 15  | 1T    | 28  | VAL  |
| 15  | 1T    | 74  | ARG  |
| 15  | 1T    | 78  | LEU  |
| 15  | 1T    | 89  | VAL  |
| 16  | 1U    | 5   | LYS  |
| 16  | 1U    | 8   | VAL  |
| 16  | 1U    | 52  | ARG  |
| 16  | 1U    | 74  | LEU  |
| 16  | 1U    | 84  | LYS  |
| 16  | 1U    | 104 | GLN  |
| 16  | 1U    | 117 | GLN  |
| 17  | 1V    | 1   | MET  |
| 17  | 1V    | 7   | THR  |
| 17  | 1V    | 21  | ARG  |
| 17  | 1V    | 44  | LYS  |
| 17  | 1V    | 46  | VAL  |
| 17  | 1V    | 52  | VAL  |
| 17  | 1V    | 61  | VAL  |
| 17  | 1V    | 79  | VAL  |
| 17  | 1V    | 82  | ARG  |
| 17  | 1V    | 91  | TYR  |
| 17  | 1V    | 95  | LEU  |
| 18  | 1W    | 17  | VAL  |
| 18  | 1W    | 19  | LEU  |
| 18  | 1W    | 67  | ASP  |
| 18  | 1W    | 100 | THR  |
| 18  | 1W    | 107 | LEU  |
| 19  | 1X    | 66  | LEU  |
| 19  | 1X    | 68  | ARG  |
| 20  | 1Y    | 23  | ARG  |
| 20  | 1Y    | 43  | ASN  |
| 20  | 1Y    | 47  | LYS  |
| 20  | 1Y    | 72  | VAL  |
| 20  | 1Y    | 107 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 21  | 1Z    | 11  | GLU  |
| 21  | 1Z    | 18  | LEU  |
| 21  | 1Z    | 20  | ARG  |
| 21  | 1Z    | 28  | MET  |
| 21  | 1Z    | 33  | LEU  |
| 21  | 1Z    | 42  | VAL  |
| 21  | 1Z    | 61  | LEU  |
| 21  | 1Z    | 72  | ARG  |
| 21  | 1Z    | 76  | LEU  |
| 21  | 1Z    | 86  | VAL  |
| 21  | 1Z    | 91  | LEU  |
| 21  | 1Z    | 103 | ARG  |
| 21  | 1Z    | 126 | VAL  |
| 21  | 1Z    | 150 | LEU  |
| 21  | 1Z    | 155 | LEU  |
| 21  | 1Z    | 162 | GLU  |
| 21  | 1Z    | 185 | GLU  |
| 21  | 1Z    | 193 | GLU  |
| 21  | 1Z    | 202 | GLU  |
| 21  | 1Z    | 203 | GLU  |
| 22  | 10    | 11  | ARG  |
| 22  | 10    | 14  | ARG  |
| 22  | 10    | 39  | ARG  |
| 22  | 10    | 43  | THR  |
| 22  | 10    | 59  | LEU  |
| 23  | 11    | 21  | ARG  |
| 23  | 11    | 30  | VAL  |
| 23  | 11    | 76  | ARG  |
| 23  | 11    | 81  | LYS  |
| 23  | 11    | 83  | GLU  |
| 24  | 12    | 3   | LEU  |
| 24  | 12    | 32  | LEU  |
| 24  | 12    | 53  | LEU  |
| 24  | 12    | 70  | GLN  |
| 25  | 13    | 8   | LEU  |
| 25  | 13    | 23  | LEU  |
| 25  | 13    | 54  | VAL  |
| 26  | 14    | 13  | ARG  |
| 26  | 14    | 27  | THR  |
| 26  | 14    | 49  | PHE  |
| 26  | 14    | 50  | VAL  |
| 26  | 14    | 59  | PHE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 26  | 14    | 60  | GLN  |
| 27  | 15    | 6   | VAL  |
| 27  | 15    | 16  | ARG  |
| 27  | 15    | 58  | LEU  |
| 28  | 16    | 48  | VAL  |
| 29  | 17    | 24  | THR  |
| 29  | 17    | 43  | THR  |
| 30  | 18    | 14  | VAL  |
| 30  | 18    | 30  | ARG  |
| 30  | 18    | 31  | HIS  |
| 30  | 18    | 32  | LEU  |
| 30  | 18    | 34  | TRP  |
| 31  | 19    | 35  | ARG  |
| 33  | 1b    | 9   | GLU  |
| 33  | 1b    | 15  | VAL  |
| 33  | 1b    | 17  | PHE  |
| 33  | 1b    | 19  | HIS  |
| 33  | 1b    | 24  | TRP  |
| 33  | 1b    | 35  | GLU  |
| 33  | 1b    | 45  | GLN  |
| 33  | 1b    | 63  | MET  |
| 33  | 1b    | 73  | THR  |
| 33  | 1b    | 75  | LYS  |
| 33  | 1b    | 76  | GLN  |
| 33  | 1b    | 82  | ARG  |
| 33  | 1b    | 111 | ARG  |
| 33  | 1b    | 126 | GLU  |
| 33  | 1b    | 144 | ARG  |
| 33  | 1b    | 158 | LEU  |
| 33  | 1b    | 160 | ASP  |
| 33  | 1b    | 172 | ILE  |
| 33  | 1b    | 178 | ARG  |
| 33  | 1b    | 221 | LEU  |
| 33  | 1b    | 226 | ARG  |
| 33  | 1b    | 231 | GLU  |
| 34  | 1c    | 3   | ASN  |
| 34  | 1c    | 54  | ARG  |
| 34  | 1c    | 64  | VAL  |
| 34  | 1c    | 70  | VAL  |
| 34  | 1c    | 89  | GLU  |
| 34  | 1c    | 104 | GLN  |
| 34  | 1c    | 105 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 34  | 1c    | 161 | GLU  |
| 34  | 1c    | 192 | THR  |
| 35  | 1d    | 31  | CYS  |
| 35  | 1d    | 85  | LYS  |
| 35  | 1d    | 86  | LYS  |
| 35  | 1d    | 107 | ARG  |
| 35  | 1d    | 108 | LEU  |
| 35  | 1d    | 122 | ARG  |
| 35  | 1d    | 127 | THR  |
| 35  | 1d    | 135 | LEU  |
| 35  | 1d    | 158 | ILE  |
| 35  | 1d    | 173 | TRP  |
| 36  | 1e    | 10  | MET  |
| 36  | 1e    | 20  | GLN  |
| 36  | 1e    | 34  | VAL  |
| 36  | 1e    | 41  | VAL  |
| 36  | 1e    | 68  | GLU  |
| 36  | 1e    | 69  | VAL  |
| 36  | 1e    | 78  | HIS  |
| 36  | 1e    | 150 | ARG  |
| 37  | 1f    | 46  | ARG  |
| 37  | 1f    | 63  | TYR  |
| 37  | 1f    | 70  | ASP  |
| 38  | 1g    | 6   | ARG  |
| 38  | 1g    | 8   | GLU  |
| 38  | 1g    | 10  | ARG  |
| 38  | 1g    | 13  | GLN  |
| 38  | 1g    | 15  | ASP  |
| 38  | 1g    | 56  | GLN  |
| 38  | 1g    | 75  | VAL  |
| 38  | 1g    | 104 | LEU  |
| 38  | 1g    | 113 | GLU  |
| 38  | 1g    | 136 | LYS  |
| 38  | 1g    | 143 | ARG  |
| 38  | 1g    | 155 | ARG  |
| 39  | 1h    | 26  | VAL  |
| 39  | 1h    | 51  | VAL  |
| 39  | 1h    | 52  | ASP  |
| 39  | 1h    | 63  | LEU  |
| 40  | 1i    | 14  | VAL  |
| 40  | 1i    | 25  | LYS  |
| 40  | 1i    | 51  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 40  | 1i    | 56  | LEU  |
| 40  | 1i    | 65  | VAL  |
| 40  | 1i    | 66  | ARG  |
| 40  | 1i    | 81  | ILE  |
| 40  | 1i    | 86  | VAL  |
| 40  | 1i    | 87  | GLN  |
| 40  | 1i    | 103 | THR  |
| 40  | 1i    | 125 | TYR  |
| 41  | 1j    | 34  | VAL  |
| 41  | 1j    | 49  | VAL  |
| 41  | 1j    | 55  | LYS  |
| 41  | 1j    | 72  | VAL  |
| 41  | 1j    | 92  | THR  |
| 41  | 1j    | 94  | VAL  |
| 41  | 1j    | 100 | THR  |
| 42  | 1k    | 14  | VAL  |
| 42  | 1k    | 84  | VAL  |
| 42  | 1k    | 109 | VAL  |
| 42  | 1k    | 114 | VAL  |
| 42  | 1k    | 124 | LYS  |
| 43  | 1l    | 27  | LEU  |
| 43  | 1l    | 33  | ARG  |
| 43  | 1l    | 47  | LYS  |
| 43  | 1l    | 67  | THR  |
| 44  | 1m    | 8   | GLU  |
| 44  | 1m    | 11  | ARG  |
| 44  | 1m    | 17  | VAL  |
| 44  | 1m    | 56  | LEU  |
| 44  | 1m    | 63  | THR  |
| 44  | 1m    | 102 | ARG  |
| 45  | 1n    | 3   | ARG  |
| 45  | 1n    | 15  | LYS  |
| 45  | 1n    | 18  | VAL  |
| 45  | 1n    | 22  | THR  |
| 45  | 1n    | 33  | VAL  |
| 45  | 1n    | 44  | LEU  |
| 46  | 1o    | 3   | ILE  |
| 46  | 1o    | 26  | GLU  |
| 46  | 1o    | 39  | LEU  |
| 46  | 1o    | 68  | ARG  |
| 47  | 1p    | 2   | VAL  |
| 47  | 1p    | 8   | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 47  | 1p    | 20  | VAL  |
| 47  | 1p    | 42  | ARG  |
| 47  | 1p    | 45  | THR  |
| 47  | 1p    | 60  | LEU  |
| 47  | 1p    | 62  | VAL  |
| 47  | 1p    | 67  | THR  |
| 47  | 1p    | 69  | THR  |
| 47  | 1p    | 74  | LEU  |
| 47  | 1p    | 79  | VAL  |
| 48  | 1q    | 16  | GLN  |
| 48  | 1q    | 87  | LYS  |
| 49  | 1r    | 65  | ILE  |
| 49  | 1r    | 76  | LEU  |
| 50  | 1s    | 3   | ARG  |
| 50  | 1s    | 4   | SER  |
| 50  | 1s    | 5   | LEU  |
| 50  | 1s    | 28  | LYS  |
| 50  | 1s    | 37  | ARG  |
| 50  | 1s    | 41  | VAL  |
| 50  | 1s    | 65  | ASN  |
| 51  | 1t    | 10  | LEU  |
| 51  | 1t    | 45  | GLN  |
| 51  | 1t    | 48  | LYS  |
| 51  | 1t    | 58  | LYS  |
| 51  | 1t    | 62  | LEU  |
| 51  | 1t    | 80  | ARG  |
| 51  | 1t    | 100 | ILE  |
| 52  | 1u    | 9   | ARG  |
| 55  | 1y    | 2   | ARG  |
| 55  | 1y    | 4   | ARG  |
| 55  | 1y    | 12  | ARG  |
| 3   | 2D    | 3   | VAL  |
| 3   | 2D    | 37  | LEU  |
| 3   | 2D    | 61  | LEU  |
| 3   | 2D    | 94  | LEU  |
| 3   | 2D    | 103 | ARG  |
| 3   | 2D    | 109 | ASP  |
| 3   | 2D    | 111 | LEU  |
| 3   | 2D    | 113 | VAL  |
| 3   | 2D    | 155 | LEU  |
| 3   | 2D    | 193 | VAL  |
| 3   | 2D    | 211 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | 2D    | 217 | ARG  |
| 3   | 2D    | 221 | VAL  |
| 3   | 2D    | 229 | VAL  |
| 3   | 2D    | 242 | ARG  |
| 3   | 2D    | 253 | GLN  |
| 3   | 2D    | 274 | ARG  |
| 3   | 2D    | 276 | LYS  |
| 4   | 2E    | 19  | ARG  |
| 4   | 2E    | 21  | VAL  |
| 4   | 2E    | 24  | THR  |
| 4   | 2E    | 33  | VAL  |
| 4   | 2E    | 73  | GLU  |
| 4   | 2E    | 75  | VAL  |
| 4   | 2E    | 78  | LEU  |
| 4   | 2E    | 97  | LYS  |
| 4   | 2E    | 101 | ARG  |
| 4   | 2E    | 116 | VAL  |
| 4   | 2E    | 144 | ARG  |
| 4   | 2E    | 154 | LYS  |
| 4   | 2E    | 167 | VAL  |
| 4   | 2E    | 170 | LEU  |
| 4   | 2E    | 181 | LEU  |
| 4   | 2E    | 195 | LEU  |
| 5   | 2F    | 33  | LEU  |
| 5   | 2F    | 57  | VAL  |
| 5   | 2F    | 74  | ARG  |
| 5   | 2F    | 112 | MET  |
| 5   | 2F    | 158 | THR  |
| 5   | 2F    | 175 | THR  |
| 5   | 2F    | 192 | LEU  |
| 5   | 2F    | 201 | VAL  |
| 6   | 2G    | 3   | LEU  |
| 6   | 2G    | 28  | VAL  |
| 6   | 2G    | 43  | LEU  |
| 6   | 2G    | 47  | LYS  |
| 6   | 2G    | 49  | ASP  |
| 6   | 2G    | 55  | LYS  |
| 6   | 2G    | 111 | LEU  |
| 6   | 2G    | 116 | ASP  |
| 6   | 2G    | 133 | LEU  |
| 6   | 2G    | 139 | LEU  |
| 6   | 2G    | 155 | MET  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | 2G    | 168 | GLU  |
| 6   | 2G    | 175 | LEU  |
| 7   | 2H    | 6   | ARG  |
| 7   | 2H    | 13  | LYS  |
| 7   | 2H    | 15  | VAL  |
| 7   | 2H    | 34  | GLU  |
| 7   | 2H    | 49  | VAL  |
| 7   | 2H    | 63  | SER  |
| 7   | 2H    | 68  | THR  |
| 7   | 2H    | 84  | SER  |
| 7   | 2H    | 95  | ARG  |
| 7   | 2H    | 105 | LEU  |
| 7   | 2H    | 122 | THR  |
| 7   | 2H    | 139 | GLN  |
| 8   | 2I    | 15  | VAL  |
| 8   | 2I    | 38  | LEU  |
| 8   | 2I    | 43  | ASN  |
| 8   | 2I    | 44  | LEU  |
| 8   | 2I    | 48  | GLU  |
| 8   | 2I    | 50  | ARG  |
| 8   | 2I    | 66  | GLU  |
| 8   | 2I    | 75  | LEU  |
| 8   | 2I    | 85  | GLU  |
| 8   | 2I    | 92  | VAL  |
| 8   | 2I    | 101 | LEU  |
| 8   | 2I    | 116 | LEU  |
| 8   | 2I    | 129 | THR  |
| 8   | 2I    | 140 | LEU  |
| 8   | 2I    | 144 | VAL  |
| 9   | 2N    | 5   | VAL  |
| 9   | 2N    | 28  | THR  |
| 9   | 2N    | 34  | LEU  |
| 9   | 2N    | 58  | ASP  |
| 9   | 2N    | 62  | VAL  |
| 9   | 2N    | 67  | LEU  |
| 9   | 2N    | 74  | ARG  |
| 9   | 2N    | 87  | LEU  |
| 9   | 2N    | 97  | ARG  |
| 9   | 2N    | 99  | LEU  |
| 9   | 2N    | 119 | ARG  |
| 9   | 2N    | 131 | GLN  |
| 9   | 2N    | 133 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9   | 2N    | 140 | VAL  |
| 10  | 2O    | 10  | VAL  |
| 10  | 2O    | 53  | LYS  |
| 10  | 2O    | 108 | GLU  |
| 11  | 2P    | 2   | LYS  |
| 11  | 2P    | 3   | LEU  |
| 11  | 2P    | 59  | LEU  |
| 11  | 2P    | 76  | LYS  |
| 11  | 2P    | 112 | LEU  |
| 11  | 2P    | 125 | VAL  |
| 11  | 2P    | 148 | LEU  |
| 12  | 2Q    | 2   | LEU  |
| 12  | 2Q    | 7   | MET  |
| 12  | 2Q    | 16  | ARG  |
| 12  | 2Q    | 98  | LYS  |
| 12  | 2Q    | 106 | VAL  |
| 12  | 2Q    | 109 | VAL  |
| 12  | 2Q    | 112 | GLU  |
| 13  | 2R    | 18  | LEU  |
| 13  | 2R    | 36  | THR  |
| 13  | 2R    | 44  | LEU  |
| 13  | 2R    | 65  | LEU  |
| 13  | 2R    | 75  | LEU  |
| 13  | 2R    | 79  | LEU  |
| 13  | 2R    | 96  | ARG  |
| 13  | 2R    | 100 | LEU  |
| 14  | 2S    | 5   | THR  |
| 14  | 2S    | 14  | VAL  |
| 14  | 2S    | 17  | ARG  |
| 14  | 2S    | 23  | ARG  |
| 14  | 2S    | 50  | SER  |
| 14  | 2S    | 75  | GLU  |
| 15  | 2T    | 13  | ARG  |
| 15  | 2T    | 16  | ARG  |
| 15  | 2T    | 23  | ARG  |
| 15  | 2T    | 28  | VAL  |
| 15  | 2T    | 49  | VAL  |
| 15  | 2T    | 74  | ARG  |
| 15  | 2T    | 89  | VAL  |
| 15  | 2T    | 96  | ARG  |
| 15  | 2T    | 108 | ARG  |
| 16  | 2U    | 31  | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 16  | 2U    | 60  | LEU  |
| 16  | 2U    | 74  | LEU  |
| 16  | 2U    | 112 | ARG  |
| 17  | 2V    | 18  | LEU  |
| 17  | 2V    | 35  | LEU  |
| 17  | 2V    | 46  | VAL  |
| 17  | 2V    | 53  | GLU  |
| 17  | 2V    | 62  | LEU  |
| 17  | 2V    | 79  | VAL  |
| 17  | 2V    | 100 | ARG  |
| 18  | 2W    | 15  | ARG  |
| 18  | 2W    | 17  | VAL  |
| 18  | 2W    | 23  | LEU  |
| 18  | 2W    | 71  | VAL  |
| 18  | 2W    | 107 | LEU  |
| 19  | 2X    | 57  | LEU  |
| 19  | 2X    | 66  | LEU  |
| 19  | 2X    | 81  | VAL  |
| 19  | 2X    | 83  | VAL  |
| 20  | 2Y    | 21  | LYS  |
| 20  | 2Y    | 72  | VAL  |
| 20  | 2Y    | 107 | ASP  |
| 21  | 2Z    | 31  | ARG  |
| 21  | 2Z    | 33  | LEU  |
| 21  | 2Z    | 42  | VAL  |
| 21  | 2Z    | 72  | ARG  |
| 21  | 2Z    | 121 | HIS  |
| 21  | 2Z    | 123 | ASP  |
| 21  | 2Z    | 126 | VAL  |
| 21  | 2Z    | 136 | PHE  |
| 21  | 2Z    | 150 | LEU  |
| 21  | 2Z    | 155 | LEU  |
| 21  | 2Z    | 170 | THR  |
| 21  | 2Z    | 182 | LYS  |
| 21  | 2Z    | 185 | GLU  |
| 22  | 20    | 14  | ARG  |
| 22  | 20    | 39  | ARG  |
| 23  | 21    | 2   | SER  |
| 23  | 21    | 23  | LYS  |
| 23  | 21    | 30  | VAL  |
| 23  | 21    | 35  | THR  |
| 23  | 21    | 81  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 23  | 21    | 85  | LEU  |
| 24  | 22    | 3   | LEU  |
| 24  | 22    | 26  | ARG  |
| 24  | 22    | 32  | LEU  |
| 24  | 22    | 40  | SER  |
| 24  | 22    | 53  | LEU  |
| 25  | 23    | 31  | LEU  |
| 25  | 23    | 54  | VAL  |
| 25  | 23    | 56  | VAL  |
| 26  | 24    | 8   | LYS  |
| 26  | 24    | 27  | THR  |
| 26  | 24    | 38  | LYS  |
| 26  | 24    | 56  | VAL  |
| 26  | 24    | 61  | ARG  |
| 26  | 24    | 63  | TYR  |
| 27  | 25    | 58  | LEU  |
| 28  | 26    | 6   | ARG  |
| 28  | 26    | 14  | THR  |
| 28  | 26    | 19  | ARG  |
| 28  | 26    | 48  | VAL  |
| 28  | 26    | 52  | VAL  |
| 29  | 27    | 43  | THR  |
| 30  | 28    | 23  | VAL  |
| 30  | 28    | 26  | LYS  |
| 30  | 28    | 31  | HIS  |
| 30  | 28    | 34  | TRP  |
| 30  | 28    | 46  | ARG  |
| 30  | 28    | 56  | GLU  |
| 33  | 2b    | 8   | LYS  |
| 33  | 2b    | 16  | HIS  |
| 33  | 2b    | 24  | TRP  |
| 33  | 2b    | 44  | LEU  |
| 33  | 2b    | 55  | PHE  |
| 33  | 2b    | 58  | ILE  |
| 33  | 2b    | 67  | THR  |
| 33  | 2b    | 71  | VAL  |
| 33  | 2b    | 87  | ARG  |
| 33  | 2b    | 93  | VAL  |
| 33  | 2b    | 128 | GLU  |
| 33  | 2b    | 135 | GLN  |
| 33  | 2b    | 136 | VAL  |
| 33  | 2b    | 157 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 33  | 2b    | 158 | LEU  |
| 33  | 2b    | 187 | LEU  |
| 33  | 2b    | 191 | ASP  |
| 33  | 2b    | 200 | ILE  |
| 33  | 2b    | 226 | ARG  |
| 33  | 2b    | 230 | VAL  |
| 34  | 2c    | 30  | ARG  |
| 34  | 2c    | 32  | LEU  |
| 34  | 2c    | 45  | LYS  |
| 34  | 2c    | 52  | LEU  |
| 34  | 2c    | 70  | VAL  |
| 34  | 2c    | 102 | ASN  |
| 34  | 2c    | 152 | ILE  |
| 34  | 2c    | 166 | GLU  |
| 34  | 2c    | 192 | THR  |
| 35  | 2d    | 5   | ILE  |
| 35  | 2d    | 8   | VAL  |
| 35  | 2d    | 13  | ARG  |
| 35  | 2d    | 49  | ARG  |
| 35  | 2d    | 65  | ARG  |
| 35  | 2d    | 96  | LEU  |
| 35  | 2d    | 106 | TYR  |
| 35  | 2d    | 108 | LEU  |
| 35  | 2d    | 127 | THR  |
| 35  | 2d    | 135 | LEU  |
| 35  | 2d    | 158 | ILE  |
| 35  | 2d    | 194 | LEU  |
| 35  | 2d    | 201 | GLN  |
| 36  | 2e    | 24  | ARG  |
| 36  | 2e    | 31  | LEU  |
| 36  | 2e    | 34  | VAL  |
| 36  | 2e    | 41  | VAL  |
| 36  | 2e    | 68  | GLU  |
| 36  | 2e    | 69  | VAL  |
| 36  | 2e    | 72  | GLN  |
| 36  | 2e    | 75  | THR  |
| 36  | 2e    | 91  | LEU  |
| 37  | 2f    | 17  | SER  |
| 37  | 2f    | 22  | GLU  |
| 37  | 2f    | 28  | ARG  |
| 37  | 2f    | 40  | VAL  |
| 37  | 2f    | 46  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 37  | 2f    | 63  | TYR  |
| 37  | 2f    | 75  | LEU  |
| 37  | 2f    | 81  | ILE  |
| 37  | 2f    | 92  | LYS  |
| 37  | 2f    | 95  | GLU  |
| 38  | 2g    | 6   | ARG  |
| 38  | 2g    | 13  | GLN  |
| 38  | 2g    | 75  | VAL  |
| 38  | 2g    | 104 | LEU  |
| 38  | 2g    | 113 | GLU  |
| 38  | 2g    | 115 | ARG  |
| 38  | 2g    | 138 | LYS  |
| 38  | 2g    | 155 | ARG  |
| 39  | 2h    | 51  | VAL  |
| 39  | 2h    | 54  | ASP  |
| 39  | 2h    | 63  | LEU  |
| 39  | 2h    | 91  | ARG  |
| 39  | 2h    | 97  | VAL  |
| 39  | 2h    | 125 | ARG  |
| 40  | 2i    | 7   | THR  |
| 40  | 2i    | 25  | LYS  |
| 40  | 2i    | 27  | THR  |
| 40  | 2i    | 42  | ARG  |
| 40  | 2i    | 50  | LEU  |
| 40  | 2i    | 53  | VAL  |
| 40  | 2i    | 64  | THR  |
| 40  | 2i    | 65  | VAL  |
| 40  | 2i    | 87  | GLN  |
| 40  | 2i    | 88  | TYR  |
| 40  | 2i    | 102 | LEU  |
| 40  | 2i    | 103 | THR  |
| 40  | 2i    | 125 | TYR  |
| 41  | 2j    | 29  | ARG  |
| 41  | 2j    | 34  | VAL  |
| 41  | 2j    | 49  | VAL  |
| 41  | 2j    | 57  | LYS  |
| 41  | 2j    | 74  | ILE  |
| 41  | 2j    | 92  | THR  |
| 42  | 2k    | 14  | VAL  |
| 42  | 2k    | 31  | THR  |
| 42  | 2k    | 81  | ASP  |
| 42  | 2k    | 109 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 42  | 2k    | 114 | VAL  |
| 43  | 2l    | 27  | LEU  |
| 43  | 2l    | 28  | LYS  |
| 43  | 2l    | 33  | ARG  |
| 43  | 2l    | 52  | LEU  |
| 43  | 2l    | 67  | THR  |
| 43  | 2l    | 117 | ARG  |
| 44  | 2m    | 4   | ILE  |
| 44  | 2m    | 8   | GLU  |
| 44  | 2m    | 17  | VAL  |
| 44  | 2m    | 27  | LYS  |
| 44  | 2m    | 65  | LYS  |
| 44  | 2m    | 88  | ARG  |
| 44  | 2m    | 103 | THR  |
| 45  | 2n    | 18  | VAL  |
| 45  | 2n    | 22  | THR  |
| 45  | 2n    | 44  | LEU  |
| 46  | 2o    | 5   | LYS  |
| 46  | 2o    | 38  | ARG  |
| 46  | 2o    | 39  | LEU  |
| 46  | 2o    | 76  | GLU  |
| 46  | 2o    | 83  | GLU  |
| 46  | 2o    | 88  | ARG  |
| 47  | 2p    | 2   | VAL  |
| 47  | 2p    | 20  | VAL  |
| 47  | 2p    | 21  | VAL  |
| 47  | 2p    | 28  | ARG  |
| 47  | 2p    | 42  | ARG  |
| 47  | 2p    | 44  | THR  |
| 47  | 2p    | 45  | THR  |
| 47  | 2p    | 54  | GLU  |
| 47  | 2p    | 62  | VAL  |
| 47  | 2p    | 67  | THR  |
| 47  | 2p    | 69  | THR  |
| 47  | 2p    | 72  | ARG  |
| 48  | 2q    | 6   | LEU  |
| 48  | 2q    | 57  | VAL  |
| 48  | 2q    | 74  | LEU  |
| 49  | 2r    | 31  | LEU  |
| 49  | 2r    | 65  | ILE  |
| 49  | 2r    | 76  | LEU  |
| 50  | 2s    | 5   | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 50  | 2s    | 41  | VAL  |
| 50  | 2s    | 64  | GLU  |
| 50  | 2s    | 77  | THR  |
| 51  | 2t    | 24  | LEU  |
| 51  | 2t    | 41  | ILE  |
| 51  | 2t    | 45  | GLN  |
| 51  | 2t    | 84  | LEU  |
| 51  | 2t    | 100 | ILE  |
| 55  | 2y    | 2   | ARG  |
| 55  | 2y    | 4   | ARG  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (96) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | 1D    | 253 | GLN  |
| 4   | 1E    | 48  | GLN  |
| 5   | 1F    | 8   | GLN  |
| 5   | 1F    | 75  | HIS  |
| 5   | 1F    | 203 | GLN  |
| 8   | 1I    | 104 | GLN  |
| 9   | 1N    | 133 | GLN  |
| 13  | 1R    | 24  | GLN  |
| 13  | 1R    | 71  | GLN  |
| 15  | 1T    | 58  | ASN  |
| 16  | 1U    | 104 | GLN  |
| 20  | 1Y    | 6   | HIS  |
| 20  | 1Y    | 43  | ASN  |
| 20  | 1Y    | 92  | ASN  |
| 21  | 1Z    | 34  | ASN  |
| 21  | 1Z    | 54  | HIS  |
| 21  | 1Z    | 73  | GLN  |
| 24  | 12    | 70  | GLN  |
| 25  | 13    | 32  | GLN  |
| 26  | 14    | 60  | GLN  |
| 34  | 1c    | 6   | HIS  |
| 34  | 1c    | 104 | GLN  |
| 34  | 1c    | 176 | HIS  |
| 35  | 1d    | 77  | ASN  |
| 35  | 1d    | 119 | GLN  |
| 35  | 1d    | 123 | HIS  |
| 35  | 1d    | 129 | ASN  |
| 36  | 1e    | 20  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 37  | 1f    | 100 | ASN  |
| 38  | 1g    | 28  | ASN  |
| 38  | 1g    | 56  | GLN  |
| 38  | 1g    | 110 | GLN  |
| 38  | 1g    | 148 | ASN  |
| 40  | 1i    | 3   | GLN  |
| 40  | 1i    | 34  | ASN  |
| 40  | 1i    | 73  | GLN  |
| 40  | 1i    | 87  | GLN  |
| 41  | 1j    | 56  | HIS  |
| 41  | 1j    | 84  | GLN  |
| 43  | 1l    | 80  | HIS  |
| 43  | 1l    | 99  | HIS  |
| 46  | 1o    | 28  | GLN  |
| 48  | 1q    | 16  | GLN  |
| 50  | 1s    | 23  | ASN  |
| 50  | 1s    | 69  | HIS  |
| 50  | 1s    | 83  | HIS  |
| 3   | 2D    | 253 | GLN  |
| 5   | 2F    | 69  | HIS  |
| 5   | 2F    | 203 | GLN  |
| 6   | 2G    | 79  | ASN  |
| 8   | 2I    | 133 | HIS  |
| 12  | 2Q    | 141 | GLN  |
| 17  | 2V    | 64  | HIS  |
| 18  | 2W    | 60  | ASN  |
| 19  | 2X    | 31  | HIS  |
| 19  | 2X    | 82  | GLN  |
| 21  | 2Z    | 73  | GLN  |
| 21  | 2Z    | 121 | HIS  |
| 22  | 20    | 70  | GLN  |
| 23  | 21    | 19  | GLN  |
| 25  | 23    | 32  | GLN  |
| 26  | 24    | 20  | ASN  |
| 26  | 24    | 46  | GLN  |
| 33  | 2b    | 19  | HIS  |
| 33  | 2b    | 76  | GLN  |
| 33  | 2b    | 135 | GLN  |
| 34  | 2c    | 6   | HIS  |
| 34  | 2c    | 136 | GLN  |
| 34  | 2c    | 176 | HIS  |
| 35  | 2d    | 77  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 35  | 2d    | 116 | GLN  |
| 35  | 2d    | 119 | GLN  |
| 35  | 2d    | 123 | HIS  |
| 35  | 2d    | 160 | GLN  |
| 35  | 2d    | 161 | ASN  |
| 35  | 2d    | 201 | GLN  |
| 36  | 2e    | 78  | HIS  |
| 36  | 2e    | 141 | GLN  |
| 37  | 2f    | 73  | ASN  |
| 37  | 2f    | 100 | ASN  |
| 38  | 2g    | 11  | GLN  |
| 38  | 2g    | 28  | ASN  |
| 38  | 2g    | 68  | ASN  |
| 38  | 2g    | 86  | GLN  |
| 40  | 2i    | 3   | GLN  |
| 40  | 2i    | 31  | GLN  |
| 40  | 2i    | 73  | GLN  |
| 40  | 2i    | 117 | HIS  |
| 41  | 2j    | 69  | ASN  |
| 44  | 2m    | 62  | ASN  |
| 46  | 2o    | 28  | GLN  |
| 48  | 2q    | 26  | GLN  |
| 50  | 2s    | 23  | ASN  |
| 50  | 2s    | 47  | HIS  |
| 50  | 2s    | 69  | HIS  |
| 50  | 2s    | 83  | HIS  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1   | 1A    | 2864/2915 (98%) | 407 (14%)         | 38 (1%)         |
| 1   | 2A    | 2857/2915 (98%) | 408 (14%)         | 33 (1%)         |
| 2   | 1B    | 119/120 (99%)   | 5 (4%)            | 0               |
| 2   | 2B    | 118/120 (98%)   | 6 (5%)            | 0               |
| 32  | 1a    | 1494/1520 (98%) | 208 (13%)         | 0               |
| 32  | 2a    | 1498/1520 (98%) | 220 (14%)         | 0               |
| 53  | 1v    | 2/3 (66%)       | 0                 | 0               |
| 53  | 2v    | 2/3 (66%)       | 0                 | 0               |
| 54  | 1x    | 75/76 (98%)     | 20 (26%)          | 0               |
| 54  | 2x    | 75/76 (98%)     | 10 (13%)          | 0               |
| All | All   | 9104/9268 (98%) | 1284 (14%)        | 71 (0%)         |

All (1284) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 1A    | 12  | U    |
| 1   | 1A    | 34  | C    |
| 1   | 1A    | 45  | C    |
| 1   | 1A    | 70  | A    |
| 1   | 1A    | 73  | A    |
| 1   | 1A    | 74  | G    |
| 1   | 1A    | 116 | A    |
| 1   | 1A    | 117 | A    |
| 1   | 1A    | 118 | U    |
| 1   | 1A    | 162 | G    |
| 1   | 1A    | 185 | A    |
| 1   | 1A    | 188 | A    |
| 1   | 1A    | 194 | G    |
| 1   | 1A    | 202 | A    |
| 1   | 1A    | 204 | G    |
| 1   | 1A    | 205 | A    |
| 1   | 1A    | 210 | A    |
| 1   | 1A    | 211 | A    |
| 1   | 1A    | 214 | A    |
| 1   | 1A    | 218 | A    |
| 1   | 1A    | 237 | G    |
| 1   | 1A    | 269 | G    |
| 1   | 1A    | 271 | U    |
| 1   | 1A    | 272 | U    |
| 1   | 1A    | 273 | G    |
| 1   | 1A    | 274 | U    |
| 1   | 1A    | 279 | G    |
| 1   | 1A    | 288 | U    |
| 1   | 1A    | 289 | G    |
| 1   | 1A    | 303 | C    |
| 1   | 1A    | 335 | A    |
| 1   | 1A    | 348 | A    |
| 1   | 1A    | 351 | G    |
| 1   | 1A    | 354 | A    |
| 1   | 1A    | 366 | G    |
| 1   | 1A    | 376 | G    |
| 1   | 1A    | 381 | A    |
| 1   | 1A    | 386 | U    |
| 1   | 1A    | 387 | G    |
| 1   | 1A    | 413 | G    |
| 1   | 1A    | 423 | G    |
| 1   | 1A    | 432 | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 1A    | 438 | G    |
| 1   | 1A    | 439 | A    |
| 1   | 1A    | 448 | U    |
| 1   | 1A    | 455 | A    |
| 1   | 1A    | 474 | U    |
| 1   | 1A    | 482 | C    |
| 1   | 1A    | 483 | A    |
| 1   | 1A    | 505 | A    |
| 1   | 1A    | 507 | G    |
| 1   | 1A    | 530 | A    |
| 1   | 1A    | 534 | C    |
| 1   | 1A    | 535 | C    |
| 1   | 1A    | 543 | G    |
| 1   | 1A    | 555 | G    |
| 1   | 1A    | 556 | C    |
| 1   | 1A    | 557 | A    |
| 1   | 1A    | 558 | G    |
| 1   | 1A    | 569 | G    |
| 1   | 1A    | 573 | G    |
| 1   | 1A    | 574 | G    |
| 1   | 1A    | 586 | G    |
| 1   | 1A    | 596 | G    |
| 1   | 1A    | 598 | A    |
| 1   | 1A    | 609 | A    |
| 1   | 1A    | 615 | G    |
| 1   | 1A    | 618 | C    |
| 1   | 1A    | 626 | A    |
| 1   | 1A    | 627 | G    |
| 1   | 1A    | 630 | U    |
| 1   | 1A    | 633 | G    |
| 1   | 1A    | 639 | G    |
| 1   | 1A    | 641 | G    |
| 1   | 1A    | 652 | A    |
| 1   | 1A    | 662 | A    |
| 1   | 1A    | 670 | C    |
| 1   | 1A    | 673 | G    |
| 1   | 1A    | 693 | G    |
| 1   | 1A    | 694 | G    |
| 1   | 1A    | 697 | C    |
| 1   | 1A    | 698 | G    |
| 1   | 1A    | 715 | G    |
| 1   | 1A    | 716 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 1A    | 733  | G    |
| 1   | 1A    | 777  | C    |
| 1   | 1A    | 822  | G    |
| 1   | 1A    | 823  | G    |
| 1   | 1A    | 829  | A    |
| 1   | 1A    | 831  | A    |
| 1   | 1A    | 832  | G    |
| 1   | 1A    | 839  | G    |
| 1   | 1A    | 852  | G    |
| 1   | 1A    | 859  | C    |
| 1   | 1A    | 874  | U    |
| 1   | 1A    | 875  | U    |
| 1   | 1A    | 906  | G    |
| 1   | 1A    | 927  | G    |
| 1   | 1A    | 933  | C    |
| 1   | 1A    | 934  | A    |
| 1   | 1A    | 935  | C    |
| 1   | 1A    | 936  | C    |
| 1   | 1A    | 937  | A    |
| 1   | 1A    | 942  | A    |
| 1   | 1A    | 945  | A    |
| 1   | 1A    | 946  | A    |
| 1   | 1A    | 947  | A    |
| 1   | 1A    | 956  | A    |
| 1   | 1A    | 977  | G    |
| 1   | 1A    | 983  | G    |
| 1   | 1A    | 990  | A    |
| 1   | 1A    | 991  | G    |
| 1   | 1A    | 1003 | U    |
| 1   | 1A    | 1004 | A    |
| 1   | 1A    | 1006 | C    |
| 1   | 1A    | 1019 | G    |
| 1   | 1A    | 1020 | C    |
| 1   | 1A    | 1021 | G    |
| 1   | 1A    | 1029 | A    |
| 1   | 1A    | 1042 | A    |
| 1   | 1A    | 1051 | C    |
| 1   | 1A    | 1058 | U    |
| 1   | 1A    | 1059 | C    |
| 1   | 1A    | 1068 | G    |
| 1   | 1A    | 1071 | G    |
| 1   | 1A    | 1072 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 1A    | 1079 | U    |
| 1   | 1A    | 1085 | G    |
| 1   | 1A    | 1088 | G    |
| 1   | 1A    | 1090 | G    |
| 1   | 1A    | 1092 | A    |
| 1   | 1A    | 1093 | G    |
| 1   | 1A    | 1094 | A    |
| 1   | 1A    | 1100 | A    |
| 1   | 1A    | 1106 | U    |
| 1   | 1A    | 1107 | U    |
| 1   | 1A    | 1108 | G    |
| 1   | 1A    | 1109 | G    |
| 1   | 1A    | 1110 | C    |
| 1   | 1A    | 1111 | U    |
| 1   | 1A    | 1112 | U    |
| 1   | 1A    | 1113 | A    |
| 1   | 1A    | 1114 | G    |
| 1   | 1A    | 1116 | A    |
| 1   | 1A    | 1117 | G    |
| 1   | 1A    | 1119 | A    |
| 1   | 1A    | 1122 | C    |
| 1   | 1A    | 1123 | A    |
| 1   | 1A    | 1124 | U    |
| 1   | 1A    | 1129 | U    |
| 1   | 1A    | 1130 | A    |
| 1   | 1A    | 1131 | A    |
| 1   | 1A    | 1134 | A    |
| 1   | 1A    | 1136 | U    |
| 1   | 1A    | 1137 | G    |
| 1   | 1A    | 1139 | G    |
| 1   | 1A    | 1141 | A    |
| 1   | 1A    | 1142 | A    |
| 1   | 1A    | 1143 | U    |
| 1   | 1A    | 1155 | C    |
| 1   | 1A    | 1156 | G    |
| 1   | 1A    | 1158 | G    |
| 1   | 1A    | 1162 | C    |
| 1   | 1A    | 1175 | A    |
| 1   | 1A    | 1176 | U    |
| 1   | 1A    | 1180 | C    |
| 1   | 1A    | 1181 | G    |
| 1   | 1A    | 1217 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 1A    | 1218 | G    |
| 1   | 1A    | 1219 | A    |
| 1   | 1A    | 1220 | U    |
| 1   | 1A    | 1221 | G    |
| 1   | 1A    | 1222 | A    |
| 1   | 1A    | 1223 | C    |
| 1   | 1A    | 1256 | U    |
| 1   | 1A    | 1265 | A    |
| 1   | 1A    | 1287 | A    |
| 1   | 1A    | 1299 | A    |
| 1   | 1A    | 1302 | G    |
| 1   | 1A    | 1317 | G    |
| 1   | 1A    | 1318 | A    |
| 1   | 1A    | 1319 | U    |
| 1   | 1A    | 1346 | U    |
| 1   | 1A    | 1347 | A    |
| 1   | 1A    | 1349 | G    |
| 1   | 1A    | 1354 | A    |
| 1   | 1A    | 1398 | U    |
| 1   | 1A    | 1405 | A    |
| 1   | 1A    | 1406 | A    |
| 1   | 1A    | 1411 | A    |
| 1   | 1A    | 1416 | C    |
| 1   | 1A    | 1430 | A    |
| 1   | 1A    | 1431 | G    |
| 1   | 1A    | 1432 | C    |
| 1   | 1A    | 1462 | G    |
| 1   | 1A    | 1463 | C    |
| 1   | 1A    | 1466 | U    |
| 1   | 1A    | 1467 | G    |
| 1   | 1A    | 1474 | C    |
| 1   | 1A    | 1491 | A    |
| 1   | 1A    | 1497 | G    |
| 1   | 1A    | 1500 | A    |
| 1   | 1A    | 1514 | C    |
| 1   | 1A    | 1518 | A    |
| 1   | 1A    | 1529 | G    |
| 1   | 1A    | 1539 | C    |
| 1   | 1A    | 1543 | U    |
| 1   | 1A    | 1554 | A    |
| 1   | 1A    | 1555 | C    |
| 1   | 1A    | 1578 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 1A    | 1589 | A    |
| 1   | 1A    | 1590 | C    |
| 1   | 1A    | 1594 | C    |
| 1   | 1A    | 1605 | A    |
| 1   | 1A    | 1613 | A    |
| 1   | 1A    | 1616 | A    |
| 1   | 1A    | 1625 | U    |
| 1   | 1A    | 1626 | A    |
| 1   | 1A    | 1628 | G    |
| 1   | 1A    | 1631 | C    |
| 1   | 1A    | 1632 | A    |
| 1   | 1A    | 1654 | A    |
| 1   | 1A    | 1655 | A    |
| 1   | 1A    | 1695 | C    |
| 1   | 1A    | 1701 | A    |
| 1   | 1A    | 1721 | G    |
| 1   | 1A    | 1743 | G    |
| 1   | 1A    | 1747 | A    |
| 1   | 1A    | 1748 | A    |
| 1   | 1A    | 1767 | A    |
| 1   | 1A    | 1787 | G    |
| 1   | 1A    | 1793 | A    |
| 1   | 1A    | 1794 | G    |
| 1   | 1A    | 1795 | G    |
| 1   | 1A    | 1804 | A    |
| 1   | 1A    | 1811 | A    |
| 1   | 1A    | 1813 | C    |
| 1   | 1A    | 1822 | A    |
| 1   | 1A    | 1831 | C    |
| 1   | 1A    | 1832 | G    |
| 1   | 1A    | 1847 | G    |
| 1   | 1A    | 1860 | A    |
| 1   | 1A    | 1870 | G    |
| 1   | 1A    | 1878 | A    |
| 1   | 1A    | 1899 | A    |
| 1   | 1A    | 1900 | G    |
| 1   | 1A    | 1911 | A    |
| 1   | 1A    | 1918 | G    |
| 1   | 1A    | 1922 | A    |
| 1   | 1A    | 1927 | C    |
| 1   | 1A    | 1928 | G    |
| 1   | 1A    | 1935 | A    |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 1          | 1A           | 1936       | C           |
| 1          | 1A           | 1951       | G           |
| 1          | 1A           | 1952       | G           |
| 1          | 1A           | 1959       | A           |
| 1          | 1A           | 1960       | A           |
| 1          | 1A           | 1977       | U           |
| 1          | 1A           | 1985       | U           |
| 1          | 1A           | 1989       | C           |
| 1          | 1A           | 1992       | A           |
| 1          | 1A           | 1993       | A           |
| 1          | 1A           | 1994       | A           |
| 1          | 1A           | 2015       | U           |
| 1          | 1A           | 2019       | G           |
| 1          | 1A           | 2042       | A           |
| 1          | 1A           | 2045       | G           |
| 1          | 1A           | 2053       | A           |
| 1          | 1A           | 2055       | A           |
| 1          | 1A           | 2061       | C           |
| 1          | 1A           | 2065       | C           |
| 1          | 1A           | 2077       | C           |
| 1          | 1A           | 2078       | G           |
| 1          | 1A           | 2082       | A           |
| 1          | 1A           | 2083       | G           |
| 1          | 1A           | 2084       | A           |
| 1          | 1A           | 2091       | G           |
| 1          | 1A           | 2115       | G           |
| 1          | 1A           | 2121       | U           |
| 1          | 1A           | 2125       | C           |
| 1          | 1A           | 2126       | G           |
| 1          | 1A           | 2129       | C           |
| 1          | 1A           | 2130       | C           |
| 1          | 1A           | 2132       | G           |
| 1          | 1A           | 2133       | C           |
| 1          | 1A           | 2134       | G           |
| 1          | 1A           | 2137       | G           |
| 1          | 1A           | 2138       | G           |
| 1          | 1A           | 2139       | A           |
| 1          | 1A           | 2140       | U           |
| 1          | 1A           | 2141       | A           |
| 1          | 1A           | 2142       | G           |
| 1          | 1A           | 2148       | A           |
| 1          | 1A           | 2149       | G           |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 1          | 1A           | 2154       | U           |
| 1          | 1A           | 2155       | G           |
| 1          | 1A           | 2156       | A           |
| 1          | 1A           | 2158       | C           |
| 1          | 1A           | 2160       | C           |
| 1          | 1A           | 2164       | C           |
| 1          | 1A           | 2166       | U           |
| 1          | 1A           | 2167       | C           |
| 1          | 1A           | 2168       | C           |
| 1          | 1A           | 2169       | G           |
| 1          | 1A           | 2170       | G           |
| 1          | 1A           | 2174       | G           |
| 1          | 1A           | 2180       | A           |
| 1          | 1A           | 2181       | G           |
| 1          | 1A           | 2182       | G           |
| 1          | 1A           | 2184       | G           |
| 1          | 1A           | 2194       | U           |
| 1          | 1A           | 2195       | A           |
| 1          | 1A           | 2200       | C           |
| 1          | 1A           | 2208       | G           |
| 1          | 1A           | 2209       | G           |
| 1          | 1A           | 2211       | U           |
| 1          | 1A           | 2212       | G           |
| 1          | 1A           | 2214       | G           |
| 1          | 1A           | 2220       | A           |
| 1          | 1A           | 2227       | G           |
| 1          | 1A           | 2228       | G           |
| 1          | 1A           | 2229       | A           |
| 1          | 1A           | 2237       | A           |
| 1          | 1A           | 2250       | G           |
| 1          | 1A           | 2251       | G           |
| 1          | 1A           | 2280       | A           |
| 1          | 1A           | 2281       | A           |
| 1          | 1A           | 2291       | G           |
| 1          | 1A           | 2295       | C           |
| 1          | 1A           | 2298       | A           |
| 1          | 1A           | 2299       | A           |
| 1          | 1A           | 2301       | G           |
| 1          | 1A           | 2317       | A           |
| 1          | 1A           | 2320       | G           |
| 1          | 1A           | 2324       | U           |
| 1          | 1A           | 2332       | A           |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 1A    | 2337 | G    |
| 1   | 1A    | 2346 | G    |
| 1   | 1A    | 2347 | A    |
| 1   | 1A    | 2348 | A    |
| 1   | 1A    | 2359 | C    |
| 1   | 1A    | 2395 | G    |
| 1   | 1A    | 2397 | C    |
| 1   | 1A    | 2408 | G    |
| 1   | 1A    | 2418 | U    |
| 1   | 1A    | 2426 | G    |
| 1   | 1A    | 2434 | A    |
| 1   | 1A    | 2435 | U    |
| 1   | 1A    | 2437 | A    |
| 1   | 1A    | 2441 | G    |
| 1   | 1A    | 2442 | A    |
| 1   | 1A    | 2443 | U    |
| 1   | 1A    | 2447 | A    |
| 1   | 1A    | 2451 | A    |
| 1   | 1A    | 2453 | C    |
| 1   | 1A    | 2460 | A    |
| 1   | 1A    | 2481 | A    |
| 1   | 1A    | 2486 | C    |
| 1   | 1A    | 2488 | A    |
| 1   | 1A    | 2514 | G    |
| 1   | 1A    | 2517 | G    |
| 1   | 1A    | 2518 | U    |
| 1   | 1A    | 2530 | A    |
| 1   | 1A    | 2532 | C    |
| 1   | 1A    | 2537 | G    |
| 1   | 1A    | 2541 | G    |
| 1   | 1A    | 2566 | U    |
| 1   | 1A    | 2578 | A    |
| 1   | 1A    | 2579 | G    |
| 1   | 1A    | 2585 | C    |
| 1   | 1A    | 2594 | G    |
| 1   | 1A    | 2597 | U    |
| 1   | 1A    | 2598 | C    |
| 1   | 1A    | 2614 | A    |
| 1   | 1A    | 2615 | G    |
| 1   | 1A    | 2621 | U    |
| 1   | 1A    | 2623 | U    |
| 1   | 1A    | 2624 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 1A    | 2642 | G    |
| 1   | 1A    | 2666 | A    |
| 1   | 1A    | 2674 | A    |
| 1   | 1A    | 2675 | G    |
| 1   | 1A    | 2694 | U    |
| 1   | 1A    | 2701 | U    |
| 1   | 1A    | 2702 | C    |
| 1   | 1A    | 2714 | U    |
| 1   | 1A    | 2715 | C    |
| 1   | 1A    | 2725 | A    |
| 1   | 1A    | 2726 | A    |
| 1   | 1A    | 2727 | G    |
| 1   | 1A    | 2739 | U    |
| 1   | 1A    | 2746 | A    |
| 1   | 1A    | 2770 | A    |
| 1   | 1A    | 2777 | A    |
| 1   | 1A    | 2778 | A    |
| 1   | 1A    | 2791 | A    |
| 1   | 1A    | 2803 | A    |
| 1   | 1A    | 2804 | C    |
| 1   | 1A    | 2813 | G    |
| 1   | 1A    | 2830 | A    |
| 1   | 1A    | 2831 | A    |
| 1   | 1A    | 2843 | G    |
| 1   | 1A    | 2845 | A    |
| 1   | 1A    | 2882 | G    |
| 1   | 1A    | 2890 | C    |
| 1   | 1A    | 2901 | A    |
| 1   | 1A    | 2903 | G    |
| 2   | 1B    | 2    | C    |
| 2   | 1B    | 30   | C    |
| 2   | 1B    | 56   | G    |
| 2   | 1B    | 73   | A    |
| 2   | 1B    | 110  | G    |
| 32  | 1a    | 9    | G    |
| 32  | 1a    | 22   | G    |
| 32  | 1a    | 32   | A    |
| 32  | 1a    | 39   | G    |
| 32  | 1a    | 47   | C    |
| 32  | 1a    | 48   | C    |
| 32  | 1a    | 51   | A    |
| 32  | 1a    | 61   | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 32  | 1a    | 78  | G    |
| 32  | 1a    | 79  | G    |
| 32  | 1a    | 101 | A    |
| 32  | 1a    | 116 | A    |
| 32  | 1a    | 121 | C    |
| 32  | 1a    | 131 | C    |
| 32  | 1a    | 159 | G    |
| 32  | 1a    | 163 | C    |
| 32  | 1a    | 173 | U    |
| 32  | 1a    | 174 | C    |
| 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    | 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    | 348 | G    |
| 32  | 1a    | 351 | G    |
| 32  | 1a    | 352 | C    |
| 32  | 1a    | 353 | A    |
| 32  | 1a    | 354 | G    |
| 32  | 1a    | 367 | U    |
| 32  | 1a    | 372 | C    |
| 32  | 1a    | 373 | A    |
| 32  | 1a    | 397 | A    |
| 32  | 1a    | 398 | C    |
| 32  | 1a    | 406 | G    |
| 32  | 1a    | 412 | A    |
| 32  | 1a    | 413 | G    |
| 32  | 1a    | 424 | G    |
| 32  | 1a    | 429 | U    |
| 32  | 1a    | 430 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 32  | 1a    | 439 | A    |
| 32  | 1a    | 442 | C    |
| 32  | 1a    | 452 | A    |
| 32  | 1a    | 458 | C    |
| 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    | 532 | A    |
| 32  | 1a    | 533 | A    |
| 32  | 1a    | 547 | A    |
| 32  | 1a    | 559 | A    |
| 32  | 1a    | 561 | U    |
| 32  | 1a    | 562 | C    |
| 32  | 1a    | 564 | C    |
| 32  | 1a    | 572 | A    |
| 32  | 1a    | 573 | A    |
| 32  | 1a    | 576 | G    |
| 32  | 1a    | 577 | G    |
| 32  | 1a    | 592 | G    |
| 32  | 1a    | 596 | C    |
| 32  | 1a    | 630 | G    |
| 32  | 1a    | 632 | A    |
| 32  | 1a    | 653 | A    |
| 32  | 1a    | 661 | G    |
| 32  | 1a    | 665 | A    |
| 32  | 1a    | 687 | A    |
| 32  | 1a    | 688 | G    |
| 32  | 1a    | 723 | U    |
| 32  | 1a    | 731 | G    |
| 32  | 1a    | 734 | G    |
| 32  | 1a    | 753 | A    |
| 32  | 1a    | 755 | G    |
| 32  | 1a    | 774 | G    |
| 32  | 1a    | 777 | A    |
| 32  | 1a    | 793 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 32  | 1a    | 794  | A    |
| 32  | 1a    | 817  | C    |
| 32  | 1a    | 821  | G    |
| 32  | 1a    | 828  | A    |
| 32  | 1a    | 829  | G    |
| 32  | 1a    | 838  | G    |
| 32  | 1a    | 840  | C    |
| 32  | 1a    | 841  | U    |
| 32  | 1a    | 848  | C    |
| 32  | 1a    | 851  | G    |
| 32  | 1a    | 859  | A    |
| 32  | 1a    | 874  | G    |
| 32  | 1a    | 902  | G    |
| 32  | 1a    | 914  | A    |
| 32  | 1a    | 926  | G    |
| 32  | 1a    | 927  | G    |
| 32  | 1a    | 934  | C    |
| 32  | 1a    | 935  | A    |
| 32  | 1a    | 960  | U    |
| 32  | 1a    | 961  | U    |
| 32  | 1a    | 967  | 5MC  |
| 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    | 994  | A    |
| 32  | 1a    | 1002 | G    |
| 32  | 1a    | 1003 | G    |
| 32  | 1a    | 1004 | A    |
| 32  | 1a    | 1005 | A    |
| 32  | 1a    | 1006 | C    |
| 32  | 1a    | 1009 | G    |
| 32  | 1a    | 1020 | U    |
| 32  | 1a    | 1022 | G    |
| 32  | 1a    | 1023 | G    |
| 32  | 1a    | 1024 | G    |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 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           | 1033       | G           |
| 32         | 1a           | 1044       | A           |
| 32         | 1a           | 1053       | G           |
| 32         | 1a           | 1054       | C           |
| 32         | 1a           | 1065       | U           |
| 32         | 1a           | 1066       | C           |
| 32         | 1a           | 1068       | G           |
| 32         | 1a           | 1081       | G           |
| 32         | 1a           | 1094       | G           |
| 32         | 1a           | 1095       | U           |
| 32         | 1a           | 1101       | A           |
| 32         | 1a           | 1125       | U           |
| 32         | 1a           | 1130       | A           |
| 32         | 1a           | 1134       | G           |
| 32         | 1a           | 1136       | U           |
| 32         | 1a           | 1137       | C           |
| 32         | 1a           | 1139       | G           |
| 32         | 1a           | 1140       | C           |
| 32         | 1a           | 1152       | A           |
| 32         | 1a           | 1159       | U           |
| 32         | 1a           | 1183       | A           |
| 32         | 1a           | 1184       | G           |
| 32         | 1a           | 1196       | U           |
| 32         | 1a           | 1197       | G           |
| 32         | 1a           | 1202       | G           |
| 32         | 1a           | 1208       | C           |
| 32         | 1a           | 1213       | A           |
| 32         | 1a           | 1224       | G           |
| 32         | 1a           | 1227       | A           |
| 32         | 1a           | 1236       | A           |
| 32         | 1a           | 1238       | A           |
| 32         | 1a           | 1250       | A           |
| 32         | 1a           | 1256       | A           |
| 32         | 1a           | 1257       | U           |
| 32         | 1a           | 1258       | G           |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 32  | 1a    | 1270    | C    |
| 32  | 1a    | 1278    | U    |
| 32  | 1a    | 1280    | A    |
| 32  | 1a    | 1286    | A    |
| 32  | 1a    | 1287    | A    |
| 32  | 1a    | 1299    | A    |
| 32  | 1a    | 1300    | G    |
| 32  | 1a    | 1302    | U    |
| 32  | 1a    | 1317    | C    |
| 32  | 1a    | 1320    | C    |
| 32  | 1a    | 1338    | G    |
| 32  | 1a    | 1346    | A    |
| 32  | 1a    | 1347    | G    |
| 32  | 1a    | 1353    | G    |
| 32  | 1a    | 1363    | C    |
| 32  | 1a    | 1370    | G    |
| 32  | 1a    | 1397    | C    |
| 32  | 1a    | 1419    | G    |
| 32  | 1a    | 1442    | G    |
| 32  | 1a    | 1442(A) | G    |
| 32  | 1a    | 1487    | G    |
| 32  | 1a    | 1493    | A    |
| 32  | 1a    | 1497    | G    |
| 32  | 1a    | 1503    | A    |
| 32  | 1a    | 1504    | G    |
| 32  | 1a    | 1505    | G    |
| 32  | 1a    | 1506    | U    |
| 32  | 1a    | 1517    | G    |
| 32  | 1a    | 1520    | G    |
| 32  | 1a    | 1529    | G    |
| 32  | 1a    | 1530    | G    |
| 32  | 1a    | 1531    | A    |
| 54  | 1x    | 3       | C    |
| 54  | 1x    | 6       | G    |
| 54  | 1x    | 9       | G    |
| 54  | 1x    | 14      | A    |
| 54  | 1x    | 16      | C    |
| 54  | 1x    | 19      | G    |
| 54  | 1x    | 20      | U    |
| 54  | 1x    | 21      | A    |
| 54  | 1x    | 30      | G    |
| 54  | 1x    | 34      | C    |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 54  | 1x    | 42     | G    |
| 54  | 1x    | 44     | A    |
| 54  | 1x    | 47     | U    |
| 54  | 1x    | 50     | U    |
| 54  | 1x    | 60     | U    |
| 54  | 1x    | 63     | G    |
| 54  | 1x    | 69     | C    |
| 54  | 1x    | 72     | A    |
| 54  | 1x    | 75     | C    |
| 54  | 1x    | 76     | A    |
| 1   | 2A    | 10     | G    |
| 1   | 2A    | 12     | U    |
| 1   | 2A    | 34     | C    |
| 1   | 2A    | 45     | C    |
| 1   | 2A    | 71     | A    |
| 1   | 2A    | 74     | A    |
| 1   | 2A    | 75     | G    |
| 1   | 2A    | 84     | A    |
| 1   | 2A    | 95     | G    |
| 1   | 2A    | 118    | A    |
| 1   | 2A    | 119    | A    |
| 1   | 2A    | 120    | U    |
| 1   | 2A    | 157    | U    |
| 1   | 2A    | 173    | G    |
| 1   | 2A    | 196    | A    |
| 1   | 2A    | 199    | A    |
| 1   | 2A    | 205    | G    |
| 1   | 2A    | 215    | G    |
| 1   | 2A    | 216    | A    |
| 1   | 2A    | 221    | A    |
| 1   | 2A    | 222    | A    |
| 1   | 2A    | 225    | A    |
| 1   | 2A    | 229    | A    |
| 1   | 2A    | 230    | U    |
| 1   | 2A    | 248    | G    |
| 1   | 2A    | 271(K) | U    |
| 1   | 2A    | 271(L) | U    |
| 1   | 2A    | 271(M) | G    |
| 1   | 2A    | 271(N) | U    |
| 1   | 2A    | 272(A) | U    |
| 1   | 2A    | 272(B) | G    |
| 1   | 2A    | 277    | C    |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | 2A    | 278    | A    |
| 1   | 2A    | 311    | A    |
| 1   | 2A    | 324    | A    |
| 1   | 2A    | 327    | G    |
| 1   | 2A    | 330    | A    |
| 1   | 2A    | 342    | G    |
| 1   | 2A    | 352    | G    |
| 1   | 2A    | 357    | A    |
| 1   | 2A    | 362    | U    |
| 1   | 2A    | 363    | G    |
| 1   | 2A    | 386    | G    |
| 1   | 2A    | 411    | G    |
| 1   | 2A    | 412    | A    |
| 1   | 2A    | 421    | U    |
| 1   | 2A    | 428    | A    |
| 1   | 2A    | 444    | C    |
| 1   | 2A    | 456    | C    |
| 1   | 2A    | 457    | A    |
| 1   | 2A    | 479    | A    |
| 1   | 2A    | 481    | G    |
| 1   | 2A    | 505    | A    |
| 1   | 2A    | 509    | C    |
| 1   | 2A    | 510    | C    |
| 1   | 2A    | 518    | G    |
| 1   | 2A    | 530    | G    |
| 1   | 2A    | 531    | C    |
| 1   | 2A    | 532    | A    |
| 1   | 2A    | 533    | G    |
| 1   | 2A    | 545    | G    |
| 1   | 2A    | 551    | G    |
| 1   | 2A    | 563    | G    |
| 1   | 2A    | 573    | G    |
| 1   | 2A    | 575    | A    |
| 1   | 2A    | 586    | A    |
| 1   | 2A    | 592    | G    |
| 1   | 2A    | 595    | C    |
| 1   | 2A    | 603    | A    |
| 1   | 2A    | 604    | G    |
| 1   | 2A    | 607    | U    |
| 1   | 2A    | 610    | G    |
| 1   | 2A    | 614(B) | G    |
| 1   | 2A    | 615    | G    |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | 2A    | 627    | A    |
| 1   | 2A    | 637    | A    |
| 1   | 2A    | 645    | C    |
| 1   | 2A    | 646    | A    |
| 1   | 2A    | 648    | G    |
| 1   | 2A    | 652(B) | A    |
| 1   | 2A    | 652(C) | G    |
| 1   | 2A    | 652(E) | G    |
| 1   | 2A    | 652(U) | G    |
| 1   | 2A    | 668    | G    |
| 1   | 2A    | 669    | G    |
| 1   | 2A    | 686    | G    |
| 1   | 2A    | 730    | C    |
| 1   | 2A    | 753    | C    |
| 1   | 2A    | 775    | G    |
| 1   | 2A    | 776    | G    |
| 1   | 2A    | 782    | A    |
| 1   | 2A    | 784    | A    |
| 1   | 2A    | 785    | G    |
| 1   | 2A    | 792    | G    |
| 1   | 2A    | 805    | G    |
| 1   | 2A    | 812    | C    |
| 1   | 2A    | 827    | U    |
| 1   | 2A    | 828    | U    |
| 1   | 2A    | 857    | C    |
| 1   | 2A    | 859    | G    |
| 1   | 2A    | 874    | G    |
| 1   | 2A    | 880    | G    |
| 1   | 2A    | 887    | A    |
| 1   | 2A    | 888    | C    |
| 1   | 2A    | 889    | C    |
| 1   | 2A    | 890    | A    |
| 1   | 2A    | 896    | A    |
| 1   | 2A    | 899    | A    |
| 1   | 2A    | 900    | A    |
| 1   | 2A    | 901    | A    |
| 1   | 2A    | 910    | A    |
| 1   | 2A    | 917    | A    |
| 1   | 2A    | 932    | G    |
| 1   | 2A    | 938    | G    |
| 1   | 2A    | 941    | A    |
| 1   | 2A    | 945    | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 2A    | 946  | G    |
| 1   | 2A    | 958  | U    |
| 1   | 2A    | 959  | A    |
| 1   | 2A    | 961  | C    |
| 1   | 2A    | 974  | G    |
| 1   | 2A    | 975  | C    |
| 1   | 2A    | 983  | A    |
| 1   | 2A    | 996  | A    |
| 1   | 2A    | 1005 | C    |
| 1   | 2A    | 1012 | U    |
| 1   | 2A    | 1013 | C    |
| 1   | 2A    | 1022 | G    |
| 1   | 2A    | 1025 | G    |
| 1   | 2A    | 1026 | U    |
| 1   | 2A    | 1033 | U    |
| 1   | 2A    | 1042 | G    |
| 1   | 2A    | 1044 | G    |
| 1   | 2A    | 1045 | A    |
| 1   | 2A    | 1046 | A    |
| 1   | 2A    | 1047 | G    |
| 1   | 2A    | 1052 | C    |
| 1   | 2A    | 1053 | C    |
| 1   | 2A    | 1054 | A    |
| 1   | 2A    | 1060 | U    |
| 1   | 2A    | 1063 | G    |
| 1   | 2A    | 1064 | C    |
| 1   | 2A    | 1065 | U    |
| 1   | 2A    | 1066 | U    |
| 1   | 2A    | 1068 | G    |
| 1   | 2A    | 1069 | A    |
| 1   | 2A    | 1070 | A    |
| 1   | 2A    | 1071 | G    |
| 1   | 2A    | 1073 | A    |
| 1   | 2A    | 1074 | G    |
| 1   | 2A    | 1076 | C    |
| 1   | 2A    | 1079 | C    |
| 1   | 2A    | 1082 | U    |
| 1   | 2A    | 1083 | U    |
| 1   | 2A    | 1084 | A    |
| 1   | 2A    | 1085 | A    |
| 1   | 2A    | 1086 | A    |
| 1   | 2A    | 1088 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 2A    | 1090 | U    |
| 1   | 2A    | 1091 | G    |
| 1   | 2A    | 1092 | C    |
| 1   | 2A    | 1093 | G    |
| 1   | 2A    | 1096 | A    |
| 1   | 2A    | 1108 | U    |
| 1   | 2A    | 1109 | C    |
| 1   | 2A    | 1110 | G    |
| 1   | 2A    | 1112 | G    |
| 1   | 2A    | 1129 | A    |
| 1   | 2A    | 1130 | U    |
| 1   | 2A    | 1135 | C    |
| 1   | 2A    | 1136 | G    |
| 1   | 2A    | 1139 | G    |
| 1   | 2A    | 1171 | G    |
| 1   | 2A    | 1211 | U    |
| 1   | 2A    | 1220 | A    |
| 1   | 2A    | 1253 | A    |
| 1   | 2A    | 1256 | G    |
| 1   | 2A    | 1271 | G    |
| 1   | 2A    | 1272 | A    |
| 1   | 2A    | 1273 | U    |
| 1   | 2A    | 1300 | U    |
| 1   | 2A    | 1301 | A    |
| 1   | 2A    | 1308 | A    |
| 1   | 2A    | 1314 | C    |
| 1   | 2A    | 1352 | U    |
| 1   | 2A    | 1359 | A    |
| 1   | 2A    | 1360 | A    |
| 1   | 2A    | 1365 | A    |
| 1   | 2A    | 1370 | C    |
| 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    | 1428 | C    |
| 1   | 2A    | 1445 | A    |
| 1   | 2A    | 1450 | G    |
| 1   | 2A    | 1467 | C    |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 1   | 2A    | 1471    | A    |
| 1   | 2A    | 1482    | G    |
| 1   | 2A    | 1493    | C    |
| 1   | 2A    | 1497    | U    |
| 1   | 2A    | 1508    | A    |
| 1   | 2A    | 1509    | C    |
| 1   | 2A    | 1509(A) | A    |
| 1   | 2A    | 1531    | C    |
| 1   | 2A    | 1533    | G    |
| 1   | 2A    | 1537    | G    |
| 1   | 2A    | 1542    | A    |
| 1   | 2A    | 1547    | C    |
| 1   | 2A    | 1558    | A    |
| 1   | 2A    | 1566    | A    |
| 1   | 2A    | 1569    | A    |
| 1   | 2A    | 1578    | U    |
| 1   | 2A    | 1579    | A    |
| 1   | 2A    | 1584    | C    |
| 1   | 2A    | 1586    | A    |
| 1   | 2A    | 1608    | A    |
| 1   | 2A    | 1609    | A    |
| 1   | 2A    | 1640    | C    |
| 1   | 2A    | 1648    | C    |
| 1   | 2A    | 1674    | G    |
| 1   | 2A    | 1696    | G    |
| 1   | 2A    | 1700    | A    |
| 1   | 2A    | 1722    | A    |
| 1   | 2A    | 1756    | G    |
| 1   | 2A    | 1762    | A    |
| 1   | 2A    | 1763    | G    |
| 1   | 2A    | 1764    | G    |
| 1   | 2A    | 1773    | A    |
| 1   | 2A    | 1780    | A    |
| 1   | 2A    | 1782    | C    |
| 1   | 2A    | 1791    | A    |
| 1   | 2A    | 1800    | C    |
| 1   | 2A    | 1801    | G    |
| 1   | 2A    | 1816    | G    |
| 1   | 2A    | 1829    | A    |
| 1   | 2A    | 1847    | A    |
| 1   | 2A    | 1848    | A    |
| 1   | 2A    | 1877    | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 2A    | 1878 | G    |
| 1   | 2A    | 1889 | A    |
| 1   | 2A    | 1896 | G    |
| 1   | 2A    | 1900 | A    |
| 1   | 2A    | 1905 | C    |
| 1   | 2A    | 1906 | G    |
| 1   | 2A    | 1914 | C    |
| 1   | 2A    | 1915 | 5MU  |
| 1   | 2A    | 1929 | G    |
| 1   | 2A    | 1930 | G    |
| 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    | 1993 | U    |
| 1   | 2A    | 1997 | G    |
| 1   | 2A    | 2020 | A    |
| 1   | 2A    | 2023 | G    |
| 1   | 2A    | 2031 | A    |
| 1   | 2A    | 2033 | A    |
| 1   | 2A    | 2039 | C    |
| 1   | 2A    | 2043 | C    |
| 1   | 2A    | 2055 | C    |
| 1   | 2A    | 2056 | G    |
| 1   | 2A    | 2060 | A    |
| 1   | 2A    | 2061 | G    |
| 1   | 2A    | 2062 | A    |
| 1   | 2A    | 2069 | G    |
| 1   | 2A    | 2096 | U    |
| 1   | 2A    | 2101 | G    |
| 1   | 2A    | 2103 | C    |
| 1   | 2A    | 2105 | C    |
| 1   | 2A    | 2107 | C    |
| 1   | 2A    | 2108 | C    |
| 1   | 2A    | 2110 | G    |
| 1   | 2A    | 2111 | C    |
| 1   | 2A    | 2116 | G    |
| 1   | 2A    | 2117 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 2A    | 2118 | U    |
| 1   | 2A    | 2119 | A    |
| 1   | 2A    | 2120 | 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    | 2136 | C    |
| 1   | 2A    | 2138 | C    |
| 1   | 2A    | 2142 | C    |
| 1   | 2A    | 2145 | C    |
| 1   | 2A    | 2146 | C    |
| 1   | 2A    | 2147 | G    |
| 1   | 2A    | 2148 | G    |
| 1   | 2A    | 2151 | G    |
| 1   | 2A    | 2152 | G    |
| 1   | 2A    | 2158 | A    |
| 1   | 2A    | 2159 | G    |
| 1   | 2A    | 2160 | G    |
| 1   | 2A    | 2162 | G    |
| 1   | 2A    | 2172 | U    |
| 1   | 2A    | 2173 | A    |
| 1   | 2A    | 2186 | G    |
| 1   | 2A    | 2187 | G    |
| 1   | 2A    | 2189 | U    |
| 1   | 2A    | 2190 | G    |
| 1   | 2A    | 2192 | G    |
| 1   | 2A    | 2198 | A    |
| 1   | 2A    | 2206 | G    |
| 1   | 2A    | 2207 | G    |
| 1   | 2A    | 2208 | A    |
| 1   | 2A    | 2218 | U    |
| 1   | 2A    | 2225 | A    |
| 1   | 2A    | 2238 | G    |
| 1   | 2A    | 2239 | G    |
| 1   | 2A    | 2268 | A    |
| 1   | 2A    | 2269 | A    |
| 1   | 2A    | 2275 | C    |
| 1   | 2A    | 2279 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 2A    | 2283 | C    |
| 1   | 2A    | 2286 | A    |
| 1   | 2A    | 2287 | A    |
| 1   | 2A    | 2305 | A    |
| 1   | 2A    | 2308 | G    |
| 1   | 2A    | 2311 | A    |
| 1   | 2A    | 2312 | U    |
| 1   | 2A    | 2320 | A    |
| 1   | 2A    | 2321 | G    |
| 1   | 2A    | 2322 | A    |
| 1   | 2A    | 2325 | G    |
| 1   | 2A    | 2334 | G    |
| 1   | 2A    | 2335 | A    |
| 1   | 2A    | 2336 | A    |
| 1   | 2A    | 2347 | C    |
| 1   | 2A    | 2383 | G    |
| 1   | 2A    | 2385 | C    |
| 1   | 2A    | 2396 | G    |
| 1   | 2A    | 2406 | U    |
| 1   | 2A    | 2414 | G    |
| 1   | 2A    | 2422 | A    |
| 1   | 2A    | 2425 | A    |
| 1   | 2A    | 2429 | G    |
| 1   | 2A    | 2430 | A    |
| 1   | 2A    | 2431 | U    |
| 1   | 2A    | 2435 | A    |
| 1   | 2A    | 2439 | A    |
| 1   | 2A    | 2441 | C    |
| 1   | 2A    | 2448 | A    |
| 1   | 2A    | 2474 | C    |
| 1   | 2A    | 2476 | A    |
| 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    | 2529 | G    |
| 1   | 2A    | 2554 | U    |
| 1   | 2A    | 2566 | A    |
| 1   | 2A    | 2567 | G    |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 1   | 2A    | 2573    | C    |
| 1   | 2A    | 2582    | G    |
| 1   | 2A    | 2585    | U    |
| 1   | 2A    | 2586    | C    |
| 1   | 2A    | 2602    | A    |
| 1   | 2A    | 2603    | G    |
| 1   | 2A    | 2609    | U    |
| 1   | 2A    | 2611    | U    |
| 1   | 2A    | 2612    | C    |
| 1   | 2A    | 2629    | A    |
| 1   | 2A    | 2630    | G    |
| 1   | 2A    | 2654    | A    |
| 1   | 2A    | 2662    | A    |
| 1   | 2A    | 2663    | G    |
| 1   | 2A    | 2682    | U    |
| 1   | 2A    | 2689    | U    |
| 1   | 2A    | 2690    | C    |
| 1   | 2A    | 2702    | U    |
| 1   | 2A    | 2703    | C    |
| 1   | 2A    | 2712(A) | A    |
| 1   | 2A    | 2713    | A    |
| 1   | 2A    | 2714    | G    |
| 1   | 2A    | 2726    | U    |
| 1   | 2A    | 2733    | A    |
| 1   | 2A    | 2757    | A    |
| 1   | 2A    | 2761    | G    |
| 1   | 2A    | 2764    | A    |
| 1   | 2A    | 2765    | A    |
| 1   | 2A    | 2778    | A    |
| 1   | 2A    | 2789    | C    |
| 1   | 2A    | 2802    | G    |
| 1   | 2A    | 2811    | G    |
| 1   | 2A    | 2820    | A    |
| 1   | 2A    | 2821    | A    |
| 1   | 2A    | 2833    | G    |
| 1   | 2A    | 2835    | A    |
| 1   | 2A    | 2872    | G    |
| 1   | 2A    | 2880    | C    |
| 1   | 2A    | 2892    | A    |
| 1   | 2A    | 2894    | G    |
| 2   | 2B    | 8       | U    |
| 2   | 2B    | 30      | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | 2B    | 56  | G    |
| 2   | 2B    | 73  | A    |
| 2   | 2B    | 84  | C    |
| 2   | 2B    | 110 | G    |
| 32  | 2a    | 5   | U    |
| 32  | 2a    | 9   | G    |
| 32  | 2a    | 22  | G    |
| 32  | 2a    | 32  | A    |
| 32  | 2a    | 39  | G    |
| 32  | 2a    | 47  | C    |
| 32  | 2a    | 48  | C    |
| 32  | 2a    | 51  | A    |
| 32  | 2a    | 61  | G    |
| 32  | 2a    | 66  | G    |
| 32  | 2a    | 80  | G    |
| 32  | 2a    | 88  | A    |
| 32  | 2a    | 89  | C    |
| 32  | 2a    | 101 | A    |
| 32  | 2a    | 116 | A    |
| 32  | 2a    | 121 | C    |
| 32  | 2a    | 131 | C    |
| 32  | 2a    | 163 | C    |
| 32  | 2a    | 173 | U    |
| 32  | 2a    | 174 | C    |
| 32  | 2a    | 182 | U    |
| 32  | 2a    | 195 | A    |
| 32  | 2a    | 197 | A    |
| 32  | 2a    | 202 | U    |
| 32  | 2a    | 203 | U    |
| 32  | 2a    | 204 | U    |
| 32  | 2a    | 216 | G    |
| 32  | 2a    | 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    | 348 | G    |
| 32  | 2a    | 351 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 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    | 397 | A    |
| 32  | 2a    | 398 | C    |
| 32  | 2a    | 406 | G    |
| 32  | 2a    | 412 | A    |
| 32  | 2a    | 413 | G    |
| 32  | 2a    | 424 | G    |
| 32  | 2a    | 429 | U    |
| 32  | 2a    | 430 | A    |
| 32  | 2a    | 439 | A    |
| 32  | 2a    | 442 | C    |
| 32  | 2a    | 452 | A    |
| 32  | 2a    | 458 | C    |
| 32  | 2a    | 461 | A    |
| 32  | 2a    | 470 | C    |
| 32  | 2a    | 485 | G    |
| 32  | 2a    | 496 | A    |
| 32  | 2a    | 498 | U    |
| 32  | 2a    | 505 | G    |
| 32  | 2a    | 510 | A    |
| 32  | 2a    | 511 | C    |
| 32  | 2a    | 518 | C    |
| 32  | 2a    | 527 | 7MG  |
| 32  | 2a    | 532 | A    |
| 32  | 2a    | 533 | A    |
| 32  | 2a    | 547 | A    |
| 32  | 2a    | 559 | A    |
| 32  | 2a    | 561 | U    |
| 32  | 2a    | 562 | C    |
| 32  | 2a    | 564 | C    |
| 32  | 2a    | 572 | A    |
| 32  | 2a    | 573 | A    |
| 32  | 2a    | 576 | G    |
| 32  | 2a    | 577 | G    |
| 32  | 2a    | 592 | G    |
| 32  | 2a    | 596 | C    |
| 32  | 2a    | 630 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 32  | 2a    | 632 | A    |
| 32  | 2a    | 653 | A    |
| 32  | 2a    | 661 | G    |
| 32  | 2a    | 665 | A    |
| 32  | 2a    | 687 | A    |
| 32  | 2a    | 688 | G    |
| 32  | 2a    | 695 | A    |
| 32  | 2a    | 723 | U    |
| 32  | 2a    | 731 | G    |
| 32  | 2a    | 753 | A    |
| 32  | 2a    | 755 | G    |
| 32  | 2a    | 774 | G    |
| 32  | 2a    | 777 | A    |
| 32  | 2a    | 793 | U    |
| 32  | 2a    | 794 | A    |
| 32  | 2a    | 815 | A    |
| 32  | 2a    | 817 | C    |
| 32  | 2a    | 821 | G    |
| 32  | 2a    | 828 | A    |
| 32  | 2a    | 829 | G    |
| 32  | 2a    | 838 | G    |
| 32  | 2a    | 840 | C    |
| 32  | 2a    | 841 | U    |
| 32  | 2a    | 848 | C    |
| 32  | 2a    | 851 | G    |
| 32  | 2a    | 859 | A    |
| 32  | 2a    | 874 | G    |
| 32  | 2a    | 902 | G    |
| 32  | 2a    | 914 | A    |
| 32  | 2a    | 926 | G    |
| 32  | 2a    | 927 | G    |
| 32  | 2a    | 934 | C    |
| 32  | 2a    | 935 | A    |
| 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    |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 32  | 2a    | 977     | A    |
| 32  | 2a    | 992     | U    |
| 32  | 2a    | 993     | G    |
| 32  | 2a    | 994     | A    |
| 32  | 2a    | 1003    | G    |
| 32  | 2a    | 1005    | A    |
| 32  | 2a    | 1006    | C    |
| 32  | 2a    | 1009    | G    |
| 32  | 2a    | 1020    | U    |
| 32  | 2a    | 1022    | G    |
| 32  | 2a    | 1023    | G    |
| 32  | 2a    | 1025    | U    |
| 32  | 2a    | 1026    | G    |
| 32  | 2a    | 1027    | C    |
| 32  | 2a    | 1028    | C    |
| 32  | 2a    | 1029    | C    |
| 32  | 2a    | 1030(A) | G    |
| 32  | 2a    | 1030(B) | C    |
| 32  | 2a    | 1036    | G    |
| 32  | 2a    | 1041    | A    |
| 32  | 2a    | 1044    | A    |
| 32  | 2a    | 1053    | G    |
| 32  | 2a    | 1054    | C    |
| 32  | 2a    | 1065    | U    |
| 32  | 2a    | 1066    | C    |
| 32  | 2a    | 1068    | G    |
| 32  | 2a    | 1081    | G    |
| 32  | 2a    | 1094    | G    |
| 32  | 2a    | 1095    | U    |
| 32  | 2a    | 1101    | A    |
| 32  | 2a    | 1117    | G    |
| 32  | 2a    | 1125    | U    |
| 32  | 2a    | 1129    | C    |
| 32  | 2a    | 1130    | A    |
| 32  | 2a    | 1132    | C    |
| 32  | 2a    | 1134    | G    |
| 32  | 2a    | 1136    | U    |
| 32  | 2a    | 1137    | C    |
| 32  | 2a    | 1139    | G    |
| 32  | 2a    | 1140    | C    |
| 32  | 2a    | 1147    | C    |
| 32  | 2a    | 1152    | A    |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 32  | 2a    | 1158    | C    |
| 32  | 2a    | 1159    | U    |
| 32  | 2a    | 1183    | A    |
| 32  | 2a    | 1184    | G    |
| 32  | 2a    | 1196    | U    |
| 32  | 2a    | 1197    | G    |
| 32  | 2a    | 1211    | U    |
| 32  | 2a    | 1212    | U    |
| 32  | 2a    | 1213    | A    |
| 32  | 2a    | 1224    | G    |
| 32  | 2a    | 1227    | A    |
| 32  | 2a    | 1236    | A    |
| 32  | 2a    | 1238    | A    |
| 32  | 2a    | 1250    | A    |
| 32  | 2a    | 1256    | A    |
| 32  | 2a    | 1257    | U    |
| 32  | 2a    | 1258    | G    |
| 32  | 2a    | 1270    | C    |
| 32  | 2a    | 1278    | U    |
| 32  | 2a    | 1280    | A    |
| 32  | 2a    | 1281    | U    |
| 32  | 2a    | 1282    | C    |
| 32  | 2a    | 1287    | A    |
| 32  | 2a    | 1299    | A    |
| 32  | 2a    | 1300    | G    |
| 32  | 2a    | 1302    | U    |
| 32  | 2a    | 1305    | G    |
| 32  | 2a    | 1317    | C    |
| 32  | 2a    | 1320    | C    |
| 32  | 2a    | 1338    | G    |
| 32  | 2a    | 1346    | A    |
| 32  | 2a    | 1347    | G    |
| 32  | 2a    | 1353    | G    |
| 32  | 2a    | 1363    | C    |
| 32  | 2a    | 1370    | G    |
| 32  | 2a    | 1397    | C    |
| 32  | 2a    | 1400    | 5MC  |
| 32  | 2a    | 1419    | G    |
| 32  | 2a    | 1442    | G    |
| 32  | 2a    | 1442(A) | G    |
| 32  | 2a    | 1447    | A    |
| 32  | 2a    | 1487    | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 32  | 2a    | 1492 | A    |
| 32  | 2a    | 1493 | A    |
| 32  | 2a    | 1497 | G    |
| 32  | 2a    | 1499 | A    |
| 32  | 2a    | 1503 | A    |
| 32  | 2a    | 1504 | G    |
| 32  | 2a    | 1505 | G    |
| 32  | 2a    | 1506 | U    |
| 32  | 2a    | 1517 | G    |
| 32  | 2a    | 1528 | U    |
| 32  | 2a    | 1529 | G    |
| 32  | 2a    | 1530 | G    |
| 32  | 2a    | 1531 | A    |
| 32  | 2a    | 1532 | U    |
| 54  | 2x    | 9    | G    |
| 54  | 2x    | 13   | C    |
| 54  | 2x    | 20   | U    |
| 54  | 2x    | 21   | A    |
| 54  | 2x    | 48   | C    |
| 54  | 2x    | 50   | U    |
| 54  | 2x    | 62   | C    |
| 54  | 2x    | 63   | G    |
| 54  | 2x    | 65   | C    |
| 54  | 2x    | 76   | A    |

All (71) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 1A    | 115 | G    |
| 1   | 1A    | 184 | A    |
| 1   | 1A    | 185 | A    |
| 1   | 1A    | 188 | A    |
| 1   | 1A    | 302 | A    |
| 1   | 1A    | 386 | U    |
| 1   | 1A    | 509 | A    |
| 1   | 1A    | 732 | A    |
| 1   | 1A    | 793 | A    |
| 1   | 1A    | 811 | A    |
| 1   | 1A    | 874 | U    |
| 1   | 1A    | 913 | A    |
| 1   | 1A    | 934 | A    |
| 1   | 1A    | 935 | C    |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | 1A    | 941    | U    |
| 1   | 1A    | 1019   | G    |
| 1   | 1A    | 1065   | U    |
| 1   | 1A    | 1067   | A    |
| 1   | 1A    | 1093   | G    |
| 1   | 1A    | 1116   | A    |
| 1   | 1A    | 1157   | A    |
| 1   | 1A    | 1201   | A    |
| 1   | 1A    | 1219   | A    |
| 1   | 1A    | 1220   | U    |
| 1   | 1A    | 1221   | G    |
| 1   | 1A    | 1255   | A    |
| 1   | 1A    | 1286   | U    |
| 1   | 1A    | 1466   | U    |
| 1   | 1A    | 1654   | A    |
| 1   | 1A    | 1700   | G    |
| 1   | 1A    | 2148   | A    |
| 1   | 1A    | 2227   | G    |
| 1   | 1A    | 2418   | U    |
| 1   | 1A    | 2434   | A    |
| 1   | 1A    | 2442   | A    |
| 1   | 1A    | 2623   | U    |
| 1   | 1A    | 2701   | U    |
| 1   | 1A    | 2769   | U    |
| 1   | 2A    | 195    | A    |
| 1   | 2A    | 196    | A    |
| 1   | 2A    | 266    | G    |
| 1   | 2A    | 271(M) | G    |
| 1   | 2A    | 277    | C    |
| 1   | 2A    | 746    | A    |
| 1   | 2A    | 752    | A    |
| 1   | 2A    | 764    | A    |
| 1   | 2A    | 827    | U    |
| 1   | 2A    | 840    | C    |
| 1   | 2A    | 856    | C    |
| 1   | 2A    | 974    | G    |
| 1   | 2A    | 1053   | C    |
| 1   | 2A    | 1065   | U    |
| 1   | 2A    | 1067   | A    |
| 1   | 2A    | 1073   | A    |
| 1   | 2A    | 1210   | A    |
| 1   | 2A    | 1399   | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 2A    | 1420 | U    |
| 1   | 2A    | 1442 | G    |
| 1   | 2A    | 1491 | G    |
| 1   | 2A    | 1608 | A    |
| 1   | 2A    | 1992 | G    |
| 1   | 2A    | 2126 | A    |
| 1   | 2A    | 2172 | U    |
| 1   | 2A    | 2206 | G    |
| 1   | 2A    | 2321 | G    |
| 1   | 2A    | 2406 | U    |
| 1   | 2A    | 2430 | A    |
| 1   | 2A    | 2585 | U    |
| 1   | 2A    | 2611 | U    |
| 1   | 2A    | 2689 | U    |
| 1   | 2A    | 2756 | U    |

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

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

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

| Mol | Type | Chain | Res  | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|------|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |      |      | Counts       | RMSZ | # $ Z  > 2$ | Counts      | RMSZ | # $ Z  > 2$ |
| 1   | PSU  | 1A    | 1933 | 1    | 15,21,22     | 2.05 | 5 (33%)     | 16,30,33    | 2.88 | 5 (31%)     |
| 1   | 5MU  | 1A    | 1937 | 1    | 13,22,23     | 1.26 | 1 (7%)      | 16,32,35    | 3.54 | 2 (12%)     |
| 1   | PSU  | 1A    | 1939 | 1,56 | 15,21,22     | 2.07 | 4 (26%)     | 16,30,33    | 2.98 | 5 (31%)     |
| 1   | OMC  | 1A    | 1942 | 1    | 15,22,23     | 2.33 | 6 (40%)     | 20,31,34    | 1.26 | 1 (5%)      |
| 1   | 5MU  | 1A    | 1961 | 1    | 13,22,23     | 1.25 | 1 (7%)      | 16,32,35    | 3.55 | 2 (12%)     |
| 1   | 5MC  | 1A    | 1964 | 1,56 | 14,22,23     | 0.78 | 0           | 17,32,35    | 0.83 | 1 (5%)      |
| 1   | 5MC  | 1A    | 1984 | 1,56 | 14,22,23     | 0.85 | 0           | 17,32,35    | 0.95 | 1 (5%)      |
| 1   | OMG  | 1A    | 2263 | 1,54 | 18,26,27     | 2.56 | 7 (38%)     | 21,38,41    | 2.23 | 6 (28%)     |
| 1   | 2MA  | 1A    | 2515 | 1,56 | 17,25,26     | 2.60 | 6 (35%)     | 18,37,40    | 4.27 | 4 (22%)     |
| 1   | OMU  | 1A    | 2564 | 1,56 | 14,22,23     | 7.79 | 8 (57%)     | 19,31,34    | 1.56 | 2 (10%)     |

| Mol | Type | Chain | Res  | Link  | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|-------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 1   | PSU  | 1A    | 2617 | 1     | 15,21,22     | 1.79 | 3 (20%)  | 16,30,33    | 2.79 | 4 (25%)  |
| 32  | 2MG  | 1a    | 1207 | 32    | 18,26,27     | 2.80 | 6 (33%)  | 21,38,41    | 3.11 | 9 (42%)  |
| 32  | 5MC  | 1a    | 1400 | 32    | 14,22,23     | 0.77 | 0        | 17,32,35    | 0.86 | 1 (5%)   |
| 32  | 4OC  | 1a    | 1402 | 32    | 15,23,24     | 2.14 | 6 (40%)  | 21,32,35    | 1.84 | 4 (19%)  |
| 32  | 5MC  | 1a    | 1404 | 32    | 14,22,23     | 0.87 | 0        | 17,32,35    | 0.84 | 1 (5%)   |
| 32  | 5MC  | 1a    | 1407 | 32    | 14,22,23     | 0.95 | 1 (7%)   | 17,32,35    | 0.99 | 1 (5%)   |
| 32  | UR3  | 1a    | 1498 | 32    | 13,22,23     | 1.90 | 3 (23%)  | 18,32,35    | 0.77 | 0        |
| 32  | MA6  | 1a    | 1518 | 32    | 18,26,27     | 0.94 | 2 (11%)  | 15,38,41    | 3.86 | 3 (20%)  |
| 32  | MA6  | 1a    | 1519 | 32    | 18,26,27     | 0.89 | 2 (11%)  | 15,38,41    | 3.80 | 3 (20%)  |
| 32  | PSU  | 1a    | 516  | 32    | 15,21,22     | 2.43 | 5 (33%)  | 16,30,33    | 3.40 | 5 (31%)  |
| 32  | 7MG  | 1a    | 527  | 32,56 | 20,26,27     | 3.04 | 7 (35%)  | 23,39,42    | 2.00 | 7 (30%)  |
| 32  | M2G  | 1a    | 966  | 32    | 18,27,28     | 2.93 | 5 (27%)  | 22,40,43    | 1.59 | 5 (22%)  |
| 32  | 5MC  | 1a    | 967  | 32    | 14,22,23     | 0.83 | 0        | 17,32,35    | 0.85 | 1 (5%)   |
| 43  | 0TD  | 1l    | 92   | 43    | 4,9,10       | 1.95 | 2 (50%)  | 4,11,13     | 2.97 | 3 (75%)  |
| 54  | 5MC  | 1x    | 32   | 54    | 14,22,23     | 0.93 | 0        | 17,32,35    | 0.82 | 1 (5%)   |
| 54  | 5MU  | 1x    | 54   | 54    | 13,22,23     | 1.22 | 1 (7%)   | 16,32,35    | 3.70 | 2 (12%)  |
| 54  | PSU  | 1x    | 55   | 54    | 15,21,22     | 2.07 | 4 (26%)  | 16,30,33    | 3.00 | 5 (31%)  |
| 54  | 4SU  | 1x    | 8    | 54    | 12,21,22     | 1.16 | 1 (8%)   | 15,30,33    | 1.79 | 1 (6%)   |
| 1   | PSU  | 2A    | 1911 | 1     | 15,21,22     | 2.06 | 4 (26%)  | 16,30,33    | 2.87 | 5 (31%)  |
| 1   | 5MU  | 2A    | 1915 | 1     | 13,22,23     | 1.29 | 1 (7%)   | 16,32,35    | 3.74 | 2 (12%)  |
| 1   | PSU  | 2A    | 1917 | 1     | 15,21,22     | 1.88 | 3 (20%)  | 16,30,33    | 2.90 | 5 (31%)  |
| 1   | OMC  | 2A    | 1920 | 1     | 15,22,23     | 2.30 | 6 (40%)  | 20,31,34    | 1.46 | 2 (10%)  |
| 1   | 5MU  | 2A    | 1939 | 1     | 13,22,23     | 1.44 | 1 (7%)   | 16,32,35    | 3.60 | 2 (12%)  |
| 1   | 5MC  | 2A    | 1942 | 1     | 14,22,23     | 0.89 | 0        | 17,32,35    | 0.92 | 1 (5%)   |
| 1   | 5MC  | 2A    | 1962 | 1,56  | 14,22,23     | 0.83 | 0        | 17,32,35    | 0.77 | 1 (5%)   |
| 1   | OMG  | 2A    | 2251 | 1,54  | 18,26,27     | 2.50 | 6 (33%)  | 21,38,41    | 2.76 | 4 (19%)  |
| 1   | 2MA  | 2A    | 2503 | 1,56  | 17,25,26     | 2.62 | 6 (35%)  | 18,37,40    | 3.86 | 4 (22%)  |
| 1   | OMU  | 2A    | 2552 | 1,56  | 14,22,23     | 7.83 | 8 (57%)  | 19,31,34    | 1.54 | 2 (10%)  |
| 1   | PSU  | 2A    | 2605 | 1     | 15,21,22     | 2.02 | 4 (26%)  | 16,30,33    | 2.95 | 5 (31%)  |
| 32  | 2MG  | 2a    | 1207 | 32    | 18,26,27     | 2.66 | 6 (33%)  | 21,38,41    | 2.70 | 7 (33%)  |
| 32  | 5MC  | 2a    | 1400 | 32    | 14,22,23     | 0.82 | 0        | 17,32,35    | 0.87 | 1 (5%)   |
| 32  | 4OC  | 2a    | 1402 | 32    | 15,23,24     | 2.09 | 6 (40%)  | 21,32,35    | 3.22 | 4 (19%)  |
| 32  | 5MC  | 2a    | 1404 | 32    | 14,22,23     | 1.03 | 1 (7%)   | 17,32,35    | 0.87 | 1 (5%)   |
| 32  | 5MC  | 2a    | 1407 | 32    | 14,22,23     | 0.92 | 0        | 17,32,35    | 0.85 | 1 (5%)   |
| 32  | UR3  | 2a    | 1498 | 32    | 13,22,23     | 2.09 | 3 (23%)  | 18,32,35    | 0.73 | 0        |



| Mol | Type | Chain | Res  | Link  | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|-------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 32  | MA6  | 2a    | 1518 | 32    | 18,26,27     | 0.94 | 2 (11%)  | 15,38,41    | 3.85 | 3 (20%)  |
| 32  | MA6  | 2a    | 1519 | 32    | 18,26,27     | 0.87 | 2 (11%)  | 15,38,41    | 3.65 | 3 (20%)  |
| 32  | PSU  | 2a    | 516  | 32    | 15,21,22     | 2.03 | 5 (33%)  | 16,30,33    | 3.13 | 5 (31%)  |
| 32  | 7MG  | 2a    | 527  | 32    | 20,26,27     | 3.23 | 7 (35%)  | 23,39,42    | 2.00 | 6 (26%)  |
| 32  | M2G  | 2a    | 966  | 32    | 18,27,28     | 3.04 | 6 (33%)  | 22,40,43    | 1.86 | 6 (27%)  |
| 32  | 5MC  | 2a    | 967  | 32    | 14,22,23     | 0.71 | 0        | 17,32,35    | 0.89 | 1 (5%)   |
| 43  | 0TD  | 2l    | 92   | 43    | 4,9,10       | 1.73 | 1 (25%)  | 4,11,13     | 2.40 | 2 (50%)  |
| 54  | 5MC  | 2x    | 32   | 54    | 14,22,23     | 0.79 | 0        | 17,32,35    | 0.81 | 1 (5%)   |
| 54  | 5MU  | 2x    | 54   | 54    | 13,22,23     | 1.42 | 1 (7%)   | 16,32,35    | 3.77 | 2 (12%)  |
| 54  | PSU  | 2x    | 55   | 54,56 | 15,21,22     | 2.10 | 3 (20%)  | 16,30,33    | 2.78 | 4 (25%)  |
| 54  | 4SU  | 2x    | 8    | 54    | 12,21,22     | 1.29 | 2 (16%)  | 15,30,33    | 2.33 | 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    | 1933 | 1     | -       | 0/7/25/26 | 0/2/2/2 |
| 1   | 5MU  | 1A    | 1937 | 1     | -       | 0/3/25/26 | 0/2/2/2 |
| 1   | PSU  | 1A    | 1939 | 1,56  | -       | 0/7/25/26 | 0/2/2/2 |
| 1   | OMC  | 1A    | 1942 | 1     | -       | 0/5/27/28 | 0/2/2/2 |
| 1   | 5MU  | 1A    | 1961 | 1     | -       | 0/3/25/26 | 0/2/2/2 |
| 1   | 5MC  | 1A    | 1964 | 1,56  | -       | 0/3/25/26 | 0/2/2/2 |
| 1   | 5MC  | 1A    | 1984 | 1,56  | -       | 0/3/25/26 | 0/2/2/2 |
| 1   | OMG  | 1A    | 2263 | 1,54  | -       | 0/5/27/28 | 0/3/3/3 |
| 1   | 2MA  | 1A    | 2515 | 1,56  | -       | 0/3/25/26 | 0/3/3/3 |
| 1   | OMU  | 1A    | 2564 | 1,56  | -       | 0/5/27/28 | 0/2/2/2 |
| 1   | PSU  | 1A    | 2617 | 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    | -       | 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 |

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| Mol | Type | Chain | Res  | Link  | Chirals | Torsions  | Rings   |
|-----|------|-------|------|-------|---------|-----------|---------|
| 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  | 5MC  | 1x    | 32   | 54    | -       | 0/3/25/26 | 0/2/2/2 |
| 54  | 5MU  | 1x    | 54   | 54    | -       | 0/3/25/26 | 0/2/2/2 |
| 54  | PSU  | 1x    | 55   | 54    | -       | 0/7/25/26 | 0/2/2/2 |
| 54  | 4SU  | 1x    | 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   | OMC  | 2A    | 1920 | 1     | -       | 0/5/27/28 | 0/2/2/2 |
| 1   | 5MU  | 2A    | 1939 | 1     | -       | 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 | 1,54  | -       | 0/5/27/28 | 0/3/3/3 |
| 1   | 2MA  | 2A    | 2503 | 1,56  | -       | 0/3/25/26 | 0/3/3/3 |
| 1   | OMU  | 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    | -       | 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    | -       | 0/3/25/26 | 0/2/2/2 |
| 43  | 0TD  | 2l    | 92   | 43    | -       | 0/2/12/14 | 0/0/0/0 |
| 54  | 5MC  | 2x    | 32   | 54    | -       | 0/3/25/26 | 0/2/2/2 |
| 54  | 5MU  | 2x    | 54   | 54    | -       | 0/3/25/26 | 0/2/2/2 |
| 54  | PSU  | 2x    | 55   | 54,56 | -       | 0/7/25/26 | 0/2/2/2 |
| 54  | 4SU  | 2x    | 8    | 54    | -       | 0/3/25/26 | 0/2/2/2 |

All (170) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|--------|-------------|----------|
| 1   | 2A    | 2552 | OMU  | C6-C5 | -12.32 | 1.11        | 1.38     |
| 1   | 1A    | 2564 | OMU  | C6-C5 | -12.24 | 1.11        | 1.38     |
| 1   | 2A    | 2552 | OMU  | C4-N3 | -11.52 | 1.12        | 1.33     |
| 1   | 1A    | 2564 | OMU  | C4-N3 | -11.33 | 1.12        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | 1A    | 2564 | OMU  | C3'-C2' | -8.50 | 1.33        | 1.53     |
| 1   | 2A    | 2552 | OMU  | C3'-C2' | -8.26 | 1.34        | 1.53     |
| 32  | 1a    | 516  | PSU  | C5-C1'  | -7.26 | 1.45        | 1.52     |
| 1   | 2A    | 2552 | OMU  | O4'-C4' | -6.24 | 1.30        | 1.45     |
| 1   | 1A    | 2564 | OMU  | O4'-C4' | -6.07 | 1.31        | 1.45     |
| 32  | 2a    | 516  | PSU  | C5-C1'  | -3.91 | 1.48        | 1.52     |
| 1   | 1A    | 1933 | PSU  | C5-C1'  | -3.71 | 1.49        | 1.52     |
| 1   | 2A    | 2605 | PSU  | C5-C1'  | -3.47 | 1.49        | 1.52     |
| 1   | 1A    | 2617 | PSU  | C6-C5   | -3.21 | 1.33        | 1.38     |
| 1   | 2A    | 2605 | PSU  | C6-C5   | -3.19 | 1.34        | 1.38     |
| 1   | 1A    | 1933 | PSU  | C6-C5   | -2.90 | 1.34        | 1.38     |
| 43  | 1l    | 92   | 0TD  | CB-SB   | -2.74 | 1.77        | 1.84     |
| 1   | 2A    | 1917 | PSU  | C6-C5   | -2.71 | 1.34        | 1.38     |
| 32  | 1a    | 516  | PSU  | O4'-C1' | -2.70 | 1.40        | 1.44     |
| 1   | 1A    | 1939 | PSU  | C5-C1'  | -2.64 | 1.49        | 1.52     |
| 32  | 2a    | 1402 | 4OC  | CM4-N4  | -2.54 | 1.40        | 1.45     |
| 1   | 1A    | 1939 | PSU  | C6-C5   | -2.50 | 1.34        | 1.38     |
| 32  | 2a    | 516  | PSU  | O4'-C1' | -2.49 | 1.40        | 1.44     |
| 54  | 2x    | 55   | PSU  | C6-C5   | -2.47 | 1.35        | 1.38     |
| 1   | 1A    | 2515 | 2MA  | C5-C4   | -2.43 | 1.35        | 1.40     |
| 1   | 1A    | 2263 | OMG  | C5-C4   | -2.43 | 1.35        | 1.40     |
| 43  | 2l    | 92   | 0TD  | CB-SB   | -2.41 | 1.78        | 1.84     |
| 32  | 1a    | 1402 | 4OC  | CM4-N4  | -2.40 | 1.40        | 1.45     |
| 32  | 2a    | 516  | PSU  | C6-C5   | -2.40 | 1.35        | 1.38     |
| 1   | 2A    | 1911 | PSU  | C6-C5   | -2.39 | 1.35        | 1.38     |
| 1   | 2A    | 2503 | 2MA  | C5-C4   | -2.38 | 1.35        | 1.40     |
| 32  | 1a    | 1518 | MA6  | C5-C4   | -2.36 | 1.35        | 1.40     |
| 1   | 2A    | 1911 | PSU  | C5-C1'  | -2.35 | 1.50        | 1.52     |
| 54  | 1x    | 55   | PSU  | C6-C5   | -2.29 | 1.35        | 1.38     |
| 32  | 1a    | 516  | PSU  | C6-C5   | -2.21 | 1.35        | 1.38     |
| 32  | 1a    | 1519 | MA6  | C5-C4   | -2.21 | 1.35        | 1.40     |
| 43  | 1l    | 92   | 0TD  | CA-N    | -2.19 | 1.41        | 1.47     |
| 1   | 2A    | 2251 | OMG  | C5-C4   | -2.15 | 1.35        | 1.40     |
| 32  | 2a    | 1519 | MA6  | C5-C4   | -2.13 | 1.35        | 1.40     |
| 32  | 2a    | 966  | M2G  | CM2-N2  | -2.11 | 1.40        | 1.45     |
| 32  | 2a    | 1518 | MA6  | C5-C4   | -2.11 | 1.35        | 1.40     |
| 32  | 1a    | 1407 | 5MC  | CM5-C5  | -2.09 | 1.46        | 1.51     |
| 1   | 1A    | 1933 | PSU  | O4'-C1' | -2.00 | 1.41        | 1.44     |
| 32  | 2a    | 1404 | 5MC  | C5-C4   | 2.05  | 1.44        | 1.41     |
| 54  | 1x    | 55   | PSU  | C2-N1   | 2.06  | 1.42        | 1.38     |
| 32  | 2a    | 1207 | 2MG  | C2-N3   | 2.08  | 1.42        | 1.34     |
| 1   | 1A    | 2263 | OMG  | C8-N7   | 2.13  | 1.38        | 1.34     |

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| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 32  | 2a    | 527  | 7MG  | C8-N9   | 2.14 | 1.48        | 1.45     |
| 32  | 1a    | 527  | 7MG  | C8-N9   | 2.14 | 1.48        | 1.45     |
| 32  | 1a    | 1207 | 2MG  | C2-N3   | 2.22 | 1.42        | 1.34     |
| 1   | 1A    | 2564 | OMU  | O2'-C2' | 2.22 | 1.48        | 1.42     |
| 32  | 1a    | 1518 | MA6  | C2-N3   | 2.23 | 1.36        | 1.32     |
| 1   | 1A    | 2617 | PSU  | C6-N1   | 2.24 | 1.39        | 1.34     |
| 1   | 1A    | 1933 | PSU  | C6-N1   | 2.27 | 1.39        | 1.34     |
| 54  | 2x    | 8    | 4SU  | C2-N3   | 2.29 | 1.42        | 1.38     |
| 32  | 2a    | 1519 | MA6  | C2-N3   | 2.32 | 1.36        | 1.32     |
| 1   | 2A    | 2605 | PSU  | C6-N1   | 2.33 | 1.39        | 1.34     |
| 1   | 2A    | 2251 | OMG  | C2-N2   | 2.36 | 1.39        | 1.34     |
| 32  | 1a    | 1519 | MA6  | C2-N3   | 2.37 | 1.36        | 1.32     |
| 1   | 1A    | 2263 | OMG  | C2-N2   | 2.50 | 1.39        | 1.34     |
| 32  | 2a    | 1518 | MA6  | C2-N3   | 2.51 | 1.36        | 1.32     |
| 1   | 1A    | 1942 | OMC  | C4-N3   | 2.58 | 1.40        | 1.35     |
| 32  | 2a    | 1498 | UR3  | C4-N3   | 2.64 | 1.42        | 1.38     |
| 1   | 2A    | 2552 | OMU  | O2'-C2' | 2.65 | 1.49        | 1.42     |
| 1   | 2A    | 1911 | PSU  | C6-N1   | 2.65 | 1.40        | 1.34     |
| 1   | 2A    | 1920 | OMC  | C4-N3   | 2.66 | 1.40        | 1.35     |
| 32  | 2a    | 1207 | 2MG  | C2-N1   | 2.70 | 1.44        | 1.34     |
| 32  | 1a    | 1207 | 2MG  | C2-N1   | 2.76 | 1.44        | 1.34     |
| 1   | 2A    | 1917 | PSU  | C6-N1   | 2.76 | 1.40        | 1.34     |
| 32  | 2a    | 1402 | 4OC  | C6-C5   | 2.80 | 1.44        | 1.38     |
| 1   | 1A    | 1939 | PSU  | C6-N1   | 2.80 | 1.40        | 1.34     |
| 32  | 2a    | 516  | PSU  | C6-N1   | 2.82 | 1.40        | 1.34     |
| 32  | 1a    | 1498 | UR3  | C4-N3   | 2.83 | 1.42        | 1.38     |
| 54  | 1x    | 8    | 4SU  | C5-C4   | 2.90 | 1.42        | 1.38     |
| 1   | 2A    | 2503 | 2MA  | C6-N1   | 2.91 | 1.40        | 1.34     |
| 32  | 1a    | 516  | PSU  | C4-N3   | 2.92 | 1.38        | 1.33     |
| 54  | 2x    | 55   | PSU  | C6-N1   | 2.93 | 1.40        | 1.34     |
| 32  | 1a    | 1402 | 4OC  | C4-N3   | 2.95 | 1.39        | 1.34     |
| 32  | 1a    | 516  | PSU  | C6-N1   | 2.96 | 1.40        | 1.34     |
| 54  | 1x    | 55   | PSU  | C6-N1   | 3.12 | 1.41        | 1.34     |
| 32  | 2a    | 1402 | 4OC  | C4-N3   | 3.13 | 1.40        | 1.34     |
| 1   | 1A    | 2515 | 2MA  | C6-N1   | 3.16 | 1.41        | 1.34     |
| 32  | 1a    | 527  | 7MG  | C2-N2   | 3.22 | 1.40        | 1.34     |
| 1   | 2A    | 1920 | OMC  | C5-C4   | 3.24 | 1.48        | 1.41     |
| 54  | 2x    | 8    | 4SU  | C5-C4   | 3.24 | 1.42        | 1.38     |
| 32  | 2a    | 1402 | 4OC  | C6-N1   | 3.28 | 1.40        | 1.35     |
| 54  | 1x    | 54   | 5MU  | C4-N3   | 3.30 | 1.39        | 1.33     |
| 32  | 1a    | 1402 | 4OC  | C2-N3   | 3.30 | 1.45        | 1.38     |
| 1   | 1A    | 1942 | OMC  | C5-C4   | 3.35 | 1.48        | 1.41     |

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| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 32  | 1a    | 1402 | 4OC  | C6-C5   | 3.38 | 1.45        | 1.38     |
| 32  | 2a    | 1207 | 2MG  | C6-N1   | 3.43 | 1.39        | 1.33     |
| 1   | 1A    | 1937 | 5MU  | C4-N3   | 3.45 | 1.39        | 1.33     |
| 1   | 2A    | 1920 | OMC  | C6-C5   | 3.47 | 1.45        | 1.38     |
| 32  | 1a    | 1207 | 2MG  | C6-N1   | 3.52 | 1.39        | 1.33     |
| 1   | 2A    | 1915 | 5MU  | C4-N3   | 3.58 | 1.39        | 1.33     |
| 1   | 1A    | 1942 | OMC  | C6-C5   | 3.60 | 1.45        | 1.38     |
| 32  | 2a    | 1402 | 4OC  | C2-N3   | 3.63 | 1.45        | 1.38     |
| 1   | 2A    | 1920 | OMC  | C2-N3   | 3.63 | 1.45        | 1.38     |
| 1   | 1A    | 1961 | 5MU  | C4-N3   | 3.65 | 1.39        | 1.33     |
| 1   | 2A    | 2251 | OMG  | C2-N1   | 3.66 | 1.42        | 1.35     |
| 32  | 2a    | 527  | 7MG  | C2-N2   | 3.66 | 1.41        | 1.34     |
| 1   | 2A    | 2552 | OMU  | C3'-C4' | 3.71 | 1.62        | 1.53     |
| 1   | 1A    | 1942 | OMC  | C2-N3   | 3.75 | 1.46        | 1.38     |
| 32  | 1a    | 1402 | 4OC  | C5-C4   | 3.82 | 1.48        | 1.39     |
| 32  | 1a    | 1207 | 2MG  | C6-C5   | 3.87 | 1.49        | 1.41     |
| 1   | 2A    | 1920 | OMC  | C6-N1   | 3.91 | 1.40        | 1.35     |
| 32  | 1a    | 1498 | UR3  | C6-C5   | 3.94 | 1.46        | 1.38     |
| 32  | 2a    | 1207 | 2MG  | C6-C5   | 3.99 | 1.49        | 1.41     |
| 1   | 1A    | 2564 | OMU  | C3'-C4' | 4.06 | 1.63        | 1.53     |
| 32  | 1a    | 527  | 7MG  | C6-N1   | 4.06 | 1.40        | 1.33     |
| 32  | 2a    | 1402 | 4OC  | C5-C4   | 4.09 | 1.48        | 1.39     |
| 32  | 1a    | 1402 | 4OC  | C6-N1   | 4.09 | 1.41        | 1.35     |
| 1   | 2A    | 2251 | OMG  | C6-C5   | 4.10 | 1.49        | 1.41     |
| 1   | 1A    | 2263 | OMG  | C2-N1   | 4.12 | 1.43        | 1.35     |
| 1   | 2A    | 1939 | 5MU  | C4-N3   | 4.14 | 1.40        | 1.33     |
| 32  | 2a    | 966  | M2G  | C6-N1   | 4.16 | 1.40        | 1.33     |
| 32  | 1a    | 527  | 7MG  | C2-N3   | 4.17 | 1.43        | 1.35     |
| 1   | 1A    | 1942 | OMC  | C6-N1   | 4.19 | 1.41        | 1.35     |
| 1   | 1A    | 1942 | OMC  | C4-N4   | 4.22 | 1.47        | 1.35     |
| 32  | 2a    | 1498 | UR3  | C6-C5   | 4.24 | 1.47        | 1.38     |
| 32  | 1a    | 527  | 7MG  | C2-N1   | 4.25 | 1.43        | 1.35     |
| 54  | 2x    | 54   | 5MU  | C4-N3   | 4.26 | 1.40        | 1.33     |
| 32  | 1a    | 966  | M2G  | C6-N1   | 4.27 | 1.40        | 1.33     |
| 32  | 2a    | 527  | 7MG  | C6-N1   | 4.35 | 1.40        | 1.33     |
| 1   | 1A    | 2515 | 2MA  | C2-N3   | 4.40 | 1.42        | 1.34     |
| 32  | 1a    | 1498 | UR3  | C6-N1   | 4.46 | 1.41        | 1.35     |
| 1   | 2A    | 2251 | OMG  | C6-N1   | 4.48 | 1.41        | 1.33     |
| 1   | 2A    | 1920 | OMC  | C4-N4   | 4.49 | 1.47        | 1.35     |
| 1   | 2A    | 2503 | 2MA  | C2-N3   | 4.61 | 1.42        | 1.34     |
| 32  | 2a    | 527  | 7MG  | C2-N3   | 4.63 | 1.44        | 1.35     |
| 32  | 2a    | 516  | PSU  | C4-N3   | 4.67 | 1.41        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | 1A    | 2263 | OMG  | C6-C5   | 4.67  | 1.50        | 1.41     |
| 1   | 1A    | 2617 | PSU  | C4-N3   | 4.70  | 1.41        | 1.33     |
| 32  | 2a    | 527  | 7MG  | C2-N1   | 4.74  | 1.44        | 1.35     |
| 1   | 1A    | 2515 | 2MA  | C4-N3   | 4.83  | 1.43        | 1.35     |
| 1   | 1A    | 2515 | 2MA  | C6-C5   | 4.85  | 1.49        | 1.40     |
| 1   | 2A    | 2503 | 2MA  | C6-C5   | 4.88  | 1.49        | 1.40     |
| 1   | 1A    | 2263 | OMG  | C6-N1   | 4.92  | 1.41        | 1.33     |
| 32  | 2a    | 966  | M2G  | C2-N1   | 4.97  | 1.43        | 1.34     |
| 1   | 2A    | 2503 | 2MA  | C2-N1   | 5.03  | 1.43        | 1.34     |
| 32  | 1a    | 966  | M2G  | C2-N1   | 5.15  | 1.43        | 1.34     |
| 32  | 1a    | 966  | M2G  | C6-C5   | 5.19  | 1.51        | 1.41     |
| 32  | 2a    | 966  | M2G  | C6-C5   | 5.25  | 1.51        | 1.41     |
| 32  | 2a    | 1498 | UR3  | C6-N1   | 5.26  | 1.42        | 1.35     |
| 1   | 1A    | 2515 | 2MA  | C2-N1   | 5.27  | 1.43        | 1.34     |
| 1   | 2A    | 2503 | 2MA  | C4-N3   | 5.34  | 1.44        | 1.35     |
| 1   | 1A    | 1933 | PSU  | C4-N3   | 5.38  | 1.42        | 1.33     |
| 1   | 2A    | 2605 | PSU  | C4-N3   | 5.40  | 1.42        | 1.33     |
| 1   | 2A    | 1917 | PSU  | C4-N3   | 5.44  | 1.42        | 1.33     |
| 32  | 1a    | 966  | M2G  | C2-N2   | 5.44  | 1.44        | 1.34     |
| 32  | 2a    | 1207 | 2MG  | C4-N3   | 5.49  | 1.44        | 1.35     |
| 1   | 1A    | 2263 | OMG  | C4-N3   | 5.70  | 1.44        | 1.35     |
| 32  | 2a    | 966  | M2G  | C2-N2   | 5.74  | 1.44        | 1.34     |
| 32  | 1a    | 1207 | 2MG  | C4-N3   | 5.84  | 1.45        | 1.35     |
| 1   | 1A    | 1939 | PSU  | C4-N3   | 5.87  | 1.43        | 1.33     |
| 54  | 1x    | 55   | PSU  | C4-N3   | 6.06  | 1.44        | 1.33     |
| 1   | 2A    | 1911 | PSU  | C4-N3   | 6.12  | 1.44        | 1.33     |
| 1   | 2A    | 2251 | OMG  | C4-N3   | 6.47  | 1.46        | 1.35     |
| 54  | 2x    | 55   | PSU  | C4-N3   | 6.52  | 1.44        | 1.33     |
| 32  | 1a    | 966  | M2G  | C4-N3   | 6.64  | 1.46        | 1.35     |
| 32  | 2a    | 1207 | 2MG  | C2-N2   | 7.10  | 1.42        | 1.34     |
| 32  | 2a    | 527  | 7MG  | C6-C5   | 7.19  | 1.51        | 1.41     |
| 32  | 1a    | 527  | 7MG  | C6-C5   | 7.27  | 1.51        | 1.41     |
| 32  | 2a    | 966  | M2G  | C4-N3   | 7.37  | 1.47        | 1.35     |
| 32  | 1a    | 1207 | 2MG  | C2-N2   | 7.58  | 1.43        | 1.34     |
| 32  | 1a    | 527  | 7MG  | C4-N3   | 7.76  | 1.44        | 1.34     |
| 32  | 2a    | 527  | 7MG  | C4-N3   | 8.55  | 1.45        | 1.34     |
| 1   | 1A    | 2564 | OMU  | O4'-C1' | 10.79 | 1.56        | 1.41     |
| 1   | 2A    | 2552 | OMU  | O4'-C1' | 11.26 | 1.57        | 1.41     |
| 1   | 2A    | 2552 | OMU  | C6-N1   | 17.70 | 1.58        | 1.35     |
| 1   | 1A    | 2564 | OMU  | C6-N1   | 17.86 | 1.58        | 1.35     |

All (166) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 32  | 2a    | 1402 | 4OC  | CM4-N4-C4   | -12.60 | 112.25      | 122.87   |
| 32  | 2a    | 1518 | MA6  | N3-C2-N1    | -10.92 | 120.29      | 128.87   |
| 54  | 2x    | 54   | 5MU  | C5-C4-N3    | -10.75 | 116.32      | 125.35   |
| 32  | 2a    | 1519 | MA6  | N3-C2-N1    | -10.70 | 120.47      | 128.87   |
| 32  | 1a    | 1518 | MA6  | N3-C2-N1    | -10.60 | 120.55      | 128.87   |
| 32  | 1a    | 1519 | MA6  | N3-C2-N1    | -10.56 | 120.58      | 128.87   |
| 1   | 2A    | 1939 | 5MU  | C5-C4-N3    | -10.53 | 116.51      | 125.35   |
| 54  | 1x    | 54   | 5MU  | C5-C4-N3    | -10.40 | 116.62      | 125.35   |
| 32  | 1a    | 1207 | 2MG  | C1'-N9-C4   | -10.40 | 115.20      | 126.81   |
| 1   | 2A    | 1915 | 5MU  | C5-C4-N3    | -10.31 | 116.70      | 125.35   |
| 1   | 1A    | 1961 | 5MU  | C5-C4-N3    | -9.88  | 117.05      | 125.35   |
| 1   | 1A    | 1937 | 5MU  | C5-C4-N3    | -9.79  | 117.13      | 125.35   |
| 32  | 1a    | 1518 | MA6  | C1'-N9-C4   | -9.70  | 115.98      | 126.81   |
| 32  | 1a    | 1519 | MA6  | C1'-N9-C4   | -9.35  | 116.37      | 126.81   |
| 32  | 2a    | 1518 | MA6  | C1'-N9-C4   | -9.27  | 116.47      | 126.81   |
| 54  | 2x    | 8    | 4SU  | C5-C4-N3    | -8.72  | 114.31      | 123.56   |
| 32  | 2a    | 1207 | 2MG  | C1'-N9-C4   | -8.59  | 117.22      | 126.81   |
| 32  | 2a    | 1519 | MA6  | C1'-N9-C4   | -8.27  | 117.58      | 126.81   |
| 54  | 1x    | 8    | 4SU  | C5-C4-N3    | -6.69  | 116.47      | 123.56   |
| 32  | 1a    | 1402 | 4OC  | CM4-N4-C4   | -6.39  | 117.48      | 122.87   |
| 32  | 1a    | 516  | PSU  | C4-C5-C1'   | -5.88  | 111.31      | 121.22   |
| 1   | 1A    | 2263 | OMG  | N3-C2-N1    | -5.68  | 119.82      | 127.56   |
| 1   | 2A    | 2251 | OMG  | N3-C2-N1    | -5.48  | 120.11      | 127.56   |
| 32  | 1a    | 527  | 7MG  | C5-C4-N3    | -5.30  | 121.34      | 126.74   |
| 32  | 2a    | 527  | 7MG  | C5-C4-N3    | -5.09  | 121.56      | 126.74   |
| 32  | 2a    | 516  | PSU  | C4-C5-C1'   | -4.25  | 114.06      | 121.22   |
| 32  | 1a    | 1207 | 2MG  | N3-C2-N1    | -4.10  | 120.05      | 126.19   |
| 1   | 1A    | 2564 | OMU  | C4'-O4'-C1' | -4.06  | 105.34      | 109.64   |
| 32  | 1a    | 516  | PSU  | C5-C6-N1    | -3.94  | 118.89      | 124.38   |
| 32  | 2a    | 1207 | 2MG  | N3-C2-N1    | -3.88  | 120.38      | 126.19   |
| 32  | 2a    | 527  | 7MG  | N1-C2-N3    | -3.58  | 119.67      | 125.51   |
| 32  | 1a    | 516  | PSU  | C5-C1'-C2'  | -3.55  | 109.40      | 115.44   |
| 32  | 2a    | 1207 | 2MG  | C5-C6-N1    | -3.55  | 118.88      | 123.52   |
| 43  | 1l    | 92   | 0TD  | CB-CA-N     | -3.43  | 102.96      | 109.83   |
| 32  | 2a    | 966  | M2G  | N3-C2-N1    | -3.41  | 120.56      | 126.35   |
| 32  | 2a    | 516  | PSU  | C5-C6-N1    | -3.24  | 119.86      | 124.38   |
| 32  | 1a    | 527  | 7MG  | N1-C2-N3    | -3.24  | 120.22      | 125.51   |
| 1   | 1A    | 1939 | PSU  | C5-C1'-C2'  | -3.18  | 110.04      | 115.44   |
| 32  | 1a    | 966  | M2G  | C5-C6-N1    | -3.17  | 119.38      | 123.52   |
| 32  | 1a    | 966  | M2G  | N3-C2-N1    | -3.03  | 121.21      | 126.35   |
| 32  | 1a    | 1207 | 2MG  | C5-C6-N1    | -3.02  | 119.57      | 123.52   |
| 54  | 1x    | 55   | PSU  | C4-C5-C1'   | -3.02  | 116.14      | 121.22   |
| 1   | 2A    | 2552 | OMU  | C4'-O4'-C1' | -2.96  | 106.51      | 109.64   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | 1A    | 2263 | OMG  | C5-C6-N1    | -2.93 | 119.69      | 123.52   |
| 1   | 1A    | 2515 | 2MA  | N3-C2-N1    | -2.92 | 119.86      | 125.60   |
| 1   | 1A    | 1933 | PSU  | C5-C1'-C2'  | -2.82 | 110.65      | 115.44   |
| 1   | 2A    | 1917 | PSU  | C5-C1'-C2'  | -2.78 | 110.72      | 115.44   |
| 32  | 2a    | 527  | 7MG  | C5-C6-N1    | -2.77 | 119.26      | 123.39   |
| 32  | 2a    | 516  | PSU  | C5-C1'-C2'  | -2.77 | 110.73      | 115.44   |
| 1   | 1A    | 2617 | PSU  | C5-C6-N1    | -2.77 | 120.52      | 124.38   |
| 43  | 2l    | 92   | 0TD  | CB-CA-N     | -2.70 | 104.42      | 109.83   |
| 32  | 1a    | 527  | 7MG  | C5-C6-N1    | -2.65 | 119.44      | 123.39   |
| 32  | 2a    | 966  | M2G  | C5-C6-N1    | -2.64 | 120.08      | 123.52   |
| 1   | 2A    | 2605 | PSU  | C5-C1'-C2'  | -2.61 | 111.01      | 115.44   |
| 1   | 2A    | 2503 | 2MA  | N3-C2-N1    | -2.59 | 120.52      | 125.60   |
| 1   | 2A    | 1917 | PSU  | C5-C6-N1    | -2.56 | 120.81      | 124.38   |
| 32  | 2a    | 1402 | 4OC  | C5-C4-N4    | -2.55 | 115.72      | 121.15   |
| 1   | 1A    | 1939 | PSU  | C5-C6-N1    | -2.55 | 120.83      | 124.38   |
| 1   | 1A    | 1939 | PSU  | C4-C5-C1'   | -2.52 | 116.98      | 121.22   |
| 1   | 1A    | 2263 | OMG  | C6-C5-C4    | -2.48 | 118.03      | 120.86   |
| 1   | 1A    | 1933 | PSU  | C5-C6-N1    | -2.42 | 121.01      | 124.38   |
| 1   | 2A    | 2605 | PSU  | C5-C6-N1    | -2.41 | 121.03      | 124.38   |
| 54  | 1x    | 55   | PSU  | C5-C6-N1    | -2.38 | 121.07      | 124.38   |
| 1   | 2A    | 1917 | PSU  | C4-C5-C1'   | -2.36 | 117.25      | 121.22   |
| 54  | 2x    | 55   | PSU  | C5-C6-N1    | -2.36 | 121.09      | 124.38   |
| 1   | 2A    | 1911 | PSU  | C4-C5-C1'   | -2.33 | 117.30      | 121.22   |
| 1   | 1A    | 1933 | PSU  | C4-C5-C1'   | -2.32 | 117.31      | 121.22   |
| 1   | 2A    | 2251 | OMG  | C5-C6-N1    | -2.30 | 120.52      | 123.52   |
| 32  | 1a    | 966  | M2G  | CM2-N2-C2   | -2.21 | 119.11      | 121.34   |
| 54  | 2x    | 55   | PSU  | C4-C5-C1'   | -2.19 | 117.53      | 121.22   |
| 1   | 2A    | 2605 | PSU  | C4-C5-C1'   | -2.17 | 117.56      | 121.22   |
| 43  | 1l    | 92   | 0TD  | O-C-CA      | -2.15 | 119.81      | 125.69   |
| 1   | 2A    | 1911 | PSU  | C5-C6-N1    | -2.12 | 121.42      | 124.38   |
| 1   | 1A    | 2617 | PSU  | C4-C5-C1'   | -2.10 | 117.68      | 121.22   |
| 1   | 2A    | 1911 | PSU  | C5-C1'-C2'  | -2.05 | 111.95      | 115.44   |
| 32  | 1a    | 1207 | 2MG  | CM2-N2-C2   | -2.04 | 120.74      | 123.03   |
| 54  | 1x    | 55   | PSU  | C5-C1'-C2'  | -2.03 | 111.99      | 115.44   |
| 32  | 2a    | 966  | M2G  | CM2-N2-C2   | -2.01 | 119.32      | 121.34   |
| 32  | 2a    | 1407 | 5MC  | C5-C4-N3    | 2.02  | 124.69      | 121.26   |
| 32  | 2a    | 1404 | 5MC  | C5-C4-N3    | 2.03  | 124.70      | 121.26   |
| 32  | 1a    | 1207 | 2MG  | O3'-C3'-C2' | 2.13  | 118.75      | 111.86   |
| 32  | 2a    | 1207 | 2MG  | N2-C2-N1    | 2.14  | 119.42      | 116.94   |
| 1   | 2A    | 1962 | 5MC  | C5-C4-N3    | 2.15  | 124.91      | 121.26   |
| 54  | 1x    | 32   | 5MC  | C5-C4-N3    | 2.15  | 124.91      | 121.26   |
| 32  | 1a    | 527  | 7MG  | C8-N9-C1'   | 2.16  | 128.92      | 122.43   |

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| Mol | Chain | Res  | Type | Atoms       | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|------|-------------|----------|
| 32  | 2a    | 1402 | 4OC  | C2-N3-C4    | 2.19 | 118.21      | 115.43   |
| 32  | 1a    | 1207 | 2MG  | N2-C2-N1    | 2.20 | 119.49      | 116.94   |
| 32  | 1a    | 966  | M2G  | N1-C2-N2    | 2.20 | 119.54      | 117.14   |
| 32  | 1a    | 1404 | 5MC  | C5-C4-N3    | 2.20 | 125.00      | 121.26   |
| 32  | 1a    | 1407 | 5MC  | C5-C4-N3    | 2.21 | 125.02      | 121.26   |
| 54  | 2x    | 32   | 5MC  | C5-C4-N3    | 2.25 | 125.08      | 121.26   |
| 32  | 1a    | 1402 | 4OC  | CM2-O2'-C2' | 2.28 | 120.98      | 114.58   |
| 1   | 2A    | 1942 | 5MC  | C5-C4-N3    | 2.29 | 125.16      | 121.26   |
| 32  | 2a    | 527  | 7MG  | N2-C2-N1    | 2.32 | 121.02      | 117.20   |
| 32  | 1a    | 1400 | 5MC  | C5-C4-N3    | 2.32 | 125.20      | 121.26   |
| 32  | 1a    | 1402 | 4OC  | C6-C5-C4    | 2.36 | 118.35      | 117.42   |
| 32  | 2a    | 966  | M2G  | C1'-N9-C4   | 2.38 | 129.46      | 126.81   |
| 32  | 1a    | 967  | 5MC  | C5-C4-N3    | 2.40 | 125.34      | 121.26   |
| 32  | 2a    | 1400 | 5MC  | C5-C4-N3    | 2.41 | 125.36      | 121.26   |
| 1   | 1A    | 1964 | 5MC  | C5-C4-N3    | 2.45 | 125.41      | 121.26   |
| 32  | 2a    | 967  | 5MC  | C5-C4-N3    | 2.46 | 125.44      | 121.26   |
| 1   | 2A    | 1917 | PSU  | O4'-C1'-C2' | 2.46 | 107.35      | 104.69   |
| 1   | 2A    | 1920 | OMC  | N4-C4-N3    | 2.52 | 120.91      | 116.50   |
| 1   | 1A    | 1984 | 5MC  | C5-C4-N3    | 2.53 | 125.56      | 121.26   |
| 32  | 1a    | 527  | 7MG  | N2-C2-N1    | 2.54 | 121.39      | 117.20   |
| 1   | 1A    | 2617 | PSU  | O4'-C1'-C2' | 2.54 | 107.44      | 104.69   |
| 1   | 2A    | 2605 | PSU  | O4'-C1'-C2' | 2.65 | 107.55      | 104.69   |
| 54  | 1x    | 55   | PSU  | O4'-C1'-C2' | 2.69 | 107.60      | 104.69   |
| 32  | 2a    | 527  | 7MG  | C5-C4-N9    | 2.69 | 110.59      | 106.25   |
| 54  | 2x    | 55   | PSU  | O4'-C1'-C2' | 2.78 | 107.69      | 104.69   |
| 32  | 2a    | 1207 | 2MG  | N2-C2-N3    | 2.80 | 120.19      | 116.94   |
| 1   | 2A    | 2503 | 2MA  | CM2-C2-N1   | 2.88 | 122.11      | 117.20   |
| 1   | 1A    | 1939 | PSU  | O4'-C1'-C2' | 2.90 | 107.83      | 104.69   |
| 1   | 2A    | 1911 | PSU  | O4'-C1'-C2' | 3.01 | 107.94      | 104.69   |
| 1   | 2A    | 2251 | OMG  | C6-N1-C2    | 3.02 | 119.42      | 115.88   |
| 32  | 1a    | 1207 | 2MG  | N2-C2-N3    | 3.03 | 120.46      | 116.94   |
| 1   | 1A    | 1933 | PSU  | O4'-C1'-C2' | 3.13 | 108.08      | 104.69   |
| 1   | 1A    | 2263 | OMG  | N2-C2-N1    | 3.20 | 122.48      | 117.20   |
| 32  | 1a    | 527  | 7MG  | C5-C4-N9    | 3.22 | 111.44      | 106.25   |
| 32  | 1a    | 1207 | 2MG  | C6-N1-C2    | 3.40 | 120.11      | 115.24   |
| 43  | 2l    | 92   | 0TD  | CSB-SB-CB   | 3.48 | 107.94      | 101.44   |
| 32  | 2a    | 1207 | 2MG  | C6-N1-C2    | 3.55 | 120.32      | 115.24   |
| 32  | 1a    | 1519 | MA6  | C2-N1-C6    | 3.58 | 120.09      | 111.64   |
| 32  | 1a    | 1518 | MA6  | C2-N1-C6    | 3.59 | 120.10      | 111.64   |
| 1   | 1A    | 2263 | OMG  | C6-N1-C2    | 3.60 | 120.10      | 115.88   |
| 32  | 1a    | 516  | PSU  | O4'-C1'-C2' | 3.60 | 108.58      | 104.69   |
| 32  | 2a    | 1519 | MA6  | C2-N1-C6    | 3.60 | 120.14      | 111.64   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 32  | 2a    | 1518 | MA6  | C2-N1-C6    | 3.65  | 120.25      | 111.64   |
| 32  | 2a    | 516  | PSU  | O4'-C1'-C2' | 3.65  | 108.64      | 104.69   |
| 32  | 1a    | 1402 | 4OC  | C2-N3-C4    | 3.71  | 120.15      | 115.43   |
| 32  | 1a    | 966  | M2G  | C2-N3-C4    | 3.88  | 119.24      | 114.99   |
| 1   | 1A    | 1942 | OMC  | C6-C5-C4    | 4.11  | 119.05      | 117.44   |
| 43  | 1l    | 92   | 0TD  | CSB-SB-CB   | 4.11  | 109.13      | 101.44   |
| 1   | 1A    | 2515 | 2MA  | CM2-C2-N1   | 4.19  | 124.35      | 117.20   |
| 32  | 1a    | 527  | 7MG  | C6-N1-C2    | 4.23  | 120.84      | 115.88   |
| 32  | 2a    | 966  | M2G  | N3-C2-N2    | 4.24  | 121.81      | 117.14   |
| 32  | 2a    | 1207 | 2MG  | C2-N3-C4    | 4.44  | 119.86      | 114.99   |
| 32  | 1a    | 1207 | 2MG  | C2-N3-C4    | 4.55  | 119.98      | 114.99   |
| 32  | 2a    | 527  | 7MG  | C6-N1-C2    | 4.62  | 121.30      | 115.88   |
| 1   | 1A    | 2564 | OMU  | C4-N3-C2    | 4.77  | 119.24      | 114.21   |
| 32  | 2a    | 966  | M2G  | C2-N3-C4    | 4.88  | 120.34      | 114.99   |
| 1   | 2A    | 1920 | OMC  | C6-C5-C4    | 5.10  | 119.43      | 117.44   |
| 1   | 2A    | 2552 | OMU  | C4-N3-C2    | 5.17  | 119.66      | 114.21   |
| 1   | 1A    | 2263 | OMG  | C1'-N9-C4   | 5.48  | 132.92      | 126.81   |
| 1   | 2A    | 2503 | 2MA  | C2-N3-C4    | 5.62  | 118.00      | 115.29   |
| 32  | 2a    | 1402 | 4OC  | C6-C5-C4    | 6.50  | 119.97      | 117.42   |
| 1   | 1A    | 2515 | 2MA  | C2-N3-C4    | 7.31  | 118.81      | 115.29   |
| 1   | 2A    | 1939 | 5MU  | C4-N3-C2    | 9.53  | 123.11      | 115.16   |
| 1   | 1A    | 1961 | 5MU  | C4-N3-C2    | 9.82  | 123.36      | 115.16   |
| 1   | 1A    | 2617 | PSU  | C4-N3-C2    | 9.83  | 123.36      | 115.16   |
| 54  | 2x    | 55   | PSU  | C4-N3-C2    | 9.84  | 123.36      | 115.16   |
| 1   | 1A    | 1937 | 5MU  | C4-N3-C2    | 9.89  | 123.41      | 115.16   |
| 1   | 1A    | 1933 | PSU  | C4-N3-C2    | 10.00 | 123.50      | 115.16   |
| 32  | 2a    | 516  | PSU  | C4-N3-C2    | 10.08 | 123.56      | 115.16   |
| 1   | 2A    | 1917 | PSU  | C4-N3-C2    | 10.12 | 123.61      | 115.16   |
| 1   | 2A    | 2251 | OMG  | C1'-N9-C4   | 10.18 | 138.16      | 126.81   |
| 54  | 2x    | 54   | 5MU  | C4-N3-C2    | 10.19 | 123.66      | 115.16   |
| 1   | 2A    | 1911 | PSU  | C4-N3-C2    | 10.21 | 123.68      | 115.16   |
| 32  | 1a    | 516  | PSU  | C4-N3-C2    | 10.27 | 123.72      | 115.16   |
| 54  | 1x    | 54   | 5MU  | C4-N3-C2    | 10.31 | 123.76      | 115.16   |
| 1   | 1A    | 1939 | PSU  | C4-N3-C2    | 10.31 | 123.76      | 115.16   |
| 1   | 2A    | 2605 | PSU  | C4-N3-C2    | 10.35 | 123.80      | 115.16   |
| 1   | 2A    | 1915 | 5MU  | C4-N3-C2    | 10.48 | 123.90      | 115.16   |
| 54  | 1x    | 55   | PSU  | C4-N3-C2    | 10.61 | 124.01      | 115.16   |
| 1   | 2A    | 2503 | 2MA  | C1'-N9-C4   | 14.72 | 143.23      | 126.81   |
| 1   | 1A    | 2515 | 2MA  | C1'-N9-C4   | 15.64 | 144.26      | 126.81   |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 14 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 1   | 1A    | 1937 | 5MU  | 1       | 0            |
| 1   | 1A    | 1961 | 5MU  | 1       | 0            |
| 1   | 1A    | 2515 | 2MA  | 1       | 0            |
| 1   | 1A    | 2564 | OMU  | 2       | 0            |
| 1   | 2A    | 1915 | 5MU  | 5       | 0            |
| 1   | 2A    | 2251 | OMG  | 1       | 0            |
| 1   | 2A    | 2503 | 2MA  | 1       | 0            |
| 1   | 2A    | 2552 | OMU  | 2       | 0            |

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 2719 ligands modelled in this entry, 2717 are monoatomic - leaving 2 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 58  | SF4  | 1d    | 501 | 35   | 0,12,12      | 0.00 | -           | 0,24,24     | 0.00 | -           |
| 58  | SF4  | 2d    | 501 | 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  | SF4  | 1d    | 501 | 35   | -       | 0/0/48/48 | 0/6/5/5 |
| 58  | SF4  | 2d    | 501 | 35   | -       | 0/0/48/48 | 0/6/5/5 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 1   | 1A    | 2861/2915 (98%) | 0.52   | 241 (8%) 14 6 | 6, 22, 80, 93         | 0     |
| 1   | 2A    | 2856/2915 (97%) | 0.67   | 270 (9%) 10 5 | 19, 41, 80, 92        | 0     |
| 2   | 1B    | 120/120 (100%)  | 0.22   | 2 (1%) 73 63  | 18, 35, 49, 69        | 0     |
| 2   | 2B    | 120/120 (100%)  | 0.71   | 11 (9%) 11 5  | 43, 60, 69, 73        | 0     |
| 3   | 1D    | 275/275 (100%)  | -0.28  | 0 100 100     | 7, 23, 36, 52         | 0     |
| 3   | 2D    | 275/275 (100%)  | -0.12  | 0 100 100     | 19, 36, 47, 63        | 0     |
| 4   | 1E    | 204/204 (100%)  | -0.21  | 0 100 100     | 7, 29, 47, 56         | 0     |
| 4   | 2E    | 204/204 (100%)  | -0.03  | 1 (0%) 91 88  | 19, 41, 55, 63        | 0     |
| 5   | 1F    | 203/203 (100%)  | -0.18  | 3 (1%) 76 68  | 7, 28, 53, 70         | 0     |
| 5   | 2F    | 203/203 (100%)  | -0.00  | 1 (0%) 91 88  | 24, 50, 63, 73        | 0     |
| 6   | 1G    | 181/181 (100%)  | -0.10  | 0 100 100     | 28, 44, 55, 69        | 0     |
| 6   | 2G    | 181/181 (100%)  | 0.82   | 30 (16%) 2 1  | 56, 65, 74, 77        | 0     |
| 7   | 1H    | 174/174 (100%)  | -0.11  | 0 100 100     | 23, 38, 49, 54        | 0     |
| 7   | 2H    | 173/174 (99%)   | 0.95   | 34 (19%) 1 1  | 50, 62, 69, 71        | 0     |
| 8   | 1I    | 147/147 (100%)  | 0.49   | 8 (5%) 29 19  | 31, 54, 66, 70        | 0     |
| 8   | 2I    | 146/147 (99%)   | 0.55   | 12 (8%) 14 7  | 39, 58, 68, 76        | 0     |
| 9   | 1N    | 140/140 (100%)  | -0.23  | 1 (0%) 89 84  | 14, 26, 44, 58        | 0     |
| 9   | 2N    | 140/140 (100%)  | -0.00  | 1 (0%) 89 84  | 28, 47, 59, 63        | 0     |
| 10  | 1O    | 122/122 (100%)  | -0.18  | 0 100 100     | 14, 26, 41, 49        | 0     |
| 10  | 2O    | 122/122 (100%)  | -0.03  | 1 (0%) 87 81  | 30, 40, 51, 56        | 0     |
| 11  | 1P    | 149/149 (100%)  | 0.10   | 3 (2%) 68 58  | 7, 32, 48, 64         | 0     |
| 11  | 2P    | 149/149 (100%)  | 0.39   | 6 (4%) 42 30  | 24, 50, 64, 71        | 0     |
| 12  | 1Q    | 141/141 (100%)  | -0.15  | 0 100 100     | 14, 26, 42, 59        | 0     |
| 12  | 2Q    | 141/141 (100%)  | -0.00  | 1 (0%) 89 84  | 31, 47, 57, 65        | 0     |

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| Mol | Chain | Analysed       | <RSRZ> | #RSRZ>2      | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|----------------|--------|--------------|-----------------------|-------|
| 13  | 1R    | 118/118 (100%) | -0.26  | 0 100 100    | 14, 22, 36, 47        | 0     |
| 13  | 2R    | 118/118 (100%) | -0.16  | 0 100 100    | 25, 37, 46, 55        | 0     |
| 14  | 1S    | 110/110 (100%) | 0.12   | 0 100 100    | 24, 36, 45, 51        | 0     |
| 14  | 2S    | 110/110 (100%) | 0.79   | 10 (9%) 11 6 | 46, 55, 62, 66        | 0     |
| 15  | 1T    | 131/131 (100%) | 0.07   | 2 (1%) 76 68 | 20, 33, 52, 64        | 0     |
| 15  | 2T    | 131/131 (100%) | 0.09   | 4 (3%) 52 40 | 36, 44, 59, 65        | 0     |
| 16  | 1U    | 116/116 (100%) | -0.20  | 0 100 100    | 9, 17, 35, 49         | 0     |
| 16  | 2U    | 116/116 (100%) | 0.44   | 5 (4%) 39 27 | 26, 45, 55, 66        | 0     |
| 17  | 1V    | 101/101 (100%) | -0.20  | 1 (0%) 84 77 | 8, 29, 44, 54         | 0     |
| 17  | 2V    | 101/101 (100%) | 0.44   | 5 (4%) 32 21 | 32, 51, 59, 67        | 0     |
| 18  | 1W    | 112/112 (100%) | -0.29  | 0 100 100    | 10, 17, 36, 66        | 0     |
| 18  | 2W    | 112/112 (100%) | -0.05  | 2 (1%) 71 61 | 25, 34, 48, 60        | 0     |
| 19  | 1X    | 95/95 (100%)   | -0.17  | 0 100 100    | 13, 24, 43, 59        | 0     |
| 19  | 2X    | 95/95 (100%)   | 0.06   | 1 (1%) 82 74 | 35, 44, 57, 60        | 0     |
| 20  | 1Y    | 107/107 (100%) | -0.29  | 0 100 100    | 24, 34, 49, 61        | 0     |
| 20  | 2Y    | 107/107 (100%) | 0.31   | 5 (4%) 35 24 | 44, 54, 62, 73        | 0     |
| 21  | 1Z    | 203/203 (100%) | 0.57   | 15 (7%) 17 9 | 28, 47, 62, 78        | 0     |
| 21  | 2Z    | 201/203 (99%)  | 0.78   | 25 (12%) 5 2 | 46, 60, 68, 71        | 0     |
| 22  | 10    | 77/77 (100%)   | 0.10   | 1 (1%) 79 71 | 17, 23, 37, 41        | 0     |
| 22  | 20    | 77/77 (100%)   | 0.37   | 3 (3%) 43 31 | 39, 45, 54, 63        | 0     |
| 23  | 11    | 97/97 (100%)   | 0.26   | 8 (8%) 14 7  | 11, 31, 54, 58        | 0     |
| 23  | 21    | 97/97 (100%)   | 0.17   | 5 (5%) 31 20 | 28, 40, 58, 64        | 0     |
| 24  | 12    | 70/70 (100%)   | -0.17  | 0 100 100    | 24, 34, 46, 56        | 0     |
| 24  | 22    | 70/70 (100%)   | 0.06   | 1 (1%) 78 69 | 42, 53, 63, 64        | 0     |
| 25  | 13    | 59/59 (100%)   | -0.14  | 0 100 100    | 15, 26, 49, 59        | 0     |
| 25  | 23    | 59/59 (100%)   | 0.42   | 5 (8%) 13 6  | 37, 46, 57, 63        | 0     |
| 26  | 14    | 69/69 (100%)   | 0.82   | 11 (15%) 3 1 | 35, 60, 72, 81        | 0     |
| 26  | 24    | 69/69 (100%)   | 2.01   | 31 (44%) 0 0 | 64, 72, 81, 84        | 0     |
| 27  | 15    | 59/59 (100%)   | -0.22  | 0 100 100    | 8, 23, 42, 51         | 0     |
| 27  | 25    | 59/59 (100%)   | -0.11  | 2 (3%) 49 36 | 23, 38, 52, 58        | 0     |
| 28  | 16    | 53/53 (100%)   | 0.11   | 0 100 100    | 24, 29, 41, 50        | 0     |

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| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 28  | 26    | 53/53 (100%)    | 0.44   | 3 (5%) 27 17  | 34, 47, 56, 58        | 0     |
| 29  | 17    | 48/48 (100%)    | -0.01  | 0 100 100     | 8, 13, 34, 42         | 0     |
| 29  | 27    | 48/48 (100%)    | 0.16   | 1 (2%) 67 56  | 21, 28, 44, 58        | 0     |
| 30  | 18    | 64/64 (100%)    | -0.20  | 0 100 100     | 15, 20, 28, 37        | 0     |
| 30  | 28    | 64/64 (100%)    | 0.10   | 0 100 100     | 31, 39, 49, 54        | 0     |
| 31  | 19    | 37/37 (100%)    | 0.03   | 0 100 100     | 19, 28, 43, 49        | 0     |
| 31  | 29    | 37/37 (100%)    | 0.59   | 0 100 100     | 39, 47, 54, 57        | 0     |
| 32  | 1a    | 1488/1520 (97%) | 0.69   | 119 (7%) 15 7 | 20, 53, 76, 91        | 0     |
| 32  | 2a    | 1492/1520 (98%) | 0.80   | 135 (9%) 12 6 | 32, 59, 77, 90        | 0     |
| 33  | 1b    | 231/231 (100%)  | 0.90   | 32 (13%) 4 2  | 50, 60, 69, 74        | 0     |
| 33  | 2b    | 231/231 (100%)  | 1.28   | 63 (27%) 1 0  | 54, 66, 71, 81        | 0     |
| 34  | 1c    | 206/206 (100%)  | 0.40   | 12 (5%) 26 16 | 47, 57, 66, 69        | 0     |
| 34  | 2c    | 206/206 (100%)  | 0.76   | 34 (16%) 2 1  | 53, 65, 71, 75        | 0     |
| 35  | 1d    | 208/208 (100%)  | 0.36   | 8 (3%) 44 32  | 41, 56, 67, 70        | 0     |
| 35  | 2d    | 208/208 (100%)  | 0.56   | 21 (10%) 9 4  | 48, 57, 64, 69        | 0     |
| 36  | 1e    | 148/148 (100%)  | 0.32   | 6 (4%) 41 29  | 33, 49, 58, 69        | 0     |
| 36  | 2e    | 148/148 (100%)  | 0.45   | 5 (3%) 49 36  | 48, 56, 63, 76        | 0     |
| 37  | 1f    | 100/100 (100%)  | 0.07   | 1 (1%) 84 77  | 46, 53, 60, 64        | 0     |
| 37  | 2f    | 100/100 (100%)  | 0.23   | 4 (4%) 42 30  | 38, 54, 62, 67        | 0     |
| 38  | 1g    | 155/155 (100%)  | 0.37   | 14 (9%) 12 6  | 47, 55, 69, 76        | 0     |
| 38  | 2g    | 155/155 (100%)  | 0.66   | 20 (12%) 5 2  | 53, 62, 71, 80        | 0     |
| 39  | 1h    | 137/137 (100%)  | 0.08   | 2 (1%) 76 68  | 40, 51, 58, 65        | 0     |
| 39  | 2h    | 137/137 (100%)  | 0.12   | 6 (4%) 38 26  | 46, 56, 62, 65        | 0     |
| 40  | 1i    | 127/127 (100%)  | 0.79   | 14 (11%) 7 3  | 40, 61, 68, 72        | 0     |
| 40  | 2i    | 126/127 (99%)   | 1.28   | 33 (26%) 1 0  | 55, 65, 72, 79        | 0     |
| 41  | 1j    | 97/97 (100%)    | 1.00   | 16 (16%) 2 1  | 44, 61, 73, 78        | 0     |
| 41  | 2j    | 96/97 (98%)     | 1.37   | 24 (25%) 1 0  | 52, 66, 72, 74        | 0     |
| 42  | 1k    | 114/114 (100%)  | 0.66   | 8 (7%) 19 11  | 29, 50, 61, 65        | 0     |
| 42  | 2k    | 114/114 (100%)  | 0.68   | 12 (10%) 8 4  | 45, 57, 64, 68        | 0     |
| 43  | 1l    | 121/122 (99%)   | 0.31   | 9 (7%) 17 9   | 32, 43, 56, 61        | 0     |
| 43  | 2l    | 121/122 (99%)   | 0.24   | 4 (3%) 50 38  | 41, 52, 60, 63        | 0     |

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| Mol | Chain | Analysed          | <RSRZ> | #RSRZ>2         | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-------------------|--------|-----------------|-----------------------|-------|
| 44  | 1m    | 116/116 (100%)    | 0.76   | 14 (12%) 6 3    | 45, 55, 64, 67        | 0     |
| 44  | 2m    | 114/116 (98%)     | 0.82   | 13 (11%) 7 3    | 56, 65, 72, 76        | 0     |
| 45  | 1n    | 60/60 (100%)      | 0.51   | 4 (6%) 21 12    | 47, 53, 59, 62        | 0     |
| 45  | 2n    | 60/60 (100%)      | 1.14   | 12 (20%) 1 1    | 58, 64, 69, 72        | 0     |
| 46  | 1o    | 88/88 (100%)      | 0.19   | 1 (1%) 82 74    | 36, 46, 58, 65        | 0     |
| 46  | 2o    | 88/88 (100%)      | 0.20   | 1 (1%) 82 74    | 45, 52, 61, 69        | 0     |
| 47  | 1p    | 82/82 (100%)      | 0.76   | 6 (7%) 18 10    | 43, 55, 62, 64        | 0     |
| 47  | 2p    | 82/82 (100%)      | 0.65   | 7 (8%) 13 6     | 46, 54, 61, 68        | 0     |
| 48  | 1q    | 99/99 (100%)      | 0.14   | 1 (1%) 84 77    | 36, 51, 61, 65        | 0     |
| 48  | 2q    | 99/99 (100%)      | 0.31   | 1 (1%) 84 77    | 43, 53, 60, 65        | 0     |
| 49  | 1r    | 68/68 (100%)      | 0.72   | 8 (11%) 6 3     | 43, 52, 62, 69        | 0     |
| 49  | 2r    | 68/68 (100%)      | 0.92   | 11 (16%) 3 1    | 48, 55, 64, 67        | 0     |
| 50  | 1s    | 83/83 (100%)      | 0.39   | 2 (2%) 62 50    | 50, 60, 67, 73        | 0     |
| 50  | 2s    | 83/83 (100%)      | 0.89   | 15 (18%) 2 1    | 55, 67, 75, 77        | 0     |
| 51  | 1t    | 96/98 (97%)       | 0.39   | 2 (2%) 67 56    | 45, 56, 65, 68        | 0     |
| 51  | 2t    | 98/98 (100%)      | 0.29   | 4 (4%) 41 29    | 46, 53, 64, 68        | 0     |
| 52  | 1u    | 23/23 (100%)      | 0.45   | 0 100 100       | 48, 52, 57, 58        | 0     |
| 52  | 2u    | 23/23 (100%)      | 1.51   | 8 (34%) 0 0     | 58, 62, 67, 68        | 0     |
| 53  | 1v    | 3/3 (100%)        | 0.17   | 0 100 100       | 37, 37, 39, 40        | 0     |
| 53  | 2v    | 3/3 (100%)        | 0.45   | 0 100 100       | 53, 53, 57, 62        | 0     |
| 54  | 1x    | 72/76 (94%)       | 0.39   | 2 (2%) 56 44    | 15, 41, 61, 71        | 0     |
| 54  | 2x    | 72/76 (94%)       | 1.06   | 16 (22%) 1 1    | 32, 57, 68, 75        | 0     |
| 55  | 1y    | 16/16 (100%)      | -0.14  | 0 100 100       | 14, 20, 32, 39        | 0     |
| 55  | 2y    | 16/16 (100%)      | 0.02   | 0 100 100       | 28, 33, 48, 48        | 0     |
| All | All   | 20755/20948 (99%) | 0.46   | 1502 (7%) 18 10 | 6, 47, 71, 93         | 0     |

All (1502) RSRZ outliers are listed below:

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | 1A    | 1133 | G    | 15.3 |
| 1   | 2A    | 2128 | C    | 14.8 |
| 1   | 1A    | 2155 | G    | 13.7 |
| 1   | 1A    | 2149 | G    | 13.6 |
| 1   | 1A    | 1135 | G    | 13.0 |

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| Mol | Chain | Res     | Type | RSRZ |
|-----|-------|---------|------|------|
| 1   | 1A    | 2180    | A    | 12.5 |
| 1   | 2A    | 2127    | G    | 12.0 |
| 1   | 1A    | 2139    | A    | 11.7 |
| 1   | 1A    | 2150    | C    | 10.7 |
| 1   | 2A    | 2112    | G    | 10.6 |
| 1   | 1A    | 2152    | U    | 10.4 |
| 1   | 2A    | 2147    | G    | 10.3 |
| 1   | 2A    | 2119    | A    | 10.2 |
| 1   | 2A    | 2159    | G    | 10.1 |
| 1   | 1A    | 2154    | U    | 10.1 |
| 1   | 2A    | 2173    | A    | 10.0 |
| 1   | 1A    | 1149    | A    | 9.9  |
| 21  | 1Z    | 192     | ALA  | 9.9  |
| 21  | 1Z    | 193     | GLU  | 9.8  |
| 1   | 2A    | 2118    | U    | 9.5  |
| 1   | 1A    | 2179    | G    | 9.4  |
| 1   | 1A    | 1134    | A    | 9.4  |
| 1   | 1A    | 1113    | A    | 9.2  |
| 1   | 1A    | 1137    | G    | 9.2  |
| 1   | 2A    | 2124    | G    | 9.1  |
| 1   | 1A    | 1112    | U    | 9.1  |
| 1   | 1A    | 1132    | A    | 9.0  |
| 1   | 2A    | 2123    | G    | 9.0  |
| 1   | 2A    | 2162    | G    | 9.0  |
| 1   | 2A    | 2168    | G    | 8.9  |
| 1   | 1A    | 1110    | C    | 8.8  |
| 1   | 1A    | 2151    | C    | 8.8  |
| 1   | 1A    | 2178    | G    | 8.8  |
| 1   | 2A    | 2133    | G    | 8.7  |
| 1   | 1A    | 1123    | A    | 8.5  |
| 1   | 1A    | 1109    | G    | 8.3  |
| 1   | 1A    | 1150    | C    | 8.3  |
| 1   | 2A    | 2129    | C    | 8.3  |
| 1   | 2A    | 2157    | G    | 8.2  |
| 1   | 2A    | 2131    | G    | 8.2  |
| 1   | 1A    | 2141    | A    | 8.2  |
| 32  | 2a    | 1030(A) | G    | 8.2  |
| 1   | 1A    | 1121    | C    | 8.2  |
| 1   | 1A    | 2146    | G    | 8.1  |
| 1   | 1A    | 2148    | A    | 8.1  |
| 1   | 1A    | 1103    | A    | 8.1  |
| 1   | 1A    | 2153    | G    | 8.1  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | 2A    | 2172 | U    | 8.0  |
| 1   | 1A    | 2145 | G    | 8.0  |
| 1   | 1A    | 2806 | G    | 8.0  |
| 1   | 1A    | 2128 | G    | 8.0  |
| 38  | 1g    | 83   | ALA  | 8.0  |
| 1   | 1A    | 1120 | G    | 7.9  |
| 1   | 2A    | 2158 | A    | 7.9  |
| 32  | 2a    | 1002 | G    | 7.7  |
| 1   | 1A    | 1122 | C    | 7.7  |
| 1   | 1A    | 2807 | C    | 7.7  |
| 1   | 2A    | 2106 | G    | 7.7  |
| 1   | 2A    | 2125 | G    | 7.6  |
| 1   | 1A    | 2181 | G    | 7.6  |
| 1   | 1A    | 1108 | G    | 7.5  |
| 20  | 2Y    | 1    | MET  | 7.5  |
| 1   | 1A    | 2195 | A    | 7.5  |
| 32  | 2a    | 1027 | C    | 7.5  |
| 1   | 2A    | 2110 | G    | 7.5  |
| 1   | 2A    | 2132 | U    | 7.4  |
| 1   | 2A    | 2179 | C    | 7.4  |
| 1   | 2A    | 2105 | C    | 7.4  |
| 1   | 2A    | 2174 | C    | 7.4  |
| 33  | 1b    | 232  | PRO  | 7.3  |
| 1   | 1A    | 1117 | G    | 7.3  |
| 1   | 1A    | 2142 | G    | 7.2  |
| 32  | 2a    | 1003 | G    | 7.1  |
| 1   | 1A    | 1139 | G    | 7.1  |
| 32  | 2a    | 1026 | G    | 7.1  |
| 1   | 1A    | 2156 | A    | 7.1  |
| 1   | 2A    | 2111 | C    | 7.1  |
| 1   | 1A    | 2147 | G    | 7.1  |
| 1   | 1A    | 1114 | G    | 7.1  |
| 32  | 1a    | 1030 | C    | 7.0  |
| 1   | 2A    | 2134 | A    | 7.0  |
| 40  | 2i    | 62   | TYR  | 7.0  |
| 1   | 1A    | 1118 | C    | 7.0  |
| 32  | 1a    | 1026 | G    | 6.9  |
| 32  | 1a    | 1027 | C    | 6.9  |
| 1   | 1A    | 2134 | G    | 6.9  |
| 21  | 1Z    | 191  | VAL  | 6.9  |
| 21  | 1Z    | 194  | PRO  | 6.9  |
| 21  | 2Z    | 193  | GLU  | 6.8  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 38  | 2g    | 84   | ASN  | 6.8  |
| 1   | 2A    | 2169 | A    | 6.8  |
| 1   | 1A    | 2177 | G    | 6.8  |
| 1   | 2A    | 2107 | C    | 6.7  |
| 1   | 2A    | 2117 | A    | 6.7  |
| 1   | 1A    | 1124 | U    | 6.7  |
| 21  | 1Z    | 202  | GLU  | 6.7  |
| 1   | 1A    | 2169 | G    | 6.7  |
| 1   | 2A    | 2802 | G    | 6.7  |
| 1   | 2A    | 1067 | A    | 6.7  |
| 1   | 1A    | 1131 | A    | 6.7  |
| 1   | 2A    | 2164 | C    | 6.6  |
| 1   | 1A    | 1111 | U    | 6.6  |
| 1   | 2A    | 1076 | C    | 6.6  |
| 32  | 1a    | 1024 | G    | 6.6  |
| 1   | 2A    | 2155 | G    | 6.5  |
| 32  | 2a    | 1034 | G    | 6.5  |
| 1   | 1A    | 1148 | C    | 6.5  |
| 1   | 2A    | 2163 | C    | 6.5  |
| 1   | 1A    | 1101 | G    | 6.5  |
| 32  | 1a    | 91   | C    | 6.5  |
| 1   | 1A    | 1130 | A    | 6.5  |
| 1   | 2A    | 2126 | A    | 6.4  |
| 1   | 1A    | 1151 | U    | 6.4  |
| 1   | 1A    | 2805 | G    | 6.4  |
| 32  | 2a    | 1005 | A    | 6.4  |
| 1   | 2A    | 2130 | U    | 6.4  |
| 1   | 1A    | 2126 | G    | 6.4  |
| 1   | 1A    | 2198 | A    | 6.3  |
| 1   | 1A    | 2191 | A    | 6.3  |
| 1   | 1A    | 932  | C    | 6.3  |
| 1   | 2A    | 1095 | A    | 6.2  |
| 1   | 2A    | 2152 | G    | 6.2  |
| 1   | 1A    | 2173 | G    | 6.2  |
| 1   | 2A    | 2156 | G    | 6.2  |
| 1   | 1A    | 2130 | C    | 6.1  |
| 1   | 1A    | 2184 | G    | 6.1  |
| 33  | 2b    | 233  | SER  | 6.1  |
| 7   | 2H    | 95   | ARG  | 6.1  |
| 1   | 2A    | 1056 | G    | 6.1  |
| 1   | 2A    | 2120 | G    | 6.0  |
| 1   | 1A    | 2140 | U    | 6.0  |

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| Mol | Chain | Res     | Type | RSRZ |
|-----|-------|---------|------|------|
| 32  | 2a    | 1001(A) | G    | 6.0  |
| 32  | 1a    | 1031    | G    | 6.0  |
| 1   | 2A    | 2108    | C    | 5.9  |
| 32  | 1a    | 1028    | C    | 5.9  |
| 33  | 2b    | 48      | MET  | 5.9  |
| 32  | 1a    | 1036    | G    | 5.9  |
| 1   | 1A    | 2183    | C    | 5.9  |
| 38  | 1g    | 84      | ASN  | 5.9  |
| 1   | 2A    | 2151    | G    | 5.9  |
| 44  | 2m    | 6       | GLY  | 5.9  |
| 1   | 2A    | 2113    | U    | 5.9  |
| 1   | 1A    | 2190    | G    | 5.9  |
| 41  | 2j    | 96      | ILE  | 5.8  |
| 1   | 1A    | 1129    | U    | 5.8  |
| 6   | 2G    | 149     | VAL  | 5.8  |
| 1   | 2A    | 2793    | G    | 5.8  |
| 33  | 2b    | 17      | PHE  | 5.8  |
| 1   | 1A    | 1127    | U    | 5.7  |
| 32  | 1a    | 1030(D) | A    | 5.7  |
| 1   | 1A    | 1119    | A    | 5.7  |
| 32  | 1a    | 1029    | C    | 5.7  |
| 1   | 1A    | 2182    | G    | 5.7  |
| 32  | 1a    | 1001(A) | G    | 5.7  |
| 32  | 2a    | 1032    | G    | 5.7  |
| 1   | 1A    | 2196    | C    | 5.7  |
| 32  | 1a    | 1034    | G    | 5.7  |
| 1   | 2A    | 2154    | G    | 5.6  |
| 1   | 2A    | 2148    | G    | 5.6  |
| 21  | 2Z    | 192     | ALA  | 5.5  |
| 32  | 2a    | 1033    | G    | 5.5  |
| 1   | 1A    | 1126    | C    | 5.5  |
| 33  | 1b    | 228     | GLY  | 5.5  |
| 1   | 1A    | 2132    | G    | 5.5  |
| 34  | 1c    | 192     | THR  | 5.5  |
| 1   | 2A    | 2805    | G    | 5.5  |
| 1   | 1A    | 2170    | G    | 5.4  |
| 1   | 1A    | 2194    | U    | 5.4  |
| 1   | 2A    | 1099    | G    | 5.4  |
| 32  | 1a    | 78      | G    | 5.4  |
| 1   | 2A    | 888     | C    | 5.4  |
| 1   | 1A    | 1102    | G    | 5.4  |
| 1   | 2A    | 2170    | A    | 5.4  |

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| Mol | Chain | Res     | Type | RSRZ |
|-----|-------|---------|------|------|
| 1   | 2A    | 2141    | G    | 5.4  |
| 1   | 1A    | 2185    | C    | 5.4  |
| 1   | 2A    | 1075    | C    | 5.4  |
| 1   | 2A    | 1058    | G    | 5.3  |
| 38  | 2g    | 81      | GLY  | 5.3  |
| 33  | 2b    | 232     | PRO  | 5.3  |
| 1   | 1A    | 2816    | G    | 5.3  |
| 1   | 1A    | 1104    | G    | 5.3  |
| 1   | 1A    | 933     | C    | 5.3  |
| 1   | 1A    | 2202    | U    | 5.3  |
| 1   | 1A    | 1116    | A    | 5.2  |
| 32  | 1a    | 1002    | G    | 5.3  |
| 1   | 1A    | 1555    | C    | 5.2  |
| 54  | 2x    | 46      | G    | 5.2  |
| 1   | 2A    | 2137    | C    | 5.2  |
| 32  | 1a    | 1030(B) | C    | 5.2  |
| 26  | 14    | 18      | CYS  | 5.2  |
| 26  | 24    | 49      | PHE  | 5.2  |
| 32  | 2a    | 91      | C    | 5.2  |
| 32  | 1a    | 92      | C    | 5.2  |
| 1   | 1A    | 2131    | U    | 5.2  |
| 1   | 2A    | 279     | C    | 5.2  |
| 32  | 2a    | 1030    | C    | 5.2  |
| 1   | 2A    | 2153    | G    | 5.2  |
| 21  | 2Z    | 194     | PRO  | 5.2  |
| 7   | 2H    | 106     | THR  | 5.1  |
| 1   | 1A    | 2133    | C    | 5.1  |
| 1   | 2A    | 1068    | G    | 5.1  |
| 1   | 1A    | 1556    | A    | 5.1  |
| 1   | 1A    | 1220    | U    | 5.1  |
| 1   | 1A    | 2197    | C    | 5.1  |
| 1   | 2A    | 2138    | C    | 5.1  |
| 26  | 24    | 67      | TYR  | 5.1  |
| 32  | 1a    | 1030(A) | G    | 5.1  |
| 1   | 1A    | 2163    | G    | 5.1  |
| 7   | 2H    | 56      | SER  | 5.0  |
| 21  | 2Z    | 201     | LYS  | 5.0  |
| 1   | 1A    | 2171    | G    | 5.0  |
| 1   | 2A    | 1509    | C    | 5.0  |
| 33  | 2b    | 139     | LYS  | 5.0  |
| 1   | 2A    | 1066    | U    | 5.0  |
| 35  | 2d    | 11      | LEU  | 5.0  |

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| Mol | Chain | Res     | Type | RSRZ |
|-----|-------|---------|------|------|
| 1   | 2A    | 889     | C    | 5.0  |
| 21  | 1Z    | 197     | ILE  | 5.0  |
| 26  | 24    | 41      | PRO  | 5.0  |
| 1   | 2A    | 2142    | C    | 5.0  |
| 1   | 2A    | 2792    | G    | 4.9  |
| 1   | 1A    | 2127    | C    | 4.9  |
| 1   | 1A    | 1141    | A    | 4.9  |
| 1   | 1A    | 1138    | C    | 4.9  |
| 32  | 2a    | 1020    | U    | 4.9  |
| 38  | 2g    | 83      | ALA  | 4.9  |
| 1   | 2A    | 2176    | A    | 4.9  |
| 32  | 1a    | 1032    | G    | 4.9  |
| 1   | 2A    | 1055    | G    | 4.9  |
| 1   | 1A    | 1128    | U    | 4.9  |
| 41  | 1j    | 98      | ILE  | 4.9  |
| 1   | 2A    | 1083    | U    | 4.9  |
| 1   | 2A    | 1064    | C    | 4.9  |
| 32  | 1a    | 77      | G    | 4.9  |
| 33  | 2b    | 190     | THR  | 4.8  |
| 1   | 1A    | 2201    | C    | 4.8  |
| 1   | 2A    | 896     | A    | 4.8  |
| 21  | 1Z    | 203     | GLU  | 4.8  |
| 1   | 2A    | 2150    | U    | 4.8  |
| 32  | 1a    | 1025    | U    | 4.8  |
| 32  | 1a    | 93      | G    | 4.8  |
| 22  | 20    | 8       | GLY  | 4.8  |
| 1   | 2A    | 2161    | C    | 4.7  |
| 41  | 1j    | 72      | VAL  | 4.7  |
| 21  | 1Z    | 196     | VAL  | 4.7  |
| 32  | 2a    | 1029    | C    | 4.7  |
| 32  | 1a    | 1023    | G    | 4.7  |
| 26  | 14    | 52      | THR  | 4.7  |
| 1   | 1A    | 934     | A    | 4.7  |
| 1   | 2A    | 2803    | C    | 4.7  |
| 32  | 2a    | 1030(B) | C    | 4.7  |
| 1   | 2A    | 2171    | A    | 4.7  |
| 1   | 1A    | 1125    | C    | 4.7  |
| 1   | 1A    | 2129    | C    | 4.7  |
| 1   | 1A    | 2208    | G    | 4.7  |
| 32  | 2a    | 1036    | G    | 4.7  |
| 1   | 1A    | 1100    | A    | 4.7  |
| 7   | 2H    | 128     | PRO  | 4.7  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 32         | 1a           | 90         | U           | 4.7         |
| 1          | 2A           | 1057       | A           | 4.7         |
| 32         | 1a           | 1033       | G           | 4.7         |
| 33         | 2b           | 49         | GLU         | 4.6         |
| 1          | 2A           | 1054       | A           | 4.6         |
| 1          | 2A           | 2160       | G           | 4.6         |
| 33         | 1b           | 48         | MET         | 4.6         |
| 33         | 2b           | 145        | LEU         | 4.6         |
| 1          | 2A           | 2114       | A           | 4.6         |
| 33         | 2b           | 231        | GLU         | 4.6         |
| 1          | 1A           | 1099       | C           | 4.6         |
| 1          | 2A           | 2136       | C           | 4.6         |
| 33         | 2b           | 44         | LEU         | 4.6         |
| 33         | 2b           | 228        | GLY         | 4.6         |
| 40         | 2i           | 29         | ASN         | 4.6         |
| 1          | 1A           | 2815       | C           | 4.6         |
| 1          | 2A           | 2801(A)    | A           | 4.6         |
| 1          | 1A           | 2804       | C           | 4.6         |
| 1          | 2A           | 2149       | G           | 4.6         |
| 8          | 1I           | 65         | ALA         | 4.6         |
| 32         | 1a           | 1037       | C           | 4.6         |
| 1          | 1A           | 1136       | U           | 4.6         |
| 1          | 1A           | 2159       | C           | 4.5         |
| 32         | 2a           | 1006       | C           | 4.5         |
| 34         | 2c           | 190        | ARG         | 4.5         |
| 32         | 1a           | 344        | A           | 4.5         |
| 32         | 1a           | 79         | G           | 4.5         |
| 16         | 2U           | 89         | GLU         | 4.5         |
| 33         | 1b           | 188        | ALA         | 4.5         |
| 1          | 2A           | 2122       | U           | 4.5         |
| 1          | 2A           | 1538       | G           | 4.5         |
| 32         | 1a           | 70         | G           | 4.5         |
| 26         | 24           | 27         | THR         | 4.5         |
| 32         | 1a           | 97         | G           | 4.5         |
| 25         | 23           | 60         | GLU         | 4.4         |
| 33         | 2b           | 118        | LEU         | 4.4         |
| 1          | 2A           | 2165       | G           | 4.4         |
| 22         | 10           | 8          | GLY         | 4.4         |
| 1          | 1A           | 936        | C           | 4.4         |
| 32         | 2a           | 1007       | C           | 4.4         |
| 1          | 1A           | 2176       | G           | 4.4         |
| 1          | 1A           | 2187       | G           | 4.4         |

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| Mol | Chain | Res    | Type | RSRZ |
|-----|-------|--------|------|------|
| 32  | 2a    | 1024   | G    | 4.4  |
| 1   | 1A    | 1879   | A    | 4.4  |
| 41  | 2j    | 34     | VAL  | 4.4  |
| 1   | 2A    | 2166   | G    | 4.4  |
| 1   | 2A    | 2167   | U    | 4.4  |
| 26  | 24    | 66     | SER  | 4.4  |
| 15  | 1T    | 38     | ASN  | 4.4  |
| 1   | 1A    | 2186   | C    | 4.4  |
| 1   | 1A    | 925    | A    | 4.4  |
| 26  | 14    | 49     | PHE  | 4.4  |
| 26  | 24    | 63     | TYR  | 4.4  |
| 41  | 2j    | 72     | VAL  | 4.4  |
| 1   | 1A    | 1143   | U    | 4.4  |
| 1   | 2A    | 2794   | C    | 4.3  |
| 26  | 14    | 45     | GLY  | 4.3  |
| 21  | 2Z    | 197    | ILE  | 4.3  |
| 1   | 2A    | 10     | G    | 4.3  |
| 1   | 2A    | 274    | G    | 4.3  |
| 32  | 2a    | 1021   | G    | 4.3  |
| 1   | 1A    | 2189   | U    | 4.3  |
| 1   | 1A    | 2210   | C    | 4.3  |
| 32  | 2a    | 1028   | C    | 4.3  |
| 50  | 2s    | 20     | LEU  | 4.3  |
| 21  | 2Z    | 200    | GLY  | 4.3  |
| 33  | 1b    | 190    | THR  | 4.3  |
| 34  | 2c    | 107    | GLN  | 4.3  |
| 1   | 1A    | 1140   | U    | 4.3  |
| 1   | 1A    | 2136   | A    | 4.3  |
| 32  | 1a    | 160    | A    | 4.3  |
| 26  | 24    | 64     | GLY  | 4.3  |
| 1   | 1A    | 930    | G    | 4.3  |
| 1   | 2A    | 229    | A    | 4.3  |
| 32  | 1a    | 1003   | G    | 4.3  |
| 1   | 1A    | 2193   | A    | 4.2  |
| 1   | 1A    | 2902   | G    | 4.2  |
| 1   | 2A    | 883    | G    | 4.2  |
| 21  | 2Z    | 191    | VAL  | 4.2  |
| 32  | 2a    | 1004   | A    | 4.2  |
| 1   | 1A    | 2209   | G    | 4.2  |
| 15  | 1T    | 37     | GLY  | 4.2  |
| 40  | 2i    | 54     | ASP  | 4.2  |
| 1   | 2A    | 652(B) | A    | 4.2  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | 2A    | 2178 | C    | 4.2  |
| 1   | 2A    | 2109 | U    | 4.2  |
| 8   | 2I    | 74   | ASN  | 4.2  |
| 21  | 1Z    | 200  | GLY  | 4.2  |
| 47  | 2p    | 51   | VAL  | 4.2  |
| 41  | 1j    | 5    | ARG  | 4.1  |
| 1   | 1A    | 935  | C    | 4.1  |
| 1   | 1A    | 2199 | C    | 4.1  |
| 1   | 2A    | 1085 | A    | 4.1  |
| 1   | 1A    | 2144 | U    | 4.1  |
| 38  | 1g    | 156  | TRP  | 4.1  |
| 1   | 2A    | 1914 | C    | 4.1  |
| 42  | 2k    | 27   | ASN  | 4.1  |
| 1   | 2A    | 2180 | U    | 4.1  |
| 1   | 2A    | 2135 | A    | 4.1  |
| 1   | 2A    | 1528 | A    | 4.1  |
| 42  | 2k    | 90   | GLY  | 4.1  |
| 1   | 1A    | 2207 | C    | 4.1  |
| 33  | 1b    | 17   | PHE  | 4.1  |
| 41  | 2j    | 26   | ALA  | 4.1  |
| 34  | 1c    | 194  | GLY  | 4.1  |
| 44  | 1m    | 56   | LEU  | 4.1  |
| 32  | 2a    | 1531 | A    | 4.1  |
| 44  | 2m    | 66   | LEU  | 4.0  |
| 32  | 1a    | 1257 | U    | 4.0  |
| 40  | 2i    | 30   | GLY  | 4.0  |
| 1   | 2A    | 2143 | C    | 4.0  |
| 1   | 2A    | 2896 | C    | 4.0  |
| 38  | 2g    | 154  | TYR  | 4.0  |
| 33  | 2b    | 123  | ALA  | 4.0  |
| 32  | 1a    | 1035 | A    | 4.0  |
| 32  | 1a    | 1447 | A    | 4.0  |
| 32  | 1a    | 1137 | C    | 4.0  |
| 1   | 1A    | 2803 | A    | 4.0  |
| 32  | 2a    | 1035 | A    | 4.0  |
| 1   | 2A    | 2145 | C    | 4.0  |
| 32  | 2a    | 77   | G    | 4.0  |
| 33  | 1b    | 231  | GLU  | 4.0  |
| 1   | 2A    | 1467 | C    | 4.0  |
| 1   | 1A    | 2138 | G    | 4.0  |
| 1   | 2A    | 11   | G    | 4.0  |
| 34  | 1c    | 193  | TYR  | 4.0  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 39  | 1h    | 117  | GLY  | 4.0  |
| 1   | 1A    | 1218 | G    | 4.0  |
| 1   | 2A    | 1450 | G    | 4.0  |
| 1   | 1A    | 2192 | A    | 4.0  |
| 32  | 1a    | 71   | C    | 4.0  |
| 33  | 2b    | 12   | GLU  | 4.0  |
| 1   | 1A    | 1905 | G    | 4.0  |
| 1   | 1A    | 1219 | A    | 3.9  |
| 32  | 2a    | 79   | G    | 3.9  |
| 8   | 2I    | 63   | ALA  | 3.9  |
| 1   | 2A    | 886  | C    | 3.9  |
| 1   | 2A    | 890  | A    | 3.9  |
| 1   | 2A    | 1103 | A    | 3.9  |
| 32  | 1a    | 152  | A    | 3.9  |
| 1   | 1A    | 2200 | C    | 3.9  |
| 1   | 2A    | 2175 | C    | 3.9  |
| 33  | 1b    | 233  | SER  | 3.9  |
| 43  | 2l    | 62   | SER  | 3.9  |
| 40  | 1i    | 81   | ILE  | 3.9  |
| 38  | 1g    | 79   | ARG  | 3.9  |
| 1   | 2A    | 877  | U    | 3.9  |
| 6   | 2G    | 41   | GLN  | 3.9  |
| 32  | 1a    | 1140 | C    | 3.9  |
| 40  | 2i    | 99   | LEU  | 3.9  |
| 54  | 2x    | 21   | A    | 3.9  |
| 32  | 1a    | 1532 | U    | 3.9  |
| 1   | 1A    | 2206 | G    | 3.9  |
| 6   | 2G    | 136  | ARG  | 3.9  |
| 1   | 1A    | 1554 | A    | 3.9  |
| 33  | 2b    | 18   | GLY  | 3.9  |
| 43  | 2l    | 64   | TYR  | 3.9  |
| 54  | 2x    | 20   | U    | 3.9  |
| 1   | 2A    | 1449 | A    | 3.9  |
| 21  | 2Z    | 114  | GLY  | 3.9  |
| 34  | 1c    | 81   | GLY  | 3.9  |
| 7   | 2H    | 126  | PRO  | 3.9  |
| 32  | 1a    | 76   | C    | 3.9  |
| 34  | 2c    | 189  | ALA  | 3.9  |
| 1   | 1A    | 2203 | G    | 3.9  |
| 7   | 2H    | 55   | PRO  | 3.8  |
| 1   | 2A    | 1087 | G    | 3.8  |
| 32  | 1a    | 1001 | A    | 3.8  |

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| Mol | Chain | Res    | Type | RSRZ |
|-----|-------|--------|------|------|
| 43  | 1l    | 63     | GLY  | 3.8  |
| 32  | 1a    | 69     | G    | 3.8  |
| 1   | 1A    | 1553   | A    | 3.8  |
| 1   | 2A    | 878    | A    | 3.8  |
| 38  | 2g    | 82     | GLY  | 3.8  |
| 1   | 2A    | 894    | C    | 3.8  |
| 32  | 1a    | 345    | C    | 3.8  |
| 32  | 2a    | 76     | C    | 3.8  |
| 39  | 2h    | 56     | LYS  | 3.8  |
| 21  | 1Z    | 201    | LYS  | 3.8  |
| 41  | 2j    | 23     | ILE  | 3.8  |
| 39  | 1h    | 115    | SER  | 3.8  |
| 1   | 1A    | 1152   | G    | 3.8  |
| 32  | 2a    | 78     | G    | 3.8  |
| 1   | 1A    | 2172   | U    | 3.8  |
| 1   | 1A    | 938    | G    | 3.8  |
| 47  | 2p    | 48     | TRP  | 3.8  |
| 52  | 2u    | 14     | TRP  | 3.8  |
| 1   | 1A    | 302    | A    | 3.8  |
| 1   | 2A    | 875    | G    | 3.8  |
| 1   | 2A    | 899    | A    | 3.8  |
| 1   | 2A    | 1102   | C    | 3.8  |
| 38  | 2g    | 4      | ARG  | 3.8  |
| 32  | 1a    | 702    | A    | 3.7  |
| 32  | 2a    | 1031   | G    | 3.7  |
| 42  | 2k    | 43     | SER  | 3.7  |
| 40  | 2i    | 90     | PRO  | 3.7  |
| 1   | 1A    | 2812   | A    | 3.7  |
| 1   | 2A    | 2181   | G    | 3.7  |
| 14  | 2S    | 58     | LEU  | 3.7  |
| 6   | 2G    | 42     | GLY  | 3.7  |
| 26  | 24    | 32     | TYR  | 3.7  |
| 40  | 1i    | 82     | ALA  | 3.7  |
| 1   | 2A    | 271(N) | U    | 3.7  |
| 1   | 2A    | 2121   | G    | 3.7  |
| 49  | 2r    | 58     | LEU  | 3.7  |
| 21  | 1Z    | 195    | GLU  | 3.7  |
| 14  | 2S    | 52     | SER  | 3.7  |
| 2   | 2B    | 4      | C    | 3.7  |
| 23  | 21    | 83     | GLU  | 3.7  |
| 32  | 2a    | 932    | C    | 3.7  |
| 32  | 2a    | 1008   | C    | 3.7  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 32  | 2a    | 1141 | C    | 3.7  |
| 52  | 2u    | 16   | GLY  | 3.7  |
| 40  | 2i    | 3    | GLN  | 3.7  |
| 1   | 2A    | 1508 | A    | 3.7  |
| 26  | 24    | 46   | GLN  | 3.6  |
| 32  | 1a    | 161  | A    | 3.6  |
| 34  | 2c    | 71   | ALA  | 3.6  |
| 40  | 2i    | 88   | TYR  | 3.6  |
| 1   | 1A    | 697  | C    | 3.6  |
| 15  | 2T    | 126  | ALA  | 3.6  |
| 1   | 2A    | 1086 | A    | 3.6  |
| 1   | 2A    | 1859 | A    | 3.6  |
| 1   | 1A    | 926  | G    | 3.6  |
| 52  | 2u    | 15   | ARG  | 3.6  |
| 44  | 1m    | 2    | ALA  | 3.6  |
| 1   | 1A    | 2123 | G    | 3.6  |
| 32  | 1a    | 1138 | G    | 3.6  |
| 32  | 2a    | 90   | U    | 3.6  |
| 50  | 2s    | 35   | SER  | 3.6  |
| 1   | 2A    | 1532 | C    | 3.6  |
| 42  | 2k    | 25   | TYR  | 3.6  |
| 44  | 2m    | 75   | ALA  | 3.6  |
| 1   | 2A    | 2804 | C    | 3.6  |
| 39  | 2h    | 52   | ASP  | 3.6  |
| 1   | 1A    | 11   | G    | 3.6  |
| 1   | 2A    | 892  | G    | 3.6  |
| 54  | 2x    | 49   | G    | 3.6  |
| 1   | 1A    | 939  | C    | 3.5  |
| 54  | 2x    | 48   | C    | 3.5  |
| 32  | 2a    | 1022 | G    | 3.5  |
| 38  | 2g    | 116  | ALA  | 3.5  |
| 43  | 1l    | 29   | GLY  | 3.5  |
| 40  | 2i    | 26   | VAL  | 3.5  |
| 32  | 2a    | 1025 | U    | 3.5  |
| 7   | 2H    | 51   | ARG  | 3.5  |
| 41  | 2j    | 6    | ILE  | 3.5  |
| 1   | 1A    | 1530 | G    | 3.5  |
| 38  | 1g    | 81   | GLY  | 3.5  |
| 1   | 2A    | 1445 | A    | 3.5  |
| 38  | 1g    | 85   | TYR  | 3.5  |
| 1   | 1A    | 386  | U    | 3.5  |
| 32  | 1a    | 145  | G    | 3.5  |

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| Mol | Chain | Res    | Type | RSRZ |
|-----|-------|--------|------|------|
| 1   | 2A    | 271(J) | C    | 3.5  |
| 1   | 2A    | 1053   | C    | 3.5  |
| 1   | 2A    | 2139   | C    | 3.5  |
| 33  | 1b    | 229    | VAL  | 3.5  |
| 52  | 2u    | 10     | ARG  | 3.5  |
| 35  | 2d    | 44     | GLY  | 3.5  |
| 1   | 2A    | 2833   | G    | 3.5  |
| 6   | 2G    | 140    | ILE  | 3.5  |
| 33  | 1b    | 237    | ALA  | 3.5  |
| 1   | 1A    | 1936   | C    | 3.5  |
| 32  | 1a    | 1531   | A    | 3.5  |
| 26  | 24    | 39     | CYS  | 3.5  |
| 33  | 2b    | 122    | PHE  | 3.5  |
| 33  | 2b    | 202    | PRO  | 3.5  |
| 6   | 2G    | 60     | LEU  | 3.5  |
| 32  | 1a    | 1007   | C    | 3.5  |
| 1   | 2A    | 2100   | G    | 3.5  |
| 32  | 2a    | 1102   | A    | 3.5  |
| 40  | 2i    | 18     | PHE  | 3.5  |
| 45  | 2n    | 10     | ALA  | 3.4  |
| 17  | 2V    | 26     | ASP  | 3.4  |
| 1   | 1A    | 1142   | A    | 3.4  |
| 51  | 1t    | 31     | SER  | 3.4  |
| 1   | 1A    | 1221   | G    | 3.4  |
| 32  | 2a    | 73     | G    | 3.4  |
| 49  | 1r    | 56     | THR  | 3.4  |
| 7   | 2H    | 94     | TYR  | 3.4  |
| 45  | 2n    | 34     | TYR  | 3.4  |
| 1   | 2A    | 1084   | A    | 3.4  |
| 44  | 1m    | 51     | ALA  | 3.4  |
| 1   | 1A    | 937    | A    | 3.4  |
| 33  | 2b    | 16     | HIS  | 3.4  |
| 33  | 2b    | 229    | VAL  | 3.4  |
| 1   | 1A    | 2188   | G    | 3.4  |
| 32  | 2a    | 1023   | G    | 3.4  |
| 26  | 24    | 4      | GLY  | 3.4  |
| 33  | 1b    | 21     | ARG  | 3.4  |
| 1   | 1A    | 931    | C    | 3.4  |
| 1   | 1A    | 2814   | C    | 3.4  |
| 32  | 2a    | 1019   | C    | 3.4  |
| 14  | 2S    | 54     | LEU  | 3.4  |
| 1   | 1A    | 269    | G    | 3.4  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | 2A    | 1541 | G    | 3.4  |
| 1   | 1A    | 943  | C    | 3.4  |
| 1   | 2A    | 2188 | C    | 3.4  |
| 44  | 1m    | 50   | GLU  | 3.4  |
| 34  | 2c    | 185  | GLY  | 3.4  |
| 1   | 1A    | 1144 | A    | 3.4  |
| 1   | 2A    | 1507 | A    | 3.4  |
| 26  | 24    | 5    | ILE  | 3.4  |
| 1   | 2A    | 1104 | C    | 3.4  |
| 50  | 2s    | 24   | ALA  | 3.4  |
| 7   | 2H    | 61   | HIS  | 3.4  |
| 34  | 1c    | 80   | GLY  | 3.4  |
| 52  | 2u    | 2    | GLY  | 3.4  |
| 40  | 2i    | 7    | THR  | 3.4  |
| 7   | 2H    | 124  | GLU  | 3.3  |
| 1   | 2A    | 1106 | G    | 3.3  |
| 32  | 1a    | 1021 | G    | 3.3  |
| 33  | 1b    | 129  | GLU  | 3.3  |
| 34  | 2c    | 72   | LYS  | 3.3  |
| 40  | 2i    | 102  | LEU  | 3.3  |
| 1   | 2A    | 901  | A    | 3.3  |
| 42  | 2k    | 44   | SER  | 3.3  |
| 7   | 2H    | 97   | ARG  | 3.3  |
| 33  | 2b    | 31   | TYR  | 3.3  |
| 35  | 2d    | 38   | TYR  | 3.3  |
| 32  | 2a    | 1130 | A    | 3.3  |
| 42  | 2k    | 29   | ILE  | 3.3  |
| 1   | 2A    | 645  | C    | 3.3  |
| 1   | 2A    | 2146 | C    | 3.3  |
| 1   | 2A    | 879  | G    | 3.3  |
| 1   | 2A    | 2897 | U    | 3.3  |
| 42  | 1k    | 57   | THR  | 3.3  |
| 33  | 2b    | 42   | ILE  | 3.3  |
| 8   | 2I    | 61   | ARG  | 3.3  |
| 33  | 1b    | 230  | VAL  | 3.3  |
| 1   | 1A    | 1935 | A    | 3.3  |
| 35  | 2d    | 43   | HIS  | 3.3  |
| 8   | 2I    | 57   | ARG  | 3.3  |
| 38  | 1g    | 4    | ARG  | 3.3  |
| 49  | 2r    | 46   | GLU  | 3.3  |
| 26  | 24    | 43   | TYR  | 3.3  |
| 32  | 2a    | 1262 | C    | 3.3  |

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| Mol | Chain | Res     | Type | RSRZ |
|-----|-------|---------|------|------|
| 1   | 2A    | 1082    | U    | 3.3  |
| 8   | 1I    | 61      | ARG  | 3.3  |
| 32  | 1a    | 73      | G    | 3.3  |
| 42  | 2k    | 42      | TRP  | 3.3  |
| 34  | 1c    | 72      | LYS  | 3.3  |
| 45  | 2n    | 25      | VAL  | 3.3  |
| 1   | 1A    | 10      | G    | 3.3  |
| 32  | 1a    | 144     | G    | 3.3  |
| 43  | 1l    | 52      | LEU  | 3.3  |
| 1   | 2A    | 1073    | A    | 3.3  |
| 1   | 1A    | 940     | C    | 3.3  |
| 1   | 2A    | 317     | G    | 3.3  |
| 26  | 24    | 40      | HIS  | 3.3  |
| 32  | 1a    | 98      | G    | 3.3  |
| 45  | 2n    | 8       | GLU  | 3.2  |
| 2   | 2B    | 3       | C    | 3.2  |
| 33  | 2b    | 92      | TYR  | 3.2  |
| 1   | 1A    | 1938    | A    | 3.2  |
| 1   | 2A    | 278     | A    | 3.2  |
| 23  | 11    | 26      | ARG  | 3.2  |
| 26  | 14    | 50      | VAL  | 3.2  |
| 32  | 2a    | 88      | A    | 3.2  |
| 32  | 2a    | 1043    | C    | 3.2  |
| 32  | 2a    | 1044    | A    | 3.2  |
| 26  | 24    | 36      | CYS  | 3.2  |
| 34  | 2c    | 105     | GLU  | 3.2  |
| 1   | 1A    | 941     | U    | 3.2  |
| 44  | 1m    | 22      | ILE  | 3.2  |
| 2   | 2B    | 2       | C    | 3.2  |
| 32  | 1a    | 72      | C    | 3.2  |
| 54  | 2x    | 16      | C    | 3.2  |
| 1   | 2A    | 1046    | A    | 3.2  |
| 34  | 2c    | 196     | LEU  | 3.2  |
| 40  | 2i    | 53      | VAL  | 3.2  |
| 1   | 2A    | 2115    | G    | 3.2  |
| 1   | 2A    | 2894    | G    | 3.2  |
| 32  | 2a    | 1030(C) | G    | 3.2  |
| 1   | 2A    | 1096    | A    | 3.2  |
| 45  | 2n    | 55      | GLY  | 3.2  |
| 6   | 2G    | 150     | ASP  | 3.2  |
| 33  | 1b    | 19      | HIS  | 3.2  |
| 34  | 2c    | 108     | ASN  | 3.2  |

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| Mol | Chain | Res     | Type | RSRZ |
|-----|-------|---------|------|------|
| 25  | 23    | 2       | PRO  | 3.2  |
| 26  | 24    | 55      | ARG  | 3.2  |
| 54  | 2x    | 59      | A    | 3.2  |
| 44  | 1m    | 4       | ILE  | 3.2  |
| 34  | 2c    | 160     | ALA  | 3.2  |
| 41  | 2j    | 27      | ALA  | 3.2  |
| 32  | 1a    | 1030(C) | G    | 3.2  |
| 45  | 1n    | 7       | ILE  | 3.2  |
| 49  | 2r    | 47      | THR  | 3.2  |
| 1   | 1A    | 2903    | G    | 3.2  |
| 32  | 2a    | 1261    | A    | 3.2  |
| 6   | 2G    | 146     | TYR  | 3.2  |
| 1   | 1A    | 1551    | C    | 3.2  |
| 1   | 1A    | 2905    | C    | 3.2  |
| 1   | 2A    | 652(T)  | C    | 3.2  |
| 45  | 2n    | 7       | ILE  | 3.1  |
| 32  | 1a    | 204     | U    | 3.1  |
| 33  | 1b    | 29      | ALA  | 3.1  |
| 35  | 2d    | 23      | GLY  | 3.1  |
| 1   | 1A    | 1145    | G    | 3.1  |
| 1   | 1A    | 2813    | G    | 3.1  |
| 1   | 2A    | 1527    | G    | 3.1  |
| 26  | 24    | 7       | PRO  | 3.1  |
| 40  | 2i    | 91      | ASP  | 3.1  |
| 21  | 1Z    | 198     | LYS  | 3.1  |
| 1   | 1A    | 1147    | U    | 3.1  |
| 42  | 1k    | 56      | GLY  | 3.1  |
| 42  | 2k    | 28      | THR  | 3.1  |
| 45  | 1n    | 22      | THR  | 3.1  |
| 1   | 2A    | 1069    | A    | 3.1  |
| 2   | 2B    | 117     | G    | 3.1  |
| 32  | 2a    | 97      | G    | 3.1  |
| 38  | 2g    | 5       | ARG  | 3.1  |
| 35  | 2d    | 33      | MET  | 3.1  |
| 1   | 2A    | 2104    | G    | 3.1  |
| 6   | 2G    | 56      | ALA  | 3.1  |
| 38  | 1g    | 82      | GLY  | 3.1  |
| 1   | 1A    | 696     | C    | 3.1  |
| 1   | 2A    | 318     | C    | 3.1  |
| 21  | 1Z    | 70      | LEU  | 3.1  |
| 40  | 2i    | 4       | TYR  | 3.1  |
| 32  | 1a    | 1004    | A    | 3.1  |

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| Mol | Chain | Res     | Type | RSRZ |
|-----|-------|---------|------|------|
| 32  | 1a    | 1493    | A    | 3.1  |
| 32  | 2a    | 1287    | A    | 3.1  |
| 1   | 1A    | 2174    | G    | 3.1  |
| 41  | 2j    | 84      | GLN  | 3.1  |
| 1   | 2A    | 652(V)  | C    | 3.1  |
| 32  | 2a    | 1249    | C    | 3.1  |
| 9   | 2N    | 9       | VAL  | 3.1  |
| 23  | 11    | 84      | GLY  | 3.1  |
| 26  | 24    | 10      | VAL  | 3.1  |
| 41  | 1j    | 97      | GLU  | 3.1  |
| 1   | 2A    | 897     | C    | 3.1  |
| 6   | 2G    | 90      | LEU  | 3.1  |
| 54  | 2x    | 9       | G    | 3.1  |
| 41  | 2j    | 87      | THR  | 3.1  |
| 44  | 1m    | 23      | TYR  | 3.1  |
| 1   | 2A    | 2189    | U    | 3.1  |
| 32  | 2a    | 1030(D) | A    | 3.1  |
| 1   | 1A    | 2162    | C    | 3.1  |
| 1   | 1A    | 1153    | G    | 3.1  |
| 26  | 14    | 17      | GLY  | 3.1  |
| 26  | 24    | 17      | GLY  | 3.1  |
| 26  | 24    | 35      | VAL  | 3.1  |
| 40  | 2i    | 31      | GLN  | 3.1  |
| 32  | 2a    | 1286    | A    | 3.1  |
| 32  | 2a    | 1447    | A    | 3.1  |
| 32  | 1a    | 1009    | G    | 3.1  |
| 51  | 2t    | 100     | ILE  | 3.1  |
| 32  | 1a    | 202     | U    | 3.0  |
| 29  | 27    | 48      | LYS  | 3.0  |
| 1   | 2A    | 2892    | A    | 3.0  |
| 7   | 2H    | 42      | ARG  | 3.0  |
| 32  | 2a    | 1001    | A    | 3.0  |
| 32  | 1a    | 153     | C    | 3.0  |
| 45  | 2n    | 27      | CYS  | 3.0  |
| 48  | 2q    | 16      | GLN  | 3.0  |
| 7   | 2H    | 96      | ALA  | 3.0  |
| 32  | 2a    | 1257    | U    | 3.0  |
| 32  | 2a    | 1392    | G    | 3.0  |
| 33  | 1b    | 210     | SER  | 3.0  |
| 40  | 1i    | 15      | ALA  | 3.0  |
| 33  | 2b    | 9       | GLU  | 3.0  |
| 1   | 2A    | 1531    | C    | 3.0  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 32         | 1a           | 154        | C           | 3.0         |
| 44         | 2m           | 42         | ALA         | 3.0         |
| 1          | 1A           | 273        | G           | 3.0         |
| 21         | 2Z           | 2          | GLU         | 3.0         |
| 26         | 24           | 57         | GLU         | 3.0         |
| 41         | 1j           | 31         | GLY         | 3.0         |
| 1          | 2A           | 280        | C           | 3.0         |
| 32         | 1a           | 841        | U           | 3.0         |
| 7          | 2H           | 98         | LEU         | 3.0         |
| 38         | 1g           | 57         | GLU         | 3.0         |
| 1          | 2A           | 652(C)     | G           | 3.0         |
| 1          | 2A           | 874        | G           | 3.0         |
| 1          | 2A           | 1059       | G           | 3.0         |
| 14         | 2S           | 35         | ILE         | 3.0         |
| 38         | 2g           | 156        | TRP         | 3.0         |
| 1          | 1A           | 2164       | C           | 3.0         |
| 1          | 2A           | 900        | A           | 3.0         |
| 32         | 1a           | 189(A)     | C           | 3.0         |
| 23         | 1l           | 27         | GLU         | 3.0         |
| 34         | 2c           | 145        | GLY         | 3.0         |
| 1          | 1A           | 1217       | G           | 3.0         |
| 1          | 1A           | 2143       | G           | 3.0         |
| 1          | 2A           | 1093       | G           | 3.0         |
| 33         | 2b           | 41         | ILE         | 3.0         |
| 17         | 2V           | 47         | VAL         | 3.0         |
| 32         | 1a           | 1446       | U           | 3.0         |
| 1          | 1A           | 1491       | A           | 3.0         |
| 1          | 2A           | 1109       | C           | 3.0         |
| 32         | 1a           | 1503       | A           | 3.0         |
| 37         | 2f           | 93         | SER         | 3.0         |
| 47         | 1p           | 17         | TYR         | 3.0         |
| 33         | 1b           | 28         | PHE         | 3.0         |
| 1          | 1A           | 2161       | C           | 3.0         |
| 1          | 2A           | 885        | C           | 3.0         |
| 33         | 2b           | 124        | SER         | 3.0         |
| 39         | 2h           | 116        | LYS         | 3.0         |
| 33         | 2b           | 136        | VAL         | 3.0         |
| 47         | 2p           | 46         | PRO         | 3.0         |
| 26         | 14           | 59         | PHE         | 3.0         |
| 26         | 24           | 42         | PHE         | 3.0         |
| 32         | 1a           | 725        | G           | 3.0         |
| 35         | 2d           | 12         | CYS         | 3.0         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 2          | 1B           | 3          | C           | 3.0         |
| 40         | 2i           | 64         | THR         | 3.0         |
| 21         | 2Z           | 195        | GLU         | 3.0         |
| 41         | 1j           | 34         | VAL         | 3.0         |
| 23         | 1l           | 54         | ALA         | 2.9         |
| 33         | 2b           | 14         | GLY         | 2.9         |
| 49         | 2r           | 55         | ARG         | 2.9         |
| 40         | 2i           | 95         | LYS         | 2.9         |
| 1          | 1A           | 1513       | G           | 2.9         |
| 1          | 2A           | 876        | C           | 2.9         |
| 32         | 1a           | 189(B)     | C           | 2.9         |
| 1          | 2A           | 2629       | A           | 2.9         |
| 5          | 2F           | 14         | PRO         | 2.9         |
| 41         | 1j           | 18         | ALA         | 2.9         |
| 21         | 1Z           | 33         | LEU         | 2.9         |
| 35         | 1d           | 166        | LYS         | 2.9         |
| 37         | 2f           | 95         | GLU         | 2.9         |
| 33         | 2b           | 47         | THR         | 2.9         |
| 44         | 2m           | 16         | ASP         | 2.9         |
| 1          | 1A           | 387        | G           | 2.9         |
| 1          | 2A           | 2893       | G           | 2.9         |
| 1          | 1A           | 945        | A           | 2.9         |
| 1          | 1A           | 2901       | A           | 2.9         |
| 1          | 2A           | 1509(A)    | A           | 2.9         |
| 1          | 2A           | 2860       | A           | 2.9         |
| 20         | 2Y           | 2          | ARG         | 2.9         |
| 32         | 2a           | 1532       | U           | 2.9         |
| 33         | 1b           | 227        | GLY         | 2.9         |
| 35         | 2d           | 158        | ILE         | 2.9         |
| 34         | 2c           | 126        | ARG         | 2.9         |
| 1          | 2A           | 275        | G           | 2.9         |
| 44         | 2m           | 51         | ALA         | 2.9         |
| 24         | 22           | 46         | GLN         | 2.9         |
| 33         | 2b           | 144        | ARG         | 2.9         |
| 1          | 2A           | 902        | C           | 2.9         |
| 32         | 1a           | 1008       | C           | 2.9         |
| 7          | 2H           | 103        | LEU         | 2.9         |
| 49         | 2r           | 62         | GLU         | 2.9         |
| 1          | 1A           | 2175       | G           | 2.9         |
| 1          | 1A           | 2641       | A           | 2.9         |
| 32         | 2a           | 142        | G           | 2.9         |
| 32         | 2a           | 189        | G           | 2.9         |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 26  | 24    | 65   | ASP  | 2.9  |
| 32  | 1a    | 1163 | C    | 2.9  |
| 33  | 2b    | 120  | ALA  | 2.9  |
| 49  | 1r    | 53   | ARG  | 2.9  |
| 36  | 1e    | 38   | GLN  | 2.9  |
| 1   | 2A    | 2190 | G    | 2.9  |
| 2   | 2B    | 118  | G    | 2.9  |
| 32  | 2a    | 532  | A    | 2.9  |
| 7   | 2H    | 48   | GLY  | 2.9  |
| 43  | 1l    | 62   | SER  | 2.9  |
| 1   | 1A    | 303  | C    | 2.9  |
| 32  | 2a    | 92   | C    | 2.9  |
| 1   | 2A    | 1090 | U    | 2.9  |
| 38  | 2g    | 28   | ASN  | 2.9  |
| 25  | 23    | 59   | VAL  | 2.9  |
| 35  | 2d    | 90   | GLY  | 2.9  |
| 44  | 1m    | 24   | GLY  | 2.9  |
| 1   | 2A    | 354  | G    | 2.9  |
| 6   | 2G    | 69   | ALA  | 2.9  |
| 6   | 2G    | 139  | LEU  | 2.9  |
| 32  | 1a    | 457  | C    | 2.8  |
| 32  | 2a    | 1129 | C    | 2.8  |
| 35  | 2d    | 37   | PRO  | 2.8  |
| 41  | 1j    | 73   | ASP  | 2.8  |
| 10  | 2O    | 57   | VAL  | 2.8  |
| 34  | 2c    | 74   | GLY  | 2.8  |
| 35  | 2d    | 36   | ARG  | 2.8  |
| 1   | 1A    | 2137 | G    | 2.8  |
| 47  | 2p    | 76   | GLN  | 2.8  |
| 1   | 2A    | 2177 | C    | 2.8  |
| 32  | 2a    | 155  | C    | 2.8  |
| 33  | 2b    | 39   | ILE  | 2.8  |
| 38  | 2g    | 3    | ARG  | 2.8  |
| 7   | 2H    | 44   | VAL  | 2.8  |
| 6   | 2G    | 43   | LEU  | 2.8  |
| 33  | 2b    | 121  | LEU  | 2.8  |
| 33  | 1b    | 79   | ASP  | 2.8  |
| 33  | 2b    | 43   | ASP  | 2.8  |
| 36  | 1e    | 114  | GLY  | 2.8  |
| 21  | 2Z    | 96   | VAL  | 2.8  |
| 33  | 1b    | 207  | ALA  | 2.8  |
| 1   | 1A    | 924  | U    | 2.8  |

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| Mol | Chain | Res    | Type | RSRZ |
|-----|-------|--------|------|------|
| 1   | 1A    | 1898   | A    | 2.8  |
| 1   | 1A    | 1512   | G    | 2.8  |
| 1   | 2A    | 1465   | G    | 2.8  |
| 7   | 2H    | 123    | PHE  | 2.8  |
| 40  | 1i    | 33     | PHE  | 2.8  |
| 50  | 2s    | 43     | GLU  | 2.8  |
| 32  | 2a    | 202    | U    | 2.8  |
| 44  | 1m    | 25     | ILE  | 2.8  |
| 1   | 2A    | 1166   | C    | 2.8  |
| 2   | 1B    | 2      | C    | 2.8  |
| 32  | 2a    | 71     | C    | 2.8  |
| 21  | 2Z    | 196    | VAL  | 2.8  |
| 32  | 1a    | 1144   | G    | 2.8  |
| 32  | 2a    | 80     | G    | 2.8  |
| 21  | 2Z    | 4      | ARG  | 2.8  |
| 41  | 2j    | 25     | GLU  | 2.8  |
| 1   | 2A    | 271(K) | U    | 2.8  |
| 1   | 2A    | 362    | U    | 2.8  |
| 1   | 2A    | 1105   | U    | 2.8  |
| 54  | 2x    | 47     | U    | 2.8  |
| 18  | 2W    | 63     | ASP  | 2.8  |
| 1   | 2A    | 1866   | C    | 2.8  |
| 44  | 2m    | 14     | ARG  | 2.8  |
| 1   | 2A    | 652(E) | G    | 2.8  |
| 1   | 2A    | 1719   | G    | 2.8  |
| 32  | 1a    | 1143   | G    | 2.8  |
| 5   | 1F    | 15     | SER  | 2.8  |
| 47  | 1p    | 19     | ILE  | 2.8  |
| 47  | 2p    | 9      | PHE  | 2.8  |
| 1   | 2A    | 1100   | C    | 2.8  |
| 32  | 2a    | 995    | C    | 2.8  |
| 49  | 1r    | 21     | LYS  | 2.8  |
| 1   | 2A    | 2191   | G    | 2.8  |
| 32  | 1a    | 993    | G    | 2.8  |
| 32  | 2a    | 1144   | G    | 2.8  |
| 40  | 2i    | 63     | ILE  | 2.8  |
| 21  | 2Z    | 198    | LYS  | 2.8  |
| 44  | 2m    | 70     | LEU  | 2.8  |
| 1   | 1A    | 2167   | C    | 2.8  |
| 1   | 2A    | 1885   | A    | 2.7  |
| 17  | 2V    | 42     | GLY  | 2.7  |
| 23  | 11    | 55     | GLY  | 2.7  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 50  | 2s    | 32   | LYS  | 2.7  |
| 1   | 2A    | 2116 | G    | 2.7  |
| 40  | 1i    | 62   | TYR  | 2.7  |
| 41  | 1j    | 27   | ALA  | 2.7  |
| 32  | 1a    | 651  | C    | 2.7  |
| 32  | 2a    | 1096 | C    | 2.7  |
| 1   | 1A    | 1466 | U    | 2.7  |
| 1   | 2A    | 1108 | U    | 2.7  |
| 52  | 2u    | 6    | ARG  | 2.7  |
| 36  | 1e    | 118  | ILE  | 2.7  |
| 33  | 1b    | 109  | SER  | 2.7  |
| 41  | 2j    | 24   | VAL  | 2.7  |
| 1   | 1A    | 698  | G    | 2.7  |
| 32  | 2a    | 1084 | G    | 2.7  |
| 54  | 2x    | 64   | G    | 2.7  |
| 1   | 2A    | 1486 | A    | 2.7  |
| 7   | 2H    | 105  | LEU  | 2.7  |
| 33  | 2b    | 216  | SER  | 2.7  |
| 34  | 2c    | 49   | SER  | 2.7  |
| 32  | 2a    | 1131 | G    | 2.7  |
| 32  | 2a    | 1202 | G    | 2.7  |
| 35  | 2d    | 6    | GLY  | 2.7  |
| 43  | 1l    | 64   | TYR  | 2.7  |
| 32  | 1a    | 203  | U    | 2.7  |
| 32  | 2a    | 1038 | C    | 2.7  |
| 32  | 2a    | 1380 | U    | 2.7  |
| 49  | 2r    | 29   | PHE  | 2.7  |
| 1   | 2A    | 1876 | A    | 2.7  |
| 32  | 1a    | 393  | A    | 2.7  |
| 35  | 1d    | 25   | ARG  | 2.7  |
| 35  | 2d    | 13   | ARG  | 2.7  |
| 1   | 1A    | 385  | G    | 2.7  |
| 32  | 2a    | 1390 | U    | 2.7  |
| 33  | 2b    | 37   | ASN  | 2.7  |
| 34  | 2c    | 124  | ILE  | 2.7  |
| 38  | 2g    | 6    | ARG  | 2.7  |
| 33  | 2b    | 133  | LYS  | 2.7  |
| 45  | 2n    | 22   | THR  | 2.7  |
| 49  | 2r    | 61   | LYS  | 2.7  |
| 1   | 1A    | 2122 | G    | 2.7  |
| 1   | 2A    | 1470 | G    | 2.7  |
| 32  | 1a    | 1039 | C    | 2.7  |

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| Mol | Chain | Res     | Type | RSRZ |
|-----|-------|---------|------|------|
| 32  | 2a    | 144     | G    | 2.7  |
| 32  | 2a    | 1097    | C    | 2.7  |
| 33  | 2b    | 45      | GLN  | 2.7  |
| 33  | 2b    | 19      | HIS  | 2.7  |
| 40  | 2i    | 52      | ALA  | 2.7  |
| 1   | 1A    | 691     | G    | 2.7  |
| 5   | 1F    | 16      | GLY  | 2.7  |
| 1   | 1A    | 700     | A    | 2.7  |
| 1   | 2A    | 1913    | A    | 2.7  |
| 32  | 2a    | 1268    | A    | 2.7  |
| 38  | 2g    | 78      | ARG  | 2.7  |
| 1   | 1A    | 272     | U    | 2.7  |
| 6   | 2G    | 58      | GLN  | 2.7  |
| 25  | 23    | 58      | VAL  | 2.7  |
| 34  | 2c    | 198     | VAL  | 2.7  |
| 49  | 2r    | 22      | VAL  | 2.7  |
| 34  | 2c    | 109     | PRO  | 2.7  |
| 51  | 2t    | 6       | PRO  | 2.7  |
| 38  | 2g    | 2       | ALA  | 2.7  |
| 26  | 24    | 68      | ARG  | 2.7  |
| 1   | 1A    | 2211    | U    | 2.6  |
| 33  | 2b    | 201     | ILE  | 2.6  |
| 41  | 2j    | 85      | LEU  | 2.6  |
| 21  | 2Z    | 175     | VAL  | 2.6  |
| 1   | 2A    | 1546    | C    | 2.6  |
| 26  | 14    | 48      | ARG  | 2.6  |
| 4   | 2E    | 87      | GLU  | 2.6  |
| 1   | 1A    | 1896    | G    | 2.6  |
| 1   | 2A    | 1107    | G    | 2.6  |
| 40  | 1i    | 47      | LEU  | 2.6  |
| 40  | 2i    | 98      | PRO  | 2.6  |
| 49  | 2r    | 60      | ALA  | 2.6  |
| 1   | 2A    | 1450(A) | C    | 2.6  |
| 1   | 2A    | 1505    | C    | 2.6  |
| 32  | 1a    | 1038    | C    | 2.6  |
| 32  | 2a    | 1126    | U    | 2.6  |
| 26  | 14    | 54      | GLY  | 2.6  |
| 44  | 1m    | 54      | VAL  | 2.6  |
| 1   | 2A    | 271(M)  | G    | 2.6  |
| 1   | 2A    | 2862    | G    | 2.6  |
| 21  | 2Z    | 95      | PRO  | 2.6  |
| 7   | 2H    | 58      | GLU  | 2.6  |

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| Mol | Chain | Res    | Type | RSRZ |
|-----|-------|--------|------|------|
| 1   | 2A    | 272(J) | C    | 2.6  |
| 32  | 1a    | 932    | C    | 2.6  |
| 32  | 1a    | 1043   | C    | 2.6  |
| 23  | 2l    | 2      | SER  | 2.6  |
| 50  | 2s    | 28     | LYS  | 2.6  |
| 1   | 2A    | 1098   | A    | 2.6  |
| 32  | 2a    | 270    | A    | 2.6  |
| 32  | 2a    | 1503   | A    | 2.6  |
| 34  | 2c    | 191    | THR  | 2.6  |
| 15  | 2T    | 39     | ARG  | 2.6  |
| 1   | 1A    | 1897   | C    | 2.6  |
| 41  | 2j    | 74     | ILE  | 2.6  |
| 32  | 2a    | 1446   | U    | 2.6  |
| 34  | 2c    | 184    | TYR  | 2.6  |
| 6   | 2G    | 108    | ASN  | 2.6  |
| 38  | 1g    | 3      | ARG  | 2.6  |
| 1   | 1A    | 929    | G    | 2.6  |
| 1   | 1A    | 1115   | A    | 2.6  |
| 1   | 2A    | 887    | A    | 2.6  |
| 32  | 2a    | 540    | G    | 2.6  |
| 32  | 2a    | 1094   | G    | 2.6  |
| 32  | 2a    | 1442   | G    | 2.6  |
| 33  | 1b    | 135    | GLN  | 2.6  |
| 41  | 2j    | 98     | ILE  | 2.6  |
| 32  | 2a    | 1037   | C    | 2.6  |
| 26  | 24    | 51     | ASP  | 2.6  |
| 26  | 24    | 59     | PHE  | 2.6  |
| 36  | 2e    | 94     | ALA  | 2.6  |
| 50  | 2s    | 29     | ARG  | 2.6  |
| 6   | 2G    | 39     | ILE  | 2.6  |
| 8   | 2I    | 54     | GLN  | 2.6  |
| 47  | 1p    | 37     | GLY  | 2.6  |
| 1   | 2A    | 652(U) | G    | 2.6  |
| 32  | 1a    | 1006   | C    | 2.6  |
| 32  | 2a    | 154    | C    | 2.6  |
| 33  | 2b    | 165    | VAL  | 2.6  |
| 21  | 2Z    | 176    | PRO  | 2.6  |
| 1   | 2A    | 271(L) | U    | 2.5  |
| 8   | 2I    | 58     | LEU  | 2.5  |
| 32  | 2a    | 427    | U    | 2.5  |
| 32  | 2a    | 841    | U    | 2.5  |
| 32  | 2a    | 1170   | A    | 2.5  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | 2A    | 1893 | C    | 2.5  |
| 1   | 2A    | 2187 | G    | 2.5  |
| 32  | 2a    | 1133 | G    | 2.5  |
| 32  | 2a    | 1143 | G    | 2.5  |
| 11  | 2P    | 123  | LEU  | 2.5  |
| 33  | 2b    | 115  | LEU  | 2.5  |
| 40  | 2i    | 27   | THR  | 2.5  |
| 41  | 1j    | 29   | ARG  | 2.5  |
| 51  | 2t    | 89   | ARG  | 2.5  |
| 26  | 14    | 51   | ASP  | 2.5  |
| 40  | 2i    | 36   | TYR  | 2.5  |
| 11  | 1P    | 143  | GLY  | 2.5  |
| 44  | 2m    | 67   | GLU  | 2.5  |
| 49  | 2r    | 51   | LEU  | 2.5  |
| 17  | 2V    | 22   | VAL  | 2.5  |
| 33  | 2b    | 140  | HIS  | 2.5  |
| 1   | 2A    | 1584 | C    | 2.5  |
| 1   | 2A    | 2140 | C    | 2.5  |
| 42  | 1k    | 60   | ALA  | 2.5  |
| 8   | 1l    | 131  | LYS  | 2.5  |
| 1   | 1A    | 389  | G    | 2.5  |
| 1   | 1A    | 1531 | G    | 2.5  |
| 1   | 2A    | 1485 | G    | 2.5  |
| 34  | 2c    | 159  | GLY  | 2.5  |
| 40  | 1i    | 8    | GLY  | 2.5  |
| 44  | 1m    | 26   | GLY  | 2.5  |
| 45  | 2n    | 38   | GLY  | 2.5  |
| 32  | 1a    | 96   | U    | 2.5  |
| 35  | 1d    | 170  | VAL  | 2.5  |
| 6   | 2G    | 55   | LYS  | 2.5  |
| 1   | 2A    | 1504 | C    | 2.5  |
| 8   | 2l    | 53   | ALA  | 2.5  |
| 1   | 2A    | 653  | A    | 2.5  |
| 7   | 2H    | 101  | ARG  | 2.5  |
| 32  | 2a    | 1236 | A    | 2.5  |
| 41  | 2j    | 8    | LEU  | 2.5  |
| 1   | 1A    | 1588 | G    | 2.5  |
| 54  | 1x    | 46   | G    | 2.5  |
| 9   | 1N    | 140  | VAL  | 2.5  |
| 16  | 2U    | 90   | VAL  | 2.5  |
| 33  | 1b    | 105  | PHE  | 2.5  |
| 33  | 2b    | 113  | HIS  | 2.5  |

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| Mol | Chain | Res    | Type | RSRZ |
|-----|-------|--------|------|------|
| 45  | 2n    | 29     | ARG  | 2.5  |
| 49  | 1r    | 24     | ALA  | 2.5  |
| 1   | 2A    | 893    | C    | 2.5  |
| 32  | 2a    | 1045   | C    | 2.5  |
| 1   | 1A    | 942    | A    | 2.5  |
| 1   | 1A    | 1591   | A    | 2.5  |
| 14  | 2S    | 56     | LEU  | 2.5  |
| 47  | 2p    | 74     | LEU  | 2.5  |
| 8   | 1I    | 19     | VAL  | 2.5  |
| 32  | 1a    | 189(K) | U    | 2.5  |
| 33  | 2b    | 83     | MET  | 2.5  |
| 35  | 2d    | 8      | VAL  | 2.5  |
| 1   | 2A    | 271(I) | G    | 2.5  |
| 32  | 2a    | 485    | G    | 2.5  |
| 22  | 20    | 11     | ARG  | 2.5  |
| 41  | 2j    | 29     | ARG  | 2.5  |
| 39  | 2h    | 55     | GLY  | 2.5  |
| 1   | 1A    | 1552   | C    | 2.5  |
| 1   | 2A    | 1080   | C    | 2.5  |
| 34  | 1c    | 87     | LEU  | 2.5  |
| 1   | 1A    | 1106   | U    | 2.5  |
| 1   | 2A    | 1060   | U    | 2.5  |
| 40  | 2i    | 28     | VAL  | 2.5  |
| 38  | 2g    | 79     | ARG  | 2.5  |
| 40  | 2i    | 20     | ARG  | 2.5  |
| 41  | 2j    | 47     | PHE  | 2.5  |
| 1   | 2A    | 361    | G    | 2.5  |
| 32  | 2a    | 145    | G    | 2.5  |
| 40  | 2i    | 94     | ALA  | 2.5  |
| 14  | 2S    | 33     | LYS  | 2.5  |
| 40  | 2i    | 92     | TYR  | 2.5  |
| 23  | 11    | 85     | LEU  | 2.5  |
| 41  | 2j    | 37     | PRO  | 2.5  |
| 6   | 2G    | 40     | ASN  | 2.5  |
| 7   | 2H    | 45     | VAL  | 2.5  |
| 12  | 2Q    | 59     | ARG  | 2.5  |
| 35  | 2d    | 159    | ARG  | 2.5  |
| 32  | 1a    | 1005   | A    | 2.5  |
| 33  | 2b    | 152    | PHE  | 2.5  |
| 7   | 2H    | 30     | LYS  | 2.5  |
| 34  | 2c    | 100    | ALA  | 2.5  |
| 1   | 2A    | 1089   | G    | 2.5  |

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| Mol | Chain | Res     | Type | RSRZ |
|-----|-------|---------|------|------|
| 32  | 2a    | 1442(A) | G    | 2.5  |
| 39  | 2h    | 29      | SER  | 2.4  |
| 45  | 1n    | 8       | GLU  | 2.4  |
| 1   | 1A    | 1507    | A    | 2.4  |
| 45  | 2n    | 2       | ALA  | 2.4  |
| 16  | 2U    | 78      | THR  | 2.4  |
| 54  | 2x    | 65      | C    | 2.4  |
| 34  | 2c    | 194     | GLY  | 2.4  |
| 26  | 24    | 48      | ARG  | 2.4  |
| 8   | 2I    | 47      | LEU  | 2.4  |
| 34  | 2c    | 188     | LEU  | 2.4  |
| 41  | 1j    | 85      | LEU  | 2.4  |
| 41  | 2j    | 38      | ILE  | 2.4  |
| 1   | 1A    | 2904    | U    | 2.4  |
| 1   | 2A    | 1110    | G    | 2.4  |
| 1   | 2A    | 1539    | G    | 2.4  |
| 1   | 2A    | 1895    | C    | 2.4  |
| 32  | 1a    | 183     | G    | 2.4  |
| 33  | 1b    | 18      | GLY  | 2.4  |
| 54  | 2x    | 15      | G    | 2.4  |
| 51  | 2t    | 93      | GLU  | 2.4  |
| 50  | 2s    | 30      | LEU  | 2.4  |
| 20  | 2Y    | 89      | PHE  | 2.4  |
| 32  | 2a    | 204     | U    | 2.4  |
| 1   | 1A    | 1550    | C    | 2.4  |
| 28  | 26    | 50      | ARG  | 2.4  |
| 1   | 2A    | 882     | G    | 2.4  |
| 1   | 2A    | 2184    | G    | 2.4  |
| 43  | 1l    | 51      | ALA  | 2.4  |
| 45  | 1n    | 2       | ALA  | 2.4  |
| 20  | 2Y    | 96      | ILE  | 2.4  |
| 36  | 2e    | 109     | ILE  | 2.4  |
| 21  | 2Z    | 177     | PRO  | 2.4  |
| 32  | 2a    | 141     | A    | 2.4  |
| 1   | 1A    | 2135    | U    | 2.4  |
| 14  | 2S    | 22      | GLY  | 2.4  |
| 23  | 11    | 28      | GLY  | 2.4  |
| 32  | 1a    | 1121    | U    | 2.4  |
| 11  | 2P    | 121     | LYS  | 2.4  |
| 18  | 2W    | 60      | ASN  | 2.4  |
| 33  | 1b    | 143     | GLU  | 2.4  |
| 1   | 1A    | 1146    | C    | 2.4  |

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| Mol | Chain | Res    | Type | RSRZ |
|-----|-------|--------|------|------|
| 1   | 1A    | 2125   | C    | 2.4  |
| 15  | 2T    | 131    | ALA  | 2.4  |
| 32  | 1a    | 1141   | C    | 2.4  |
| 1   | 2A    | 1042   | G    | 2.4  |
| 1   | 2A    | 1525   | G    | 2.4  |
| 6   | 2G    | 19     | LEU  | 2.4  |
| 32  | 2a    | 1142   | G    | 2.4  |
| 33  | 2b    | 138    | LEU  | 2.4  |
| 33  | 2b    | 142    | LEU  | 2.4  |
| 6   | 2G    | 57     | ALA  | 2.4  |
| 1   | 2A    | 652(D) | C    | 2.4  |
| 32  | 2a    | 848    | C    | 2.4  |
| 33  | 2b    | 10     | LEU  | 2.4  |
| 1   | 1A    | 1494   | G    | 2.4  |
| 5   | 1F    | 14     | PRO  | 2.4  |
| 26  | 24    | 54     | GLY  | 2.4  |
| 49  | 1r    | 22     | VAL  | 2.4  |
| 1   | 1A    | 274    | U    | 2.4  |
| 42  | 1k    | 28     | THR  | 2.4  |
| 43  | 1l    | 112    | ASP  | 2.4  |
| 23  | 2l    | 82     | LEU  | 2.4  |
| 54  | 2x    | 17     | C    | 2.4  |
| 38  | 2g    | 14     | PRO  | 2.4  |
| 32  | 2a    | 1088   | G    | 2.4  |
| 6   | 2G    | 155    | MET  | 2.4  |
| 11  | 1P    | 135    | LEU  | 2.4  |
| 23  | 2l    | 78     | LYS  | 2.4  |
| 35  | 2d    | 10     | ARG  | 2.4  |
| 40  | 2i    | 16     | ARG  | 2.4  |
| 1   | 2A    | 1040   | C    | 2.4  |
| 1   | 2A    | 1049   | C    | 2.4  |
| 50  | 2s    | 26     | GLY  | 2.3  |
| 6   | 2G    | 2      | PRO  | 2.3  |
| 40  | 2i    | 123    | PRO  | 2.3  |
| 1   | 1A    | 1572   | G    | 2.3  |
| 1   | 2A    | 1466   | G    | 2.3  |
| 1   | 2A    | 2101   | G    | 2.3  |
| 32  | 1a    | 146    | G    | 2.3  |
| 33  | 2b    | 132    | LYS  | 2.3  |
| 45  | 2n    | 11     | LYS  | 2.3  |
| 50  | 2s    | 50     | ALA  | 2.3  |
| 32  | 1a    | 163    | C    | 2.3  |

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| Mol | Chain | Res     | Type | RSRZ |
|-----|-------|---------|------|------|
| 44  | 1m    | 15      | VAL  | 2.3  |
| 38  | 1g    | 78      | ARG  | 2.3  |
| 6   | 2G    | 64      | THR  | 2.3  |
| 34  | 2c    | 65      | ALA  | 2.3  |
| 33  | 1b    | 44      | LEU  | 2.3  |
| 40  | 2i    | 19      | LEU  | 2.3  |
| 1   | 2A    | 1529    | G    | 2.3  |
| 33  | 2b    | 38      | GLY  | 2.3  |
| 1   | 2A    | 1179    | C    | 2.3  |
| 14  | 2S    | 34      | HIS  | 2.3  |
| 32  | 1a    | 419     | C    | 2.3  |
| 34  | 2c    | 106     | VAL  | 2.3  |
| 40  | 2i    | 124     | GLN  | 2.3  |
| 41  | 2j    | 20      | ALA  | 2.3  |
| 8   | 1l    | 12      | LEU  | 2.3  |
| 41  | 2j    | 97      | GLU  | 2.3  |
| 42  | 1k    | 98      | LEU  | 2.3  |
| 1   | 1A    | 1529    | G    | 2.3  |
| 2   | 2B    | 58      | A    | 2.3  |
| 2   | 2B    | 63      | G    | 2.3  |
| 32  | 2a    | 994     | A    | 2.3  |
| 33  | 2b    | 207     | ALA  | 2.3  |
| 41  | 1j    | 20      | ALA  | 2.3  |
| 50  | 2s    | 82      | GLY  | 2.3  |
| 7   | 2H    | 50      | VAL  | 2.3  |
| 47  | 1p    | 76      | GLN  | 2.3  |
| 7   | 2H    | 111     | HIS  | 2.3  |
| 2   | 2B    | 62      | C    | 2.3  |
| 32  | 1a    | 1022    | G    | 2.3  |
| 32  | 2a    | 996     | A    | 2.3  |
| 32  | 2a    | 1442(B) | A    | 2.3  |
| 33  | 1b    | 16      | HIS  | 2.3  |
| 35  | 2d    | 163     | GLU  | 2.3  |
| 6   | 2G    | 115     | ARG  | 2.3  |
| 7   | 2H    | 129     | THR  | 2.3  |
| 33  | 1b    | 15      | VAL  | 2.3  |
| 33  | 2b    | 24      | TRP  | 2.3  |
| 27  | 25    | 59      | GLU  | 2.3  |
| 37  | 2f    | 38      | GLU  | 2.3  |
| 1   | 2A    | 1469    | A    | 2.3  |
| 1   | 2A    | 2859    | G    | 2.3  |
| 32  | 1a    | 68      | G    | 2.3  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 32         | 1a           | 1263       | C           | 2.3         |
| 32         | 2a           | 93         | G           | 2.3         |
| 21         | 2Z           | 70         | LEU         | 2.3         |
| 11         | 1P           | 118        | GLY         | 2.3         |
| 38         | 1g           | 55         | GLY         | 2.3         |
| 37         | 2f           | 90         | VAL         | 2.3         |
| 38         | 1g           | 53         | LYS         | 2.3         |
| 6          | 2G           | 49         | ASP         | 2.3         |
| 1          | 2A           | 1077       | A           | 2.3         |
| 1          | 2A           | 1916       | A           | 2.3         |
| 34         | 2c           | 157        | ILE         | 2.3         |
| 36         | 2e           | 76         | ILE         | 2.3         |
| 11         | 2P           | 119        | GLU         | 2.3         |
| 40         | 1i           | 78         | LYS         | 2.3         |
| 33         | 2b           | 235        | SER         | 2.3         |
| 33         | 1b           | 130        | ARG         | 2.3         |
| 40         | 1i           | 83         | ARG         | 2.3         |
| 1          | 2A           | 1848       | A           | 2.3         |
| 1          | 2A           | 1112       | G           | 2.3         |
| 43         | 1l           | 43         | VAL         | 2.2         |
| 50         | 2s           | 23         | ASN         | 2.2         |
| 32         | 2a           | 952        | U           | 2.2         |
| 33         | 2b           | 13         | ALA         | 2.2         |
| 33         | 1b           | 126        | GLU         | 2.2         |
| 7          | 2H           | 54         | ARG         | 2.2         |
| 32         | 1a           | 156        | G           | 2.2         |
| 32         | 1a           | 1142       | G           | 2.2         |
| 32         | 2a           | 1294       | G           | 2.2         |
| 42         | 1k           | 53         | SER         | 2.2         |
| 1          | 1A           | 271        | U           | 2.2         |
| 35         | 2d           | 26         | CYS         | 2.2         |
| 40         | 1i           | 79         | LEU         | 2.2         |
| 42         | 2k           | 89         | ALA         | 2.2         |
| 50         | 1s           | 50         | ALA         | 2.2         |
| 21         | 2Z           | 146        | ILE         | 2.2         |
| 33         | 2b           | 143        | GLU         | 2.2         |
| 34         | 2c           | 122        | GLU         | 2.2         |
| 1          | 1A           | 699        | C           | 2.2         |
| 32         | 2a           | 962        | C           | 2.2         |
| 1          | 2A           | 1544       | A           | 2.2         |
| 1          | 2A           | 1877       | A           | 2.2         |
| 1          | 2A           | 9          | U           | 2.2         |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 6   | 2G    | 147  | ASP  | 2.2  |
| 1   | 2A    | 1062 | G    | 2.2  |
| 32  | 1a    | 1133 | G    | 2.2  |
| 50  | 2s    | 27   | GLU  | 2.2  |
| 2   | 2B    | 5    | C    | 2.2  |
| 1   | 2A    | 1460 | A    | 2.2  |
| 1   | 2A    | 1884 | A    | 2.2  |
| 11  | 2P    | 116  | GLY  | 2.2  |
| 32  | 2a    | 1492 | A    | 2.2  |
| 32  | 1a    | 921  | U    | 2.2  |
| 42  | 1k    | 81   | ASP  | 2.2  |
| 25  | 23    | 42   | ALA  | 2.2  |
| 34  | 1c    | 196  | LEU  | 2.2  |
| 46  | 2o    | 80   | ALA  | 2.2  |
| 32  | 1a    | 1120 | G    | 2.2  |
| 38  | 2g    | 115  | ARG  | 2.2  |
| 21  | 2Z    | 56   | VAL  | 2.2  |
| 34  | 2c    | 158  | GLY  | 2.2  |
| 1   | 2A    | 2895 | U    | 2.2  |
| 36  | 1e    | 43   | LEU  | 2.2  |
| 36  | 1e    | 112  | LEU  | 2.2  |
| 52  | 2u    | 23   | PRO  | 2.2  |
| 1   | 1A    | 927  | G    | 2.2  |
| 1   | 2A    | 1044 | G    | 2.2  |
| 27  | 25    | 60   | VAL  | 2.2  |
| 1   | 1A    | 270  | C    | 2.2  |
| 1   | 1A    | 1514 | C    | 2.2  |
| 1   | 1A    | 1595 | C    | 2.2  |
| 32  | 2a    | 1263 | C    | 2.2  |
| 34  | 1c    | 2    | GLY  | 2.2  |
| 38  | 2g    | 19   | GLY  | 2.2  |
| 42  | 1k    | 92   | GLU  | 2.2  |
| 1   | 1A    | 1154 | U    | 2.2  |
| 41  | 2j    | 73   | ASP  | 2.2  |
| 26  | 24    | 28   | LYS  | 2.2  |
| 43  | 1l    | 44   | THR  | 2.2  |
| 35  | 2d    | 4    | TYR  | 2.2  |
| 1   | 2A    | 355  | G    | 2.2  |
| 32  | 2a    | 69   | G    | 2.2  |
| 32  | 2a    | 70   | G    | 2.2  |
| 32  | 2a    | 460  | G    | 2.2  |
| 32  | 2a    | 1385 | G    | 2.2  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | 1A    | 304  | C    | 2.2  |
| 1   | 1A    | 1904 | C    | 2.2  |
| 32  | 1a    | 188  | C    | 2.2  |
| 32  | 1a    | 417  | C    | 2.2  |
| 32  | 2a    | 1395 | C    | 2.2  |
| 38  | 2g    | 114  | ARG  | 2.2  |
| 36  | 1e    | 117  | ASP  | 2.2  |
| 54  | 2x    | 61   | C    | 2.2  |
| 32  | 1a    | 591  | U    | 2.2  |
| 8   | 2I    | 88   | ILE  | 2.2  |
| 33  | 2b    | 214  | ILE  | 2.2  |
| 36  | 2e    | 75   | THR  | 2.2  |
| 42  | 2k    | 31   | THR  | 2.2  |
| 1   | 1A    | 388  | A    | 2.2  |
| 32  | 1a    | 270  | A    | 2.2  |
| 32  | 2a    | 1248 | A    | 2.2  |
| 32  | 2a    | 1275 | A    | 2.2  |
| 21  | 1Z    | 126  | VAL  | 2.2  |
| 33  | 2b    | 33   | TYR  | 2.2  |
| 23  | 2I    | 79   | GLY  | 2.2  |
| 34  | 2c    | 2    | GLY  | 2.2  |
| 6   | 2G    | 29   | TRP  | 2.2  |
| 1   | 1A    | 928  | G    | 2.2  |
| 1   | 2A    | 1894 | C    | 2.2  |
| 2   | 2B    | 107  | G    | 2.2  |
| 19  | 2X    | 92   | LEU  | 2.2  |
| 21  | 2Z    | 125  | LEU  | 2.2  |
| 32  | 1a    | 1082 | G    | 2.2  |
| 32  | 1a    | 1533 | C    | 2.2  |
| 7   | 2H    | 102  | ALA  | 2.2  |
| 40  | 1i    | 52   | ALA  | 2.2  |
| 54  | 2x    | 50   | U    | 2.2  |
| 33  | 1b    | 214  | ILE  | 2.2  |
| 7   | 2H    | 130  | ARG  | 2.2  |
| 1   | 2A    | 1220 | A    | 2.2  |
| 17  | 2V    | 5    | VAL  | 2.2  |
| 38  | 1g    | 80   | VAL  | 2.2  |
| 1   | 2A    | 284  | U    | 2.1  |
| 33  | 2b    | 28   | PHE  | 2.1  |
| 40  | 1i    | 50   | LEU  | 2.1  |
| 32  | 1a    | 155  | C    | 2.1  |
| 34  | 2c    | 187  | ALA  | 2.1  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 33  | 2b    | 111  | ARG  | 2.1  |
| 41  | 1j    | 35   | SER  | 2.1  |
| 34  | 2c    | 192  | THR  | 2.1  |
| 35  | 2d    | 89   | THR  | 2.1  |
| 6   | 2G    | 70   | VAL  | 2.1  |
| 1   | 2A    | 654  | A    | 2.1  |
| 2   | 2B    | 1    | U    | 2.1  |
| 33  | 1b    | 222  | ILE  | 2.1  |
| 49  | 2r    | 21   | LYS  | 2.1  |
| 32  | 2a    | 89   | C    | 2.1  |
| 37  | 1f    | 36   | ARG  | 2.1  |
| 1   | 1A    | 1467 | G    | 2.1  |
| 32  | 1a    | 471  | G    | 2.1  |
| 32  | 2a    | 447  | G    | 2.1  |
| 32  | 2a    | 1164 | G    | 2.1  |
| 7   | 2H    | 100  | GLY  | 2.1  |
| 34  | 1c    | 78   | GLY  | 2.1  |
| 35  | 1d    | 4    | TYR  | 2.1  |
| 40  | 1i    | 4    | TYR  | 2.1  |
| 8   | 2I    | 71   | ILE  | 2.1  |
| 28  | 26    | 37   | ARG  | 2.1  |
| 1   | 1A    | 692  | C    | 2.1  |
| 8   | 2I    | 134  | PRO  | 2.1  |
| 20  | 2Y    | 93   | GLY  | 2.1  |
| 33  | 2b    | 230  | VAL  | 2.1  |
| 47  | 1p    | 61   | SER  | 2.1  |
| 49  | 1r    | 57   | GLY  | 2.1  |
| 32  | 1a    | 1274 | G    | 2.1  |
| 32  | 2a    | 216  | G    | 2.1  |
| 47  | 2p    | 49   | LEU  | 2.1  |
| 15  | 2T    | 42   | ILE  | 2.1  |
| 32  | 2a    | 1085 | U    | 2.1  |
| 1   | 2A    | 289  | A    | 2.1  |
| 17  | 1V    | 27   | ALA  | 2.1  |
| 32  | 1a    | 1046 | A    | 2.1  |
| 39  | 2h    | 28   | ALA  | 2.1  |
| 8   | 1I    | 8    | PRO  | 2.1  |
| 11  | 2P    | 24   | GLY  | 2.1  |
| 43  | 2l    | 63   | GLY  | 2.1  |
| 34  | 1c    | 154  | SER  | 2.1  |
| 41  | 2j    | 68   | HIS  | 2.1  |
| 43  | 2l    | 123  | LYS  | 2.1  |

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| Mol | Chain | Res     | Type | RSRZ |
|-----|-------|---------|------|------|
| 21  | 2Z    | 155     | LEU  | 2.1  |
| 35  | 1d    | 138     | TYR  | 2.1  |
| 40  | 1i    | 128     | ARG  | 2.1  |
| 40  | 2i    | 125     | TYR  | 2.1  |
| 1   | 2A    | 1063    | G    | 2.1  |
| 42  | 2k    | 92      | GLU  | 2.1  |
| 41  | 1j    | 75      | ILE  | 2.1  |
| 32  | 2a    | 640     | A    | 2.1  |
| 34  | 2c    | 51      | GLY  | 2.1  |
| 51  | 1t    | 75      | ASN  | 2.1  |
| 41  | 1j    | 77      | PRO  | 2.1  |
| 1   | 1A    | 1511    | C    | 2.1  |
| 32  | 1a    | 178     | C    | 2.1  |
| 38  | 2g    | 9       | VAL  | 2.1  |
| 44  | 2m    | 17      | VAL  | 2.1  |
| 49  | 1r    | 87      | ARG  | 2.1  |
| 34  | 1c    | 43      | LEU  | 2.1  |
| 44  | 1m    | 19      | LEU  | 2.1  |
| 33  | 2b    | 127     | ILE  | 2.1  |
| 54  | 2x    | 60      | U    | 2.1  |
| 1   | 1A    | 694     | G    | 2.1  |
| 1   | 2A    | 271(H)  | G    | 2.1  |
| 32  | 2a    | 1258    | G    | 2.1  |
| 1   | 1A    | 1906    | A    | 2.1  |
| 32  | 1a    | 532     | A    | 2.1  |
| 32  | 1a    | 443     | C    | 2.1  |
| 14  | 2S    | 73      | LEU  | 2.1  |
| 16  | 2U    | 76      | TYR  | 2.1  |
| 36  | 2e    | 16      | THR  | 2.1  |
| 44  | 2m    | 49      | THR  | 2.1  |
| 1   | 2A    | 1065    | U    | 2.1  |
| 32  | 1a    | 182     | U    | 2.1  |
| 54  | 1x    | 20      | U    | 2.1  |
| 1   | 2A    | 1747(A) | G    | 2.1  |
| 11  | 2P    | 122     | PRO  | 2.1  |
| 26  | 24    | 50      | VAL  | 2.1  |
| 32  | 2a    | 1011    | G    | 2.1  |
| 32  | 2a    | 1266    | G    | 2.1  |
| 50  | 2s    | 53      | ASN  | 2.1  |
| 47  | 1p    | 54      | GLU  | 2.1  |
| 1   | 1A    | 2165    | C    | 2.1  |
| 1   | 2A    | 1111    | A    | 2.1  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 32  | 1a    | 162  | A    | 2.1  |
| 16  | 2U    | 88   | ILE  | 2.1  |
| 21  | 2Z    | 93   | ASP  | 2.1  |
| 21  | 2Z    | 133  | ILE  | 2.1  |
| 28  | 26    | 54   | ILE  | 2.1  |
| 41  | 2j    | 89   | ASP  | 2.1  |
| 35  | 1d    | 41   | GLY  | 2.1  |
| 52  | 2u    | 24   | ARG  | 2.1  |
| 8   | 1I    | 64   | GLU  | 2.1  |
| 35  | 2d    | 24   | GLU  | 2.1  |
| 35  | 1d    | 37   | PRO  | 2.1  |
| 44  | 2m    | 7    | VAL  | 2.1  |
| 48  | 1q    | 14   | LYS  | 2.1  |
| 1   | 2A    | 281  | G    | 2.1  |
| 32  | 1a    | 1042 | G    | 2.1  |
| 32  | 2a    | 630  | G    | 2.1  |
| 32  | 2a    | 1173 | G    | 2.1  |
| 32  | 1a    | 999  | C    | 2.0  |
| 32  | 2a    | 153  | C    | 2.0  |
| 8   | 1I    | 63   | ALA  | 2.0  |
| 23  | 1I    | 89   | GLU  | 2.0  |
| 33  | 2b    | 141  | GLU  | 2.0  |
| 42  | 2k    | 26   | ASN  | 2.0  |
| 50  | 1s    | 30   | LEU  | 2.0  |
| 1   | 2A    | 1170 | G    | 2.0  |
| 14  | 2S    | 108  | GLY  | 2.0  |
| 26  | 14    | 43   | TYR  | 2.0  |
| 32  | 2a    | 51   | A    | 2.0  |
| 32  | 2a    | 840  | C    | 2.0  |
| 32  | 2a    | 955  | U    | 2.0  |
| 7   | 2H    | 125  | VAL  | 2.0  |
| 6   | 2G    | 142  | PRO  | 2.0  |
| 7   | 2H    | 8    | PRO  | 2.0  |
| 35  | 1d    | 165  | MET  | 2.0  |
| 22  | 20    | 55   | ARG  | 2.0  |
| 26  | 24    | 6    | HIS  | 2.0  |
| 44  | 1m    | 55   | ARG  | 2.0  |
| 7   | 2H    | 110  | SER  | 2.0  |
| 44  | 2m    | 78   | ILE  | 2.0  |
| 1   | 1A    | 391  | G    | 2.0  |
| 1   | 1A    | 923  | C    | 2.0  |
| 1   | 1A    | 1495 | G    | 2.0  |

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| Mol | Chain | Res    | Type | RSRZ |
|-----|-------|--------|------|------|
| 1   | 1A    | 2158   | C    | 2.0  |
| 1   | 2A    | 272(H) | C    | 2.0  |
| 1   | 2A    | 1113   | U    | 2.0  |
| 32  | 2a    | 1091   | U    | 2.0  |
| 1   | 2A    | 1048   | A    | 2.0  |
| 32  | 2a    | 1300   | G    | 2.0  |
| 46  | 1o    | 69     | TYR  | 2.0  |
| 6   | 2G    | 160    | VAL  | 2.0  |
| 7   | 2H    | 99     | VAL  | 2.0  |
| 34  | 2c    | 195    | VAL  | 2.0  |
| 40  | 2i    | 21     | PRO  | 2.0  |
| 41  | 1j    | 17     | ASP  | 2.0  |
| 1   | 1A    | 2160   | C    | 2.0  |
| 1   | 2A    | 884    | C    | 2.0  |
| 32  | 2a    | 1391   | U    | 2.0  |
| 50  | 2s    | 52     | TYR  | 2.0  |
| 1   | 1A    | 1899   | A    | 2.0  |
| 1   | 2A    | 1114   | G    | 2.0  |
| 1   | 2A    | 1388   | G    | 2.0  |
| 1   | 2A    | 1490   | A    | 2.0  |
| 8   | 2I    | 81     | VAL  | 2.0  |
| 32  | 1a    | 189    | G    | 2.0  |
| 32  | 1a    | 472    | A    | 2.0  |
| 32  | 1a    | 540    | G    | 2.0  |
| 33  | 2b    | 21     | ARG  | 2.0  |
| 34  | 2c    | 186    | PHE  | 2.0  |
| 49  | 1r    | 42     | ARG  | 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(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|----------------------------|-------|
| 32  | 5MC  | 1a    | 1400 | 21/22 | 0.93 | 0.17 | -    | 39,42,46,48                | 0     |
| 1   | 2MA  | 2A    | 2503 | 23/24 | 0.97 | 0.21 | -    | 18,21,24,27                | 0     |
| 32  | 4OC  | 2a    | 1402 | 22/23 | 0.92 | 0.23 | -    | 44,50,53,56                | 0     |
| 32  | 4OC  | 1a    | 1402 | 22/23 | 0.95 | 0.19 | -    | 31,35,37,39                | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 54  | 4SU  | 1x    | 8    | 20/21 | 0.95 | 0.15 | -    | 36,42,44,45                 | 0     |
| 1   | 5MC  | 2A    | 1962 | 21/22 | 0.95 | 0.19 | -    | 30,33,36,42                 | 0     |
| 1   | PSU  | 2A    | 1911 | 20/21 | 0.95 | 0.25 | -    | 45,51,57,60                 | 0     |
| 54  | 5MC  | 2x    | 32   | 21/22 | 0.95 | 0.16 | -    | 46,55,57,59                 | 0     |
| 1   | PSU  | 1A    | 1933 | 20/21 | 0.96 | 0.21 | -    | 31,43,46,49                 | 0     |
| 1   | 5MU  | 2A    | 1915 | 21/22 | 0.85 | 0.41 | -    | 58,65,81,94                 | 0     |
| 32  | MA6  | 1a    | 1518 | 24/25 | 0.96 | 0.19 | -    | 23,27,28,29                 | 0     |
| 32  | 2MG  | 2a    | 1207 | 24/25 | 0.87 | 0.26 | -    | 58,64,73,77                 | 0     |
| 32  | PSU  | 1a    | 516  | 20/21 | 0.93 | 0.20 | -    | 39,48,50,50                 | 0     |
| 1   | 5MU  | 2A    | 1939 | 21/22 | 0.97 | 0.15 | -    | 26,28,30,31                 | 0     |
| 1   | 5MC  | 2A    | 1942 | 21/22 | 0.96 | 0.13 | -    | 35,37,40,45                 | 0     |
| 1   | PSU  | 1A    | 2617 | 20/21 | 0.96 | 0.19 | -    | 10,12,14,16                 | 0     |
| 1   | 5MU  | 1A    | 1961 | 21/22 | 0.97 | 0.18 | -    | 12,16,19,21                 | 0     |
| 54  | 5MC  | 1x    | 32   | 21/22 | 0.95 | 0.18 | -    | 36,39,43,49                 | 0     |
| 32  | 5MC  | 1a    | 1404 | 21/22 | 0.95 | 0.17 | -    | 27,31,34,45                 | 0     |
| 32  | 5MC  | 2a    | 967  | 21/22 | 0.91 | 0.21 | -    | 52,56,63,69                 | 0     |
| 54  | PSU  | 1x    | 55   | 20/21 | 0.93 | 0.19 | -    | 37,44,48,52                 | 0     |
| 1   | OMC  | 2A    | 1920 | 21/22 | 0.94 | 0.21 | -    | 39,46,48,50                 | 0     |
| 32  | M2G  | 1a    | 966  | 25/26 | 0.94 | 0.19 | -    | 34,37,46,48                 | 0     |
| 1   | OMU  | 2A    | 2552 | 21/22 | 0.97 | 0.20 | -    | 26,27,29,31                 | 0     |
| 32  | MA6  | 2a    | 1519 | 24/25 | 0.96 | 0.22 | -    | 37,43,46,49                 | 0     |
| 1   | PSU  | 1A    | 1939 | 20/21 | 0.90 | 0.30 | -    | 34,47,52,52                 | 0     |
| 1   | PSU  | 2A    | 2605 | 20/21 | 0.96 | 0.18 | -    | 22,26,27,27                 | 0     |
| 1   | 5MC  | 1A    | 1984 | 21/22 | 0.98 | 0.17 | -    | 19,23,25,30                 | 0     |
| 32  | M2G  | 2a    | 966  | 25/26 | 0.91 | 0.19 | -    | 48,53,60,61                 | 0     |
| 1   | OMU  | 1A    | 2564 | 21/22 | 0.97 | 0.19 | -    | 14,18,20,21                 | 0     |
| 32  | 7MG  | 2a    | 527  | 24/25 | 0.93 | 0.17 | -    | 52,56,62,67                 | 0     |
| 32  | 5MC  | 2a    | 1407 | 21/22 | 0.94 | 0.16 | -    | 35,44,46,47                 | 0     |
| 32  | 5MC  | 1a    | 1407 | 21/22 | 0.94 | 0.18 | -    | 27,31,35,36                 | 0     |
| 32  | 5MC  | 1a    | 967  | 21/22 | 0.94 | 0.17 | -    | 35,43,47,49                 | 0     |
| 43  | 0TD  | 2l    | 92   | 10/11 | 0.89 | 0.17 | -    | 50,53,56,61                 | 0     |
| 1   | 5MU  | 1A    | 1937 | 21/22 | 0.90 | 0.44 | -    | 50,57,72,76                 | 0     |
| 32  | 7MG  | 1a    | 527  | 24/25 | 0.94 | 0.18 | -    | 33,38,43,46                 | 0     |
| 54  | PSU  | 2x    | 55   | 20/21 | 0.88 | 0.15 | -    | 54,59,67,69                 | 0     |
| 43  | 0TD  | 1l    | 92   | 10/11 | 0.94 | 0.15 | -    | 41,43,47,48                 | 0     |
| 1   | PSU  | 2A    | 1917 | 20/21 | 0.91 | 0.26 | -    | 46,58,67,72                 | 0     |
| 32  | MA6  | 1a    | 1519 | 24/25 | 0.97 | 0.18 | -    | 24,28,29,31                 | 0     |
| 54  | 5MU  | 2x    | 54   | 21/22 | 0.91 | 0.19 | -    | 56,60,63,66                 | 0     |
| 32  | UR3  | 2a    | 1498 | 21/22 | 0.95 | 0.23 | -    | 39,44,48,51                 | 0     |
| 1   | 5MC  | 1A    | 1964 | 21/22 | 0.97 | 0.14 | -    | 25,29,33,40                 | 0     |
| 32  | 5MC  | 2a    | 1400 | 21/22 | 0.95 | 0.16 | -    | 54,59,62,64                 | 0     |
| 32  | MA6  | 2a    | 1518 | 24/25 | 0.95 | 0.17 | -    | 41,45,47,48                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 32  | 5MC  | 2a    | 1404 | 21/22 | 0.94 | 0.17 | -    | 36,41,44,47                 | 0     |
| 32  | UR3  | 1a    | 1498 | 21/22 | 0.97 | 0.17 | -    | 26,29,32,33                 | 0     |
| 1   | OMG  | 1A    | 2263 | 24/25 | 0.97 | 0.17 | -    | 9,10,12,12                  | 0     |
| 54  | 5MU  | 1x    | 54   | 21/22 | 0.95 | 0.18 | -    | 43,48,53,60                 | 0     |
| 54  | 4SU  | 2x    | 8    | 20/21 | 0.91 | 0.23 | -    | 51,57,61,61                 | 0     |
| 1   | OMG  | 2A    | 2251 | 24/25 | 0.97 | 0.18 | -    | 19,25,27,28                 | 0     |
| 32  | 2MG  | 1a    | 1207 | 24/25 | 0.91 | 0.29 | -    | 54,58,61,69                 | 0     |
| 1   | 2MA  | 1A    | 2515 | 23/24 | 0.98 | 0.18 | -    | 5,9,11,15                   | 0     |
| 1   | OMC  | 1A    | 1942 | 21/22 | 0.97 | 0.21 | -    | 26,34,40,42                 | 0     |
| 32  | PSU  | 2a    | 516  | 20/21 | 0.89 | 0.34 | -    | 58,63,69,71                 | 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   | 2A    | 3029 | 1/1   | 0.89 | 1.02 | 118.47 | 31,31,31,31                 | 0     |
| 56  | MG   | 2A    | 3131 | 1/1   | 0.91 | 1.10 | 60.43  | 33,33,33,33                 | 0     |
| 56  | MG   | 2A    | 3946 | 1/1   | 0.93 | 0.69 | 39.51  | 29,29,29,29                 | 0     |
| 56  | MG   | 2a    | 1725 | 1/1   | 0.20 | 0.87 | 34.04  | 71,71,71,71                 | 0     |
| 56  | MG   | 1A    | 8045 | 1/1   | 0.86 | 0.55 | 33.81  | 11,11,11,11                 | 0     |
| 56  | MG   | 2A    | 3244 | 1/1   | 0.96 | 0.43 | 32.27  | 30,30,30,30                 | 0     |
| 56  | MG   | 1A    | 8806 | 1/1   | 0.95 | 0.45 | 31.77  | 16,16,16,16                 | 0     |
| 56  | MG   | 1A    | 8647 | 1/1   | 0.96 | 0.43 | 30.52  | 14,14,14,14                 | 0     |
| 56  | MG   | 2A    | 3261 | 1/1   | 0.88 | 1.14 | 29.90  | 42,42,42,42                 | 0     |
| 56  | MG   | 2A    | 3203 | 1/1   | 0.91 | 0.56 | 29.78  | 28,28,28,28                 | 0     |
| 56  | MG   | 2A    | 3948 | 1/1   | 0.90 | 0.47 | 26.27  | 42,42,42,42                 | 0     |
| 56  | MG   | 2A    | 3611 | 1/1   | 0.96 | 0.58 | 26.18  | 34,34,34,34                 | 0     |
| 56  | MG   | 2A    | 3956 | 1/1   | 0.95 | 0.49 | 23.19  | 35,35,35,35                 | 0     |
| 56  | MG   | 2F    | 307  | 1/1   | 0.94 | 0.60 | 22.92  | 37,37,37,37                 | 0     |
| 56  | MG   | 2A    | 3774 | 1/1   | 0.96 | 0.49 | 22.91  | 56,56,56,56                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|----------------------------|-------|
| 56  | MG   | 2A    | 3199 | 1/1   | 0.84 | 0.43 | 22.57 | 30,30,30,30                | 0     |
| 56  | MG   | 1A    | 8917 | 1/1   | 0.91 | 0.45 | 22.54 | 21,21,21,21                | 0     |
| 56  | MG   | 1A    | 8291 | 1/1   | 0.91 | 0.46 | 21.94 | 13,13,13,13                | 0     |
| 56  | MG   | 1A    | 8753 | 1/1   | 0.83 | 0.40 | 21.87 | 13,13,13,13                | 0     |
| 56  | MG   | 2A    | 3944 | 1/1   | 0.90 | 0.49 | 21.14 | 28,28,28,28                | 0     |
| 56  | MG   | 2A    | 3024 | 1/1   | 0.95 | 0.40 | 20.28 | 30,30,30,30                | 0     |
| 56  | MG   | 2A    | 3530 | 1/1   | 0.92 | 0.59 | 19.40 | 45,45,45,45                | 0     |
| 56  | MG   | 2A    | 3938 | 1/1   | 0.97 | 0.46 | 19.28 | 38,38,38,38                | 0     |
| 56  | MG   | 1A    | 8024 | 1/1   | 0.92 | 0.29 | 18.84 | 8,8,8,8                    | 0     |
| 56  | MG   | 1A    | 8161 | 1/1   | 0.93 | 0.42 | 18.78 | 10,10,10,10                | 0     |
| 56  | MG   | 2A    | 3092 | 1/1   | 0.77 | 0.61 | 18.65 | 48,48,48,48                | 0     |
| 56  | MG   | 1A    | 8276 | 1/1   | 0.88 | 0.36 | 18.52 | 15,15,15,15                | 0     |
| 56  | MG   | 1A    | 8167 | 1/1   | 0.97 | 0.40 | 18.21 | 17,17,17,17                | 0     |
| 56  | MG   | 2A    | 3086 | 1/1   | 0.95 | 0.56 | 18.20 | 40,40,40,40                | 0     |
| 56  | MG   | 1A    | 8589 | 1/1   | 0.96 | 0.32 | 17.50 | 13,13,13,13                | 0     |
| 56  | MG   | 2A    | 3804 | 1/1   | 0.90 | 0.56 | 17.26 | 33,33,33,33                | 0     |
| 56  | MG   | 19    | 101  | 1/1   | 0.95 | 0.58 | 17.09 | 24,24,24,24                | 0     |
| 56  | MG   | 2A    | 3169 | 1/1   | 0.94 | 0.49 | 16.92 | 31,31,31,31                | 0     |
| 56  | MG   | 1A    | 8759 | 1/1   | 0.92 | 0.26 | 16.91 | 15,15,15,15                | 0     |
| 56  | MG   | 2A    | 3151 | 1/1   | 0.92 | 0.60 | 16.82 | 32,32,32,32                | 0     |
| 56  | MG   | 2A    | 3744 | 1/1   | 0.26 | 0.57 | 16.26 | 45,45,45,45                | 0     |
| 56  | MG   | 2A    | 3558 | 1/1   | 0.94 | 0.44 | 16.15 | 32,32,32,32                | 0     |
| 56  | MG   | 1A    | 8484 | 1/1   | 0.77 | 0.38 | 16.01 | 17,17,17,17                | 0     |
| 56  | MG   | 2A    | 3070 | 1/1   | 0.95 | 0.42 | 15.66 | 39,39,39,39                | 0     |
| 56  | MG   | 2A    | 3984 | 1/1   | 0.90 | 0.54 | 15.42 | 37,37,37,37                | 0     |
| 56  | MG   | 1A    | 8025 | 1/1   | 0.93 | 0.59 | 15.17 | 23,23,23,23                | 0     |
| 56  | MG   | 2A    | 3482 | 1/1   | 0.85 | 0.30 | 13.92 | 43,43,43,43                | 0     |
| 56  | MG   | 1A    | 8026 | 1/1   | 0.89 | 0.32 | 13.85 | 10,10,10,10                | 0     |
| 56  | MG   | 1a    | 1649 | 1/1   | 0.92 | 0.36 | 13.79 | 32,32,32,32                | 0     |
| 56  | MG   | 2a    | 1667 | 1/1   | 0.18 | 0.70 | 13.76 | 79,79,79,79                | 0     |
| 56  | MG   | 2a    | 1810 | 1/1   | 0.84 | 0.89 | 13.64 | 53,53,53,53                | 0     |
| 56  | MG   | 1A    | 8223 | 1/1   | 0.96 | 0.46 | 13.38 | 18,18,18,18                | 0     |
| 56  | MG   | 1A    | 8098 | 1/1   | 0.83 | 0.39 | 12.72 | 19,19,19,19                | 0     |
| 56  | MG   | 1A    | 8478 | 1/1   | 0.91 | 0.44 | 12.51 | 9,9,9,9                    | 0     |
| 56  | MG   | 2x    | 104  | 1/1   | 0.76 | 1.18 | 12.40 | 68,68,68,68                | 0     |
| 56  | MG   | 2A    | 3291 | 1/1   | 0.96 | 0.34 | 12.28 | 19,19,19,19                | 0     |
| 56  | MG   | 2A    | 3955 | 1/1   | 0.90 | 0.38 | 12.07 | 35,35,35,35                | 0     |
| 56  | MG   | 2A    | 3917 | 1/1   | 0.81 | 0.62 | 11.78 | 49,49,49,49                | 0     |
| 56  | MG   | 2a    | 1718 | 1/1   | 0.79 | 0.73 | 11.64 | 72,72,72,72                | 0     |
| 56  | MG   | 1A    | 8949 | 1/1   | 0.94 | 0.37 | 11.54 | 16,16,16,16                | 0     |
| 56  | MG   | 1A    | 8110 | 1/1   | 0.83 | 0.34 | 11.32 | 14,14,14,14                | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 56  | MG   | 1A    | 8147 | 1/1   | 0.95 | 0.33 | 11.28 | 18,18,18,18                 | 0     |
| 56  | MG   | 2a    | 1635 | 1/1   | 0.67 | 0.70 | 11.01 | 69,69,69,69                 | 0     |
| 56  | MG   | 1A    | 8108 | 1/1   | 0.94 | 0.38 | 10.94 | 18,18,18,18                 | 0     |
| 56  | MG   | 2a    | 1780 | 1/1   | 0.28 | 0.89 | 10.51 | 77,77,77,77                 | 0     |
| 56  | MG   | 1A    | 8021 | 1/1   | 0.97 | 0.31 | 10.23 | 12,12,12,12                 | 0     |
| 56  | MG   | 2A    | 3954 | 1/1   | 0.91 | 0.54 | 10.12 | 41,41,41,41                 | 0     |
| 56  | MG   | 1A    | 8952 | 1/1   | 0.91 | 0.28 | 9.97  | 17,17,17,17                 | 0     |
| 56  | MG   | 1a    | 1833 | 1/1   | 0.94 | 0.30 | 9.97  | 39,39,39,39                 | 0     |
| 56  | MG   | 1A    | 8658 | 1/1   | 0.97 | 0.28 | 9.85  | 9,9,9,9                     | 0     |
| 56  | MG   | 1a    | 1669 | 1/1   | 0.88 | 0.38 | 9.76  | 42,42,42,42                 | 0     |
| 56  | MG   | 2A    | 3585 | 1/1   | 0.94 | 0.35 | 9.60  | 33,33,33,33                 | 0     |
| 56  | MG   | 2A    | 3947 | 1/1   | 0.88 | 0.30 | 9.60  | 24,24,24,24                 | 0     |
| 56  | MG   | 1A    | 8532 | 1/1   | 0.89 | 0.27 | 9.59  | 15,15,15,15                 | 0     |
| 56  | MG   | 2A    | 3138 | 1/1   | 0.88 | 0.23 | 9.51  | 31,31,31,31                 | 0     |
| 56  | MG   | 1A    | 8091 | 1/1   | 0.92 | 0.28 | 9.50  | 16,16,16,16                 | 0     |
| 56  | MG   | 1a    | 1613 | 1/1   | 0.93 | 0.26 | 9.29  | 15,15,15,15                 | 0     |
| 56  | MG   | 1a    | 1740 | 1/1   | 0.87 | 0.40 | 9.23  | 54,54,54,54                 | 0     |
| 56  | MG   | 2A    | 3177 | 1/1   | 0.93 | 0.52 | 8.93  | 56,56,56,56                 | 0     |
| 56  | MG   | 1A    | 8922 | 1/1   | 0.75 | 0.26 | 8.81  | 16,16,16,16                 | 0     |
| 56  | MG   | 2A    | 3106 | 1/1   | 0.82 | 0.31 | 8.76  | 31,31,31,31                 | 0     |
| 56  | MG   | 2A    | 3702 | 1/1   | 0.79 | 0.34 | 8.75  | 55,55,55,55                 | 0     |
| 56  | MG   | 1A    | 8943 | 1/1   | 0.98 | 0.34 | 8.62  | 19,19,19,19                 | 0     |
| 56  | MG   | 2F    | 308  | 1/1   | 0.98 | 0.37 | 8.52  | 46,46,46,46                 | 0     |
| 56  | MG   | 1a    | 1836 | 1/1   | 0.95 | 0.35 | 8.47  | 36,36,36,36                 | 0     |
| 56  | MG   | 2a    | 1712 | 1/1   | 0.87 | 0.32 | 8.43  | 64,64,64,64                 | 0     |
| 56  | MG   | 1A    | 8683 | 1/1   | 0.88 | 0.28 | 8.40  | 30,30,30,30                 | 0     |
| 56  | MG   | 1o    | 101  | 1/1   | 0.84 | 0.35 | 8.33  | 50,50,50,50                 | 0     |
| 56  | MG   | 2A    | 3016 | 1/1   | 0.89 | 0.54 | 8.15  | 34,34,34,34                 | 0     |
| 56  | MG   | 1A    | 8743 | 1/1   | 0.96 | 0.28 | 8.11  | 14,14,14,14                 | 0     |
| 56  | MG   | 2A    | 3656 | 1/1   | 0.97 | 0.33 | 7.97  | 24,24,24,24                 | 0     |
| 56  | MG   | 1A    | 8173 | 1/1   | 0.95 | 0.28 | 7.94  | 15,15,15,15                 | 0     |
| 56  | MG   | 1A    | 8256 | 1/1   | 0.95 | 0.26 | 7.74  | 14,14,14,14                 | 0     |
| 56  | MG   | 2A    | 3061 | 1/1   | 0.57 | 0.60 | 7.67  | 68,68,68,68                 | 0     |
| 56  | MG   | 1A    | 8107 | 1/1   | 0.89 | 0.25 | 7.51  | 18,18,18,18                 | 0     |
| 56  | MG   | 2A    | 3575 | 1/1   | 0.92 | 0.28 | 7.49  | 42,42,42,42                 | 0     |
| 56  | MG   | 1A    | 8258 | 1/1   | 0.93 | 0.40 | 7.46  | 24,24,24,24                 | 0     |
| 56  | MG   | 2A    | 3028 | 1/1   | 0.92 | 0.41 | 7.45  | 34,34,34,34                 | 0     |
| 56  | MG   | 1A    | 8741 | 1/1   | 0.90 | 0.34 | 7.33  | 25,25,25,25                 | 0     |
| 56  | MG   | 2A    | 3654 | 1/1   | 0.94 | 0.44 | 7.16  | 41,41,41,41                 | 0     |
| 56  | MG   | 2A    | 3951 | 1/1   | 0.92 | 0.31 | 7.09  | 30,30,30,30                 | 0     |
| 56  | MG   | 1A    | 8565 | 1/1   | 0.94 | 0.27 | 7.07  | 17,17,17,17                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|----------------------------|-------|
| 56  | MG   | 1A    | 8217 | 1/1   | 0.95 | 0.22 | 6.97 | 11,11,11,11                | 0     |
| 56  | MG   | 2A    | 3269 | 1/1   | 0.95 | 0.41 | 6.79 | 44,44,44,44                | 0     |
| 56  | MG   | 2a    | 1661 | 1/1   | 0.81 | 0.35 | 6.69 | 43,43,43,43                | 0     |
| 56  | MG   | 2A    | 3142 | 1/1   | 0.90 | 0.26 | 6.69 | 36,36,36,36                | 0     |
| 56  | MG   | 2a    | 1728 | 1/1   | 0.91 | 0.34 | 6.56 | 64,64,64,64                | 0     |
| 56  | MG   | 1A    | 8597 | 1/1   | 0.93 | 0.27 | 6.42 | 14,14,14,14                | 0     |
| 56  | MG   | 2a    | 1765 | 1/1   | 0.92 | 0.38 | 6.38 | 47,47,47,47                | 0     |
| 56  | MG   | 1A    | 8080 | 1/1   | 0.87 | 0.25 | 6.32 | 18,18,18,18                | 0     |
| 56  | MG   | 1A    | 8494 | 1/1   | 0.98 | 0.31 | 6.08 | 17,17,17,17                | 0     |
| 56  | MG   | 1A    | 8933 | 1/1   | 0.98 | 0.30 | 6.02 | 20,20,20,20                | 0     |
| 56  | MG   | 1A    | 8117 | 1/1   | 0.95 | 0.24 | 5.97 | 27,27,27,27                | 0     |
| 56  | MG   | 1A    | 8832 | 1/1   | 0.98 | 0.24 | 5.87 | 12,12,12,12                | 0     |
| 56  | MG   | 1D    | 307  | 1/1   | 0.79 | 0.29 | 5.86 | 20,20,20,20                | 0     |
| 56  | MG   | 1A    | 8070 | 1/1   | 0.96 | 0.23 | 5.86 | 16,16,16,16                | 0     |
| 56  | MG   | 2A    | 3957 | 1/1   | 0.87 | 0.34 | 5.80 | 41,41,41,41                | 0     |
| 56  | MG   | 2A    | 3629 | 1/1   | 0.82 | 0.20 | 5.79 | 25,25,25,25                | 0     |
| 56  | MG   | 2A    | 3211 | 1/1   | 0.92 | 0.29 | 5.72 | 35,35,35,35                | 0     |
| 56  | MG   | 2A    | 3150 | 1/1   | 0.95 | 0.30 | 5.72 | 35,35,35,35                | 0     |
| 56  | MG   | 1A    | 8207 | 1/1   | 0.95 | 0.23 | 5.61 | 11,11,11,11                | 0     |
| 56  | MG   | 25    | 103  | 1/1   | 0.83 | 0.30 | 5.56 | 46,46,46,46                | 0     |
| 56  | MG   | 2A    | 3523 | 1/1   | 0.85 | 0.29 | 5.43 | 38,38,38,38                | 0     |
| 56  | MG   | 2A    | 3981 | 1/1   | 0.97 | 0.62 | 5.42 | 41,41,41,41                | 0     |
| 56  | MG   | 1a    | 1625 | 1/1   | 0.79 | 0.35 | 5.41 | 47,47,47,47                | 0     |
| 56  | MG   | 2a    | 1767 | 1/1   | 0.72 | 0.37 | 5.32 | 65,65,65,65                | 0     |
| 56  | MG   | 20    | 105  | 1/1   | 0.77 | 0.35 | 5.28 | 50,50,50,50                | 0     |
| 56  | MG   | 1A    | 8111 | 1/1   | 0.96 | 0.26 | 5.27 | 12,12,12,12                | 0     |
| 56  | MG   | 2A    | 3757 | 1/1   | 0.82 | 0.23 | 5.17 | 32,32,32,32                | 0     |
| 56  | MG   | 1A    | 8131 | 1/1   | 0.95 | 0.23 | 5.14 | 12,12,12,12                | 0     |
| 56  | MG   | 2A    | 3108 | 1/1   | 0.97 | 0.31 | 5.13 | 27,27,27,27                | 0     |
| 56  | MG   | 1A    | 8972 | 1/1   | 0.87 | 0.25 | 5.08 | 20,20,20,20                | 0     |
| 56  | MG   | 1A    | 8657 | 1/1   | 0.87 | 0.22 | 5.06 | 19,19,19,19                | 0     |
| 56  | MG   | 2a    | 1657 | 1/1   | 0.93 | 0.37 | 5.02 | 38,38,38,38                | 0     |
| 56  | MG   | 1A    | 8927 | 1/1   | 0.95 | 0.29 | 5.02 | 8,8,8,8                    | 0     |
| 56  | MG   | 2A    | 3084 | 1/1   | 0.97 | 0.32 | 5.01 | 21,21,21,21                | 0     |
| 56  | MG   | 2B    | 3020 | 1/1   | 0.66 | 0.27 | 4.96 | 54,54,54,54                | 0     |
| 56  | MG   | 2A    | 3561 | 1/1   | 0.95 | 0.31 | 4.94 | 32,32,32,32                | 0     |
| 56  | MG   | 2A    | 3350 | 1/1   | 0.82 | 0.24 | 4.94 | 28,28,28,28                | 0     |
| 56  | MG   | 1E    | 305  | 1/1   | 0.96 | 0.30 | 4.93 | 12,12,12,12                | 0     |
| 56  | MG   | 2A    | 3949 | 1/1   | 0.97 | 0.23 | 4.92 | 26,26,26,26                | 0     |
| 56  | MG   | 2B    | 3014 | 1/1   | 0.65 | 0.46 | 4.90 | 66,66,66,66                | 0     |
| 56  | MG   | 2A    | 3187 | 1/1   | 0.95 | 0.30 | 4.87 | 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    | 8032 | 1/1   | 0.92 | 0.19 | 4.87 | 6,6,6,6                     | 0     |
| 56  | MG   | 1A    | 8969 | 1/1   | 0.97 | 0.23 | 4.86 | 12,12,12,12                 | 0     |
| 56  | MG   | 2A    | 3657 | 1/1   | 0.87 | 0.41 | 4.85 | 33,33,33,33                 | 0     |
| 56  | MG   | 2A    | 3961 | 1/1   | 0.97 | 0.44 | 4.79 | 35,35,35,35                 | 0     |
| 56  | MG   | 1A    | 8911 | 1/1   | 0.91 | 0.30 | 4.77 | 32,32,32,32                 | 0     |
| 56  | MG   | 1A    | 8030 | 1/1   | 0.84 | 0.33 | 4.66 | 20,20,20,20                 | 0     |
| 56  | MG   | 2A    | 3080 | 1/1   | 0.94 | 0.29 | 4.64 | 31,31,31,31                 | 0     |
| 56  | MG   | 1A    | 8726 | 1/1   | 0.94 | 0.27 | 4.63 | 17,17,17,17                 | 0     |
| 56  | MG   | 2A    | 3921 | 1/1   | 0.91 | 0.34 | 4.61 | 19,19,19,19                 | 0     |
| 56  | MG   | 1A    | 8556 | 1/1   | 0.93 | 0.28 | 4.61 | 17,17,17,17                 | 0     |
| 56  | MG   | 1A    | 8215 | 1/1   | 0.88 | 0.25 | 4.58 | 12,12,12,12                 | 0     |
| 56  | MG   | 2A    | 3113 | 1/1   | 0.99 | 0.25 | 4.58 | 29,29,29,29                 | 0     |
| 56  | MG   | 1A    | 8268 | 1/1   | 0.94 | 0.26 | 4.52 | 15,15,15,15                 | 0     |
| 56  | MG   | 1A    | 8363 | 1/1   | 0.95 | 0.23 | 4.52 | 15,15,15,15                 | 0     |
| 56  | MG   | 1F    | 303  | 1/1   | 0.94 | 0.22 | 4.49 | 19,19,19,19                 | 0     |
| 56  | MG   | 2A    | 3831 | 1/1   | 0.96 | 0.31 | 4.49 | 35,35,35,35                 | 0     |
| 56  | MG   | 1F    | 301  | 1/1   | 0.73 | 0.25 | 4.36 | 21,21,21,21                 | 0     |
| 56  | MG   | 2F    | 302  | 1/1   | 0.91 | 0.33 | 4.35 | 28,28,28,28                 | 0     |
| 56  | MG   | 1A    | 8965 | 1/1   | 0.96 | 0.25 | 4.22 | 14,14,14,14                 | 0     |
| 56  | MG   | 2A    | 3976 | 1/1   | 0.96 | 0.30 | 4.20 | 28,28,28,28                 | 0     |
| 56  | MG   | 2A    | 3348 | 1/1   | 0.94 | 0.24 | 4.15 | 19,19,19,19                 | 0     |
| 56  | MG   | 1A    | 8955 | 1/1   | 0.86 | 0.27 | 4.12 | 11,11,11,11                 | 0     |
| 56  | MG   | 2A    | 3667 | 1/1   | 0.76 | 0.36 | 4.11 | 58,58,58,58                 | 0     |
| 56  | MG   | 2A    | 3391 | 1/1   | 0.94 | 0.27 | 4.09 | 20,20,20,20                 | 0     |
| 56  | MG   | 2A    | 3854 | 1/1   | 0.81 | 0.20 | 4.04 | 32,32,32,32                 | 0     |
| 56  | MG   | 2A    | 3926 | 1/1   | 0.96 | 0.28 | 4.02 | 36,36,36,36                 | 0     |
| 56  | MG   | 1A    | 8212 | 1/1   | 0.97 | 0.33 | 4.01 | 33,33,33,33                 | 0     |
| 56  | MG   | 1A    | 8126 | 1/1   | 0.91 | 0.22 | 3.95 | 12,12,12,12                 | 0     |
| 56  | MG   | 1a    | 1682 | 1/1   | 0.89 | 0.47 | 3.90 | 45,45,45,45                 | 0     |
| 56  | MG   | 2A    | 3748 | 1/1   | 0.97 | 0.19 | 3.89 | 47,47,47,47                 | 0     |
| 56  | MG   | 2A    | 3977 | 1/1   | 0.87 | 0.26 | 3.78 | 30,30,30,30                 | 0     |
| 56  | MG   | 1A    | 8022 | 1/1   | 0.99 | 0.23 | 3.78 | 12,12,12,12                 | 0     |
| 56  | MG   | 1A    | 8020 | 1/1   | 0.95 | 0.23 | 3.78 | 8,8,8,8                     | 0     |
| 56  | MG   | 2A    | 3971 | 1/1   | 0.91 | 0.48 | 3.71 | 41,41,41,41                 | 0     |
| 56  | MG   | 2A    | 3934 | 1/1   | 0.92 | 0.35 | 3.70 | 32,32,32,32                 | 0     |
| 56  | MG   | 2A    | 3964 | 1/1   | 0.96 | 0.36 | 3.69 | 37,37,37,37                 | 0     |
| 56  | MG   | 1A    | 8936 | 1/1   | 0.93 | 0.23 | 3.64 | 11,11,11,11                 | 0     |
| 56  | MG   | 18    | 101  | 1/1   | 0.82 | 0.28 | 3.63 | 49,49,49,49                 | 0     |
| 56  | MG   | 1A    | 8928 | 1/1   | 0.95 | 0.37 | 3.61 | 16,16,16,16                 | 0     |
| 56  | MG   | 2A    | 3593 | 1/1   | 0.93 | 0.27 | 3.56 | 24,24,24,24                 | 0     |
| 56  | MG   | 1A    | 8275 | 1/1   | 0.95 | 0.23 | 3.52 | 10,10,10,10                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56  | MG   | 1A    | 8266 | 1/1   | 0.87 | 0.21 | 3.45 | 13,13,13,13                 | 0     |
| 56  | MG   | 2A    | 3572 | 1/1   | 0.96 | 0.23 | 3.42 | 56,56,56,56                 | 0     |
| 56  | MG   | 15    | 105  | 1/1   | 0.95 | 0.24 | 3.41 | 12,12,12,12                 | 0     |
| 56  | MG   | 2A    | 3487 | 1/1   | 0.94 | 0.23 | 3.37 | 26,26,26,26                 | 0     |
| 56  | MG   | 1A    | 8008 | 1/1   | 0.97 | 0.25 | 3.35 | 23,23,23,23                 | 0     |
| 56  | MG   | 1A    | 8210 | 1/1   | 0.87 | 0.22 | 3.28 | 14,14,14,14                 | 0     |
| 56  | MG   | 1F    | 302  | 1/1   | 0.95 | 0.22 | 3.27 | 16,16,16,16                 | 0     |
| 56  | MG   | 2R    | 201  | 1/1   | 0.69 | 0.27 | 3.27 | 42,42,42,42                 | 0     |
| 56  | MG   | 2A    | 3959 | 1/1   | 0.98 | 0.34 | 3.24 | 38,38,38,38                 | 0     |
| 56  | MG   | 2A    | 3939 | 1/1   | 0.93 | 0.27 | 3.19 | 43,43,43,43                 | 0     |
| 56  | MG   | 1A    | 8178 | 1/1   | 0.94 | 0.26 | 3.10 | 14,14,14,14                 | 0     |
| 56  | MG   | 2A    | 3196 | 1/1   | 0.92 | 0.31 | 3.06 | 31,31,31,31                 | 0     |
| 56  | MG   | 2a    | 1729 | 1/1   | 0.91 | 0.33 | 3.05 | 62,62,62,62                 | 0     |
| 56  | MG   | 2A    | 3563 | 1/1   | 0.82 | 0.31 | 2.99 | 51,51,51,51                 | 0     |
| 56  | MG   | 1A    | 8970 | 1/1   | 0.81 | 0.25 | 2.92 | 29,29,29,29                 | 0     |
| 56  | MG   | 2A    | 3641 | 1/1   | 0.98 | 0.28 | 2.89 | 35,35,35,35                 | 0     |
| 56  | MG   | 2A    | 3405 | 1/1   | 0.97 | 0.23 | 2.84 | 28,28,28,28                 | 0     |
| 56  | MG   | 2a    | 1660 | 1/1   | 0.79 | 0.40 | 2.82 | 59,59,59,59                 | 0     |
| 56  | MG   | 1A    | 8467 | 1/1   | 0.95 | 0.18 | 2.81 | 9,9,9,9                     | 0     |
| 56  | MG   | 1D    | 314  | 1/1   | 0.79 | 0.22 | 2.73 | 31,31,31,31                 | 0     |
| 56  | MG   | 2A    | 3227 | 1/1   | 0.93 | 0.25 | 2.69 | 34,34,34,34                 | 0     |
| 56  | MG   | 2A    | 3740 | 1/1   | 0.91 | 0.40 | 2.69 | 39,39,39,39                 | 0     |
| 56  | MG   | 1A    | 8347 | 1/1   | 0.96 | 0.22 | 2.69 | 13,13,13,13                 | 0     |
| 56  | MG   | 1A    | 8041 | 1/1   | 0.93 | 0.22 | 2.67 | 24,24,24,24                 | 0     |
| 56  | MG   | 2U    | 204  | 1/1   | 0.74 | 0.30 | 2.65 | 52,52,52,52                 | 0     |
| 56  | MG   | 2A    | 3527 | 1/1   | 0.66 | 0.17 | 2.64 | 42,42,42,42                 | 0     |
| 56  | MG   | 1a    | 1751 | 1/1   | 0.88 | 0.32 | 2.63 | 59,59,59,59                 | 0     |
| 56  | MG   | 2A    | 3090 | 1/1   | 0.93 | 0.27 | 2.62 | 39,39,39,39                 | 0     |
| 56  | MG   | 2A    | 3219 | 1/1   | 0.87 | 0.21 | 2.61 | 29,29,29,29                 | 0     |
| 56  | MG   | 1a    | 1653 | 1/1   | 0.96 | 0.21 | 2.56 | 32,32,32,32                 | 0     |
| 56  | MG   | 1A    | 8973 | 1/1   | 0.95 | 0.24 | 2.56 | 12,12,12,12                 | 0     |
| 56  | MG   | 2A    | 3330 | 1/1   | 0.97 | 0.21 | 2.54 | 23,23,23,23                 | 0     |
| 56  | MG   | 2A    | 3987 | 1/1   | 0.94 | 0.28 | 2.53 | 28,28,28,28                 | 0     |
| 56  | MG   | 2A    | 3891 | 1/1   | 0.90 | 0.23 | 2.52 | 43,43,43,43                 | 0     |
| 56  | MG   | 2A    | 3924 | 1/1   | 0.81 | 0.26 | 2.52 | 26,26,26,26                 | 0     |
| 56  | MG   | 1A    | 8920 | 1/1   | 0.95 | 0.22 | 2.37 | 6,6,6,6                     | 0     |
| 56  | MG   | 2A    | 3364 | 1/1   | 0.86 | 0.26 | 2.35 | 42,42,42,42                 | 0     |
| 56  | MG   | 1A    | 8208 | 1/1   | 0.95 | 0.19 | 2.27 | 11,11,11,11                 | 0     |
| 56  | MG   | 2A    | 3833 | 1/1   | 0.67 | 0.24 | 2.22 | 28,28,28,28                 | 0     |
| 56  | MG   | 1A    | 8489 | 1/1   | 0.99 | 0.20 | 2.16 | 9,9,9,9                     | 0     |
| 56  | MG   | 2N    | 201  | 1/1   | 0.88 | 0.21 | 2.14 | 50,50,50,50                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|----------------------------|-------|
| 56  | MG   | 1B    | 3005 | 1/1   | 0.95 | 0.27 | 2.11 | 34,34,34,34                | 0     |
| 56  | MG   | 2B    | 3008 | 1/1   | 0.86 | 0.22 | 2.09 | 52,52,52,52                | 0     |
| 56  | MG   | 2A    | 3727 | 1/1   | 0.89 | 0.20 | 2.08 | 44,44,44,44                | 0     |
| 56  | MG   | 1A    | 8855 | 1/1   | 0.82 | 0.21 | 2.08 | 29,29,29,29                | 0     |
| 56  | MG   | 1A    | 8798 | 1/1   | 0.85 | 0.21 | 2.07 | 24,24,24,24                | 0     |
| 56  | MG   | 2a    | 1799 | 1/1   | 0.87 | 0.19 | 2.00 | 57,57,57,57                | 0     |
| 56  | MG   | 1a    | 1668 | 1/1   | 0.89 | 0.26 | 2.00 | 47,47,47,47                | 0     |
| 56  | MG   | 2A    | 3834 | 1/1   | 0.89 | 0.28 | 1.98 | 55,55,55,55                | 0     |
| 56  | MG   | 1D    | 305  | 1/1   | 0.93 | 0.19 | 1.97 | 18,18,18,18                | 0     |
| 56  | MG   | 1A    | 8146 | 1/1   | 0.97 | 0.19 | 1.96 | 13,13,13,13                | 0     |
| 56  | MG   | 1a    | 1755 | 1/1   | 0.80 | 0.25 | 1.86 | 60,60,60,60                | 0     |
| 56  | MG   | 1d    | 503  | 1/1   | 0.93 | 0.27 | 1.86 | 38,38,38,38                | 0     |
| 56  | MG   | 2A    | 3937 | 1/1   | 0.90 | 0.26 | 1.85 | 38,38,38,38                | 0     |
| 56  | MG   | 2A    | 3116 | 1/1   | 0.98 | 0.22 | 1.84 | 36,36,36,36                | 0     |
| 56  | MG   | 2A    | 3300 | 1/1   | 0.92 | 0.21 | 1.84 | 30,30,30,30                | 0     |
| 56  | MG   | 1a    | 1618 | 1/1   | 0.91 | 0.20 | 1.82 | 57,57,57,57                | 0     |
| 56  | MG   | 2D    | 314  | 1/1   | 0.87 | 0.22 | 1.79 | 25,25,25,25                | 0     |
| 56  | MG   | 1A    | 8561 | 1/1   | 0.97 | 0.22 | 1.74 | 17,17,17,17                | 0     |
| 56  | MG   | 1F    | 307  | 1/1   | 0.92 | 0.20 | 1.73 | 13,13,13,13                | 0     |
| 56  | MG   | 1A    | 8049 | 1/1   | 0.98 | 0.21 | 1.71 | 12,12,12,12                | 0     |
| 56  | MG   | 2D    | 304  | 1/1   | 0.93 | 0.21 | 1.70 | 41,41,41,41                | 0     |
| 56  | MG   | 29    | 502  | 1/1   | 0.93 | 0.23 | 1.66 | 53,53,53,53                | 0     |
| 56  | MG   | 2D    | 302  | 1/1   | 0.89 | 0.32 | 1.63 | 44,44,44,44                | 0     |
| 56  | MG   | 2A    | 3678 | 1/1   | 0.88 | 0.32 | 1.61 | 49,49,49,49                | 0     |
| 56  | MG   | 2A    | 3568 | 1/1   | 0.93 | 0.22 | 1.61 | 22,22,22,22                | 0     |
| 56  | MG   | 2a    | 1727 | 1/1   | 0.88 | 0.22 | 1.55 | 49,49,49,49                | 0     |
| 56  | MG   | 2A    | 3786 | 1/1   | 0.74 | 0.27 | 1.53 | 62,62,62,62                | 0     |
| 56  | MG   | 2A    | 3974 | 1/1   | 0.95 | 0.22 | 1.51 | 27,27,27,27                | 0     |
| 56  | MG   | 2A    | 3779 | 1/1   | 0.89 | 0.21 | 1.51 | 34,34,34,34                | 0     |
| 56  | MG   | 1A    | 8175 | 1/1   | 0.91 | 0.19 | 1.49 | 25,25,25,25                | 0     |
| 56  | MG   | 2A    | 3909 | 1/1   | 0.96 | 0.24 | 1.46 | 29,29,29,29                | 0     |
| 56  | MG   | 1a    | 1676 | 1/1   | 0.92 | 0.21 | 1.46 | 30,30,30,30                | 0     |
| 56  | MG   | 2A    | 3881 | 1/1   | 0.89 | 0.26 | 1.45 | 56,56,56,56                | 0     |
| 56  | MG   | 1a    | 1645 | 1/1   | 0.95 | 0.20 | 1.42 | 34,34,34,34                | 0     |
| 56  | MG   | 2A    | 3623 | 1/1   | 0.85 | 0.36 | 1.42 | 53,53,53,53                | 0     |
| 56  | MG   | 2A    | 3784 | 1/1   | 0.95 | 0.19 | 1.40 | 45,45,45,45                | 0     |
| 56  | MG   | 2A    | 3565 | 1/1   | 0.94 | 0.19 | 1.37 | 32,32,32,32                | 0     |
| 56  | MG   | 2A    | 3472 | 1/1   | 0.92 | 0.22 | 1.32 | 29,29,29,29                | 0     |
| 56  | MG   | 1a    | 1619 | 1/1   | 0.77 | 0.22 | 1.30 | 45,45,45,45                | 0     |
| 56  | MG   | 2A    | 3802 | 1/1   | 0.90 | 0.32 | 1.29 | 54,54,54,54                | 0     |
| 56  | MG   | 1A    | 8096 | 1/1   | 0.90 | 0.19 | 1.25 | 10,10,10,10                | 0     |
| 56  | MG   | 1A    | 8198 | 1/1   | 0.90 | 0.19 | 1.24 | 8,8,8,8                    | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56  | MG   | 1A    | 8957 | 1/1   | 0.95 | 0.20 | 1.22 | 26,26,26,26                 | 0     |
| 56  | MG   | 1A    | 8156 | 1/1   | 0.94 | 0.41 | 1.18 | 25,25,25,25                 | 0     |
| 56  | MG   | 2n    | 502  | 1/1   | 0.82 | 0.31 | 1.18 | 55,55,55,55                 | 0     |
| 56  | MG   | 1A    | 8925 | 1/1   | 0.91 | 0.20 | 1.16 | 32,32,32,32                 | 0     |
| 56  | MG   | 2a    | 1653 | 1/1   | 0.94 | 0.24 | 1.15 | 40,40,40,40                 | 0     |
| 56  | MG   | 2A    | 3605 | 1/1   | 0.73 | 0.16 | 1.15 | 35,35,35,35                 | 0     |
| 56  | MG   | 10    | 101  | 1/1   | 0.91 | 0.22 | 1.12 | 42,42,42,42                 | 0     |
| 56  | MG   | 1A    | 8971 | 1/1   | 0.91 | 0.21 | 1.12 | 9,9,9,9                     | 0     |
| 56  | MG   | 2A    | 3034 | 1/1   | 0.90 | 0.19 | 1.06 | 23,23,23,23                 | 0     |
| 56  | MG   | 1A    | 8014 | 1/1   | 0.93 | 0.18 | 1.01 | 5,5,5,5                     | 0     |
| 56  | MG   | 2A    | 3424 | 1/1   | 0.87 | 0.30 | 1.00 | 50,50,50,50                 | 0     |
| 56  | MG   | 2A    | 3661 | 1/1   | 0.95 | 0.19 | 0.93 | 36,36,36,36                 | 0     |
| 56  | MG   | 2a    | 1623 | 1/1   | 0.76 | 0.28 | 0.93 | 41,41,41,41                 | 0     |
| 56  | MG   | 2A    | 3465 | 1/1   | 0.93 | 0.18 | 0.93 | 23,23,23,23                 | 0     |
| 56  | MG   | 2A    | 3032 | 1/1   | 0.92 | 0.27 | 0.92 | 43,43,43,43                 | 0     |
| 56  | MG   | 1A    | 8953 | 1/1   | 0.95 | 0.20 | 0.85 | 13,13,13,13                 | 0     |
| 56  | MG   | 1A    | 8127 | 1/1   | 0.97 | 0.19 | 0.84 | 11,11,11,11                 | 0     |
| 56  | MG   | 2E    | 304  | 1/1   | 0.97 | 0.20 | 0.83 | 21,21,21,21                 | 0     |
| 56  | MG   | 2B    | 3005 | 1/1   | 0.79 | 0.30 | 0.80 | 55,55,55,55                 | 0     |
| 56  | MG   | 1A    | 8271 | 1/1   | 0.93 | 0.20 | 0.78 | 21,21,21,21                 | 0     |
| 56  | MG   | 2a    | 1695 | 1/1   | 0.92 | 0.26 | 0.71 | 53,53,53,53                 | 0     |
| 56  | MG   | 2a    | 1641 | 1/1   | 0.85 | 0.27 | 0.69 | 59,59,59,59                 | 0     |
| 56  | MG   | 2A    | 3110 | 1/1   | 0.98 | 0.25 | 0.66 | 35,35,35,35                 | 0     |
| 56  | MG   | 1R    | 202  | 1/1   | 0.95 | 0.20 | 0.65 | 26,26,26,26                 | 0     |
| 56  | MG   | 2Q    | 203  | 1/1   | 0.90 | 0.24 | 0.64 | 33,33,33,33                 | 0     |
| 56  | MG   | 2A    | 3027 | 1/1   | 0.92 | 0.18 | 0.63 | 31,31,31,31                 | 0     |
| 56  | MG   | 1a    | 1809 | 1/1   | 0.92 | 0.18 | 0.63 | 51,51,51,51                 | 0     |
| 56  | MG   | 2A    | 3272 | 1/1   | 0.96 | 0.17 | 0.62 | 30,30,30,30                 | 0     |
| 56  | MG   | 2a    | 1688 | 1/1   | 0.98 | 0.23 | 0.62 | 53,53,53,53                 | 0     |
| 56  | MG   | 2A    | 3492 | 1/1   | 0.96 | 0.21 | 0.61 | 35,35,35,35                 | 0     |
| 56  | MG   | 1A    | 8840 | 1/1   | 0.79 | 0.17 | 0.58 | 9,9,9,9                     | 0     |
| 56  | MG   | 2A    | 3063 | 1/1   | 0.70 | 0.22 | 0.55 | 38,38,38,38                 | 0     |
| 56  | MG   | 1A    | 8114 | 1/1   | 0.93 | 0.18 | 0.55 | 20,20,20,20                 | 0     |
| 56  | MG   | 2A    | 3968 | 1/1   | 0.92 | 0.20 | 0.47 | 38,38,38,38                 | 0     |
| 56  | MG   | 2D    | 312  | 1/1   | 0.86 | 0.19 | 0.45 | 39,39,39,39                 | 0     |
| 56  | MG   | 1A    | 8962 | 1/1   | 0.97 | 0.18 | 0.43 | 11,11,11,11                 | 0     |
| 56  | MG   | 2A    | 3338 | 1/1   | 0.95 | 0.20 | 0.43 | 40,40,40,40                 | 0     |
| 56  | MG   | 1A    | 8350 | 1/1   | 0.92 | 0.17 | 0.42 | 8,8,8,8                     | 0     |
| 56  | MG   | 1Q    | 201  | 1/1   | 0.87 | 0.20 | 0.42 | 17,17,17,17                 | 0     |
| 56  | MG   | 1A    | 8089 | 1/1   | 0.97 | 0.20 | 0.39 | 20,20,20,20                 | 0     |
| 56  | MG   | 2A    | 3307 | 1/1   | 0.99 | 0.18 | 0.36 | 43,43,43,43                 | 0     |
| 56  | MG   | 1A    | 8029 | 1/1   | 0.91 | 0.18 | 0.33 | 15,15,15,15                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 56  | MG   | 2A    | 3966 | 1/1   | 0.93 | 0.23 | 0.32  | 50,50,50,50                 | 0     |
| 56  | MG   | 2D    | 313  | 1/1   | 0.92 | 0.21 | 0.32  | 32,32,32,32                 | 0     |
| 56  | MG   | 1A    | 8918 | 1/1   | 0.91 | 0.17 | 0.31  | 16,16,16,16                 | 0     |
| 56  | MG   | 1a    | 1635 | 1/1   | 0.78 | 0.19 | 0.31  | 38,38,38,38                 | 0     |
| 56  | MG   | 2A    | 3213 | 1/1   | 0.88 | 0.21 | 0.31  | 32,32,32,32                 | 0     |
| 56  | MG   | 2A    | 3015 | 1/1   | 0.89 | 0.18 | 0.30  | 18,18,18,18                 | 0     |
| 56  | MG   | 2A    | 3608 | 1/1   | 0.95 | 0.18 | 0.28  | 21,21,21,21                 | 0     |
| 56  | MG   | 2A    | 3295 | 1/1   | 0.94 | 0.23 | 0.25  | 43,43,43,43                 | 0     |
| 56  | MG   | 1a    | 1821 | 1/1   | 0.91 | 0.19 | 0.24  | 39,39,39,39                 | 0     |
| 56  | MG   | 1A    | 8244 | 1/1   | 0.90 | 0.19 | 0.23  | 11,11,11,11                 | 0     |
| 56  | MG   | 2a    | 1814 | 1/1   | 0.95 | 0.26 | 0.21  | 40,40,40,40                 | 0     |
| 56  | MG   | 1A    | 8370 | 1/1   | 0.70 | 0.17 | 0.20  | 10,10,10,10                 | 0     |
| 56  | MG   | 1A    | 8495 | 1/1   | 0.89 | 0.16 | 0.18  | 14,14,14,14                 | 0     |
| 56  | MG   | 1A    | 8948 | 1/1   | 0.92 | 0.17 | 0.17  | 35,35,35,35                 | 0     |
| 56  | MG   | 1A    | 8320 | 1/1   | 0.76 | 0.18 | 0.16  | 7,7,7,7                     | 0     |
| 56  | MG   | 2A    | 3314 | 1/1   | 0.90 | 0.17 | 0.14  | 22,22,22,22                 | 0     |
| 56  | MG   | 2U    | 205  | 1/1   | 0.88 | 0.23 | 0.12  | 49,49,49,49                 | 0     |
| 56  | MG   | 1A    | 8144 | 1/1   | 0.89 | 0.15 | 0.05  | 35,35,35,35                 | 0     |
| 56  | MG   | 1A    | 8153 | 1/1   | 0.94 | 0.16 | 0.03  | 12,12,12,12                 | 0     |
| 56  | MG   | 1A    | 8128 | 1/1   | 0.90 | 0.25 | 0.03  | 40,40,40,40                 | 0     |
| 56  | MG   | 2A    | 3985 | 1/1   | 0.83 | 0.18 | 0.02  | 39,39,39,39                 | 0     |
| 56  | MG   | 1x    | 3005 | 1/1   | 0.86 | 0.23 | -0.00 | 51,51,51,51                 | 0     |
| 56  | MG   | 1A    | 8669 | 1/1   | 0.95 | 0.20 | -0.04 | 27,27,27,27                 | 0     |
| 56  | MG   | 2A    | 3323 | 1/1   | 0.77 | 0.22 | -0.07 | 47,47,47,47                 | 0     |
| 56  | MG   | 1A    | 8939 | 1/1   | 0.94 | 0.18 | -0.09 | 12,12,12,12                 | 0     |
| 56  | MG   | 2A    | 3916 | 1/1   | 0.79 | 0.35 | -0.10 | 86,86,86,86                 | 0     |
| 56  | MG   | 20    | 101  | 1/1   | 0.95 | 0.23 | -0.11 | 46,46,46,46                 | 0     |
| 56  | MG   | 1A    | 8272 | 1/1   | 0.96 | 0.17 | -0.11 | 27,27,27,27                 | 0     |
| 56  | MG   | 2P    | 202  | 1/1   | 0.97 | 0.24 | -0.12 | 37,37,37,37                 | 0     |
| 56  | MG   | 2A    | 3577 | 1/1   | 0.91 | 0.18 | -0.12 | 25,25,25,25                 | 0     |
| 56  | MG   | 1A    | 8703 | 1/1   | 0.93 | 0.18 | -0.23 | 28,28,28,28                 | 0     |
| 56  | MG   | 2a    | 1777 | 1/1   | 0.91 | 0.20 | -0.23 | 45,45,45,45                 | 0     |
| 56  | MG   | 1a    | 1839 | 1/1   | 0.79 | 0.22 | -0.25 | 48,48,48,48                 | 0     |
| 56  | MG   | 2A    | 3162 | 1/1   | 0.93 | 0.16 | -0.27 | 39,39,39,39                 | 0     |
| 56  | MG   | 2A    | 3168 | 1/1   | 0.94 | 0.17 | -0.28 | 24,24,24,24                 | 0     |
| 56  | MG   | 1a    | 1716 | 1/1   | 0.94 | 0.17 | -0.32 | 52,52,52,52                 | 0     |
| 56  | MG   | 1A    | 8353 | 1/1   | 0.95 | 0.16 | -0.32 | 7,7,7,7                     | 0     |
| 56  | MG   | 2d    | 505  | 1/1   | 0.47 | 0.21 | -0.35 | 73,73,73,73                 | 0     |
| 56  | MG   | 1A    | 8011 | 1/1   | 0.98 | 0.16 | -0.36 | 27,27,27,27                 | 0     |
| 56  | MG   | 1a    | 1692 | 1/1   | 0.93 | 0.19 | -0.36 | 40,40,40,40                 | 0     |
| 56  | MG   | 2A    | 3986 | 1/1   | 0.96 | 0.18 | -0.36 | 37,37,37,37                 | 0     |
| 56  | MG   | 1a    | 1609 | 1/1   | 0.95 | 0.21 | -0.37 | 43,43,43,43                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|----------------------------|-------|
| 56  | MG   | 2a    | 1659 | 1/1   | 0.92 | 0.15 | -0.37 | 46,46,46,46                | 0     |
| 56  | MG   | 1A    | 8627 | 1/1   | 0.94 | 0.25 | -0.39 | 48,48,48,48                | 0     |
| 56  | MG   | 1A    | 8930 | 1/1   | 0.93 | 0.17 | -0.42 | 23,23,23,23                | 0     |
| 56  | MG   | 2P    | 201  | 1/1   | 0.90 | 0.24 | -0.43 | 38,38,38,38                | 0     |
| 56  | MG   | 2A    | 3310 | 1/1   | 0.93 | 0.18 | -0.44 | 25,25,25,25                | 0     |
| 56  | MG   | 2A    | 3044 | 1/1   | 0.89 | 0.17 | -0.44 | 39,39,39,39                | 0     |
| 56  | MG   | 1A    | 8663 | 1/1   | 0.94 | 0.16 | -0.44 | 21,21,21,21                | 0     |
| 56  | MG   | 1A    | 8073 | 1/1   | 0.98 | 0.16 | -0.45 | 17,17,17,17                | 0     |
| 56  | MG   | 2A    | 3670 | 1/1   | 0.86 | 0.19 | -0.47 | 32,32,32,32                | 0     |
| 56  | MG   | 2A    | 3655 | 1/1   | 0.96 | 0.18 | -0.48 | 25,25,25,25                | 0     |
| 56  | MG   | 1A    | 8486 | 1/1   | 0.95 | 0.16 | -0.48 | 26,26,26,26                | 0     |
| 56  | MG   | 2A    | 3795 | 1/1   | 0.86 | 0.18 | -0.49 | 28,28,28,28                | 0     |
| 56  | MG   | 2A    | 3460 | 1/1   | 0.91 | 0.19 | -0.51 | 25,25,25,25                | 0     |
| 56  | MG   | 1A    | 8659 | 1/1   | 0.95 | 0.16 | -0.54 | 23,23,23,23                | 0     |
| 56  | MG   | 2A    | 3068 | 1/1   | 0.96 | 0.20 | -0.54 | 34,34,34,34                | 0     |
| 56  | MG   | 1a    | 1803 | 1/1   | 0.73 | 0.17 | -0.54 | 47,47,47,47                | 0     |
| 56  | MG   | 2A    | 3352 | 1/1   | 0.92 | 0.15 | -0.55 | 60,60,60,60                | 0     |
| 56  | MG   | 1A    | 8300 | 1/1   | 0.91 | 0.17 | -0.55 | 23,23,23,23                | 0     |
| 56  | MG   | 2A    | 3442 | 1/1   | 0.90 | 0.18 | -0.55 | 23,23,23,23                | 0     |
| 56  | MG   | 1A    | 8929 | 1/1   | 0.93 | 0.18 | -0.56 | 17,17,17,17                | 0     |
| 56  | MG   | 1A    | 8559 | 1/1   | 0.90 | 0.16 | -0.57 | 43,43,43,43                | 0     |
| 56  | MG   | 1x    | 3002 | 1/1   | 0.89 | 0.19 | -0.57 | 44,44,44,44                | 0     |
| 56  | MG   | 2A    | 3385 | 1/1   | 0.84 | 0.17 | -0.62 | 24,24,24,24                | 0     |
| 56  | MG   | 2A    | 3796 | 1/1   | 0.90 | 0.18 | -0.62 | 29,29,29,29                | 0     |
| 56  | MG   | 2A    | 3427 | 1/1   | 0.88 | 0.18 | -0.64 | 22,22,22,22                | 0     |
| 56  | MG   | 1d    | 506  | 1/1   | 0.51 | 0.17 | -0.65 | 77,77,77,77                | 0     |
| 56  | MG   | 2A    | 3154 | 1/1   | 0.96 | 0.16 | -0.67 | 31,31,31,31                | 0     |
| 56  | MG   | 1A    | 8468 | 1/1   | 0.66 | 0.15 | -0.67 | 29,29,29,29                | 0     |
| 56  | MG   | 1A    | 8964 | 1/1   | 0.97 | 0.16 | -0.69 | 12,12,12,12                | 0     |
| 56  | MG   | 2A    | 3869 | 1/1   | 0.81 | 0.17 | -0.69 | 38,38,38,38                | 0     |
| 56  | MG   | 1A    | 8068 | 1/1   | 0.96 | 0.19 | -0.70 | 16,16,16,16                | 0     |
| 56  | MG   | 2A    | 3380 | 1/1   | 0.92 | 0.17 | -0.75 | 25,25,25,25                | 0     |
| 56  | MG   | 1a    | 1622 | 1/1   | 0.94 | 0.17 | -0.85 | 32,32,32,32                | 0     |
| 56  | MG   | 1A    | 8443 | 1/1   | 0.90 | 0.17 | -0.86 | 13,13,13,13                | 0     |
| 56  | MG   | 2A    | 3320 | 1/1   | 0.84 | 0.18 | -0.88 | 27,27,27,27                | 0     |
| 56  | MG   | 1a    | 1655 | 1/1   | 0.98 | 0.15 | -0.88 | 28,28,28,28                | 0     |
| 56  | MG   | 1A    | 8355 | 1/1   | 0.93 | 0.17 | -0.89 | 7,7,7,7                    | 0     |
| 56  | MG   | 2a    | 1672 | 1/1   | 0.86 | 0.17 | -0.91 | 64,64,64,64                | 0     |
| 56  | MG   | 1A    | 8075 | 1/1   | 0.94 | 0.16 | -0.91 | 20,20,20,20                | 0     |
| 56  | MG   | 1U    | 203  | 1/1   | 0.96 | 0.17 | -0.92 | 13,13,13,13                | 0     |
| 56  | MG   | 1B    | 3008 | 1/1   | 0.91 | 0.15 | -0.93 | 35,35,35,35                | 0     |
| 56  | MG   | 2a    | 1604 | 1/1   | 0.86 | 0.19 | -0.94 | 44,44,44,44                | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|----------------------------|-------|
| 56  | MG   | 2B    | 3024 | 1/1   | 0.60 | 0.21 | -0.96 | 61,61,61,61                | 0     |
| 56  | MG   | 2A    | 3607 | 1/1   | 0.93 | 0.15 | -0.98 | 37,37,37,37                | 0     |
| 56  | MG   | 1A    | 8043 | 1/1   | 0.96 | 0.17 | -1.00 | 24,24,24,24                | 0     |
| 56  | MG   | 2A    | 3490 | 1/1   | 0.91 | 0.18 | -1.01 | 39,39,39,39                | 0     |
| 56  | MG   | 1a    | 1626 | 1/1   | 0.92 | 0.16 | -1.01 | 38,38,38,38                | 0     |
| 56  | MG   | 2A    | 3353 | 1/1   | 0.93 | 0.17 | -1.01 | 27,27,27,27                | 0     |
| 56  | MG   | 2A    | 3715 | 1/1   | 0.91 | 0.15 | -1.02 | 28,28,28,28                | 0     |
| 56  | MG   | 2A    | 3214 | 1/1   | 0.94 | 0.15 | -1.04 | 32,32,32,32                | 0     |
| 56  | MG   | 2A    | 3584 | 1/1   | 0.89 | 0.17 | -1.04 | 30,30,30,30                | 0     |
| 56  | MG   | 2A    | 3164 | 1/1   | 0.96 | 0.16 | -1.06 | 29,29,29,29                | 0     |
| 56  | MG   | 2x    | 101  | 1/1   | 0.94 | 0.22 | -1.11 | 48,48,48,48                | 0     |
| 56  | MG   | 1D    | 302  | 1/1   | 0.99 | 0.16 | -1.11 | 11,11,11,11                | 0     |
| 56  | MG   | 2Q    | 201  | 1/1   | 0.97 | 0.16 | -1.13 | 38,38,38,38                | 0     |
| 56  | MG   | 2f    | 8001 | 1/1   | 0.95 | 0.14 | -1.15 | 43,43,43,43                | 0     |
| 56  | MG   | 2b    | 3001 | 1/1   | 0.90 | 0.16 | -1.15 | 56,56,56,56                | 0     |
| 56  | MG   | 2G    | 3003 | 1/1   | 0.73 | 0.16 | -1.19 | 59,59,59,59                | 0     |
| 56  | MG   | 1A    | 8162 | 1/1   | 0.97 | 0.14 | -1.20 | 10,10,10,10                | 0     |
| 56  | MG   | 1A    | 8427 | 1/1   | 0.95 | 0.17 | -1.22 | 7,7,7,7                    | 0     |
| 56  | MG   | 2Q    | 204  | 1/1   | 0.96 | 0.14 | -1.25 | 42,42,42,42                | 0     |
| 56  | MG   | 1A    | 8412 | 1/1   | 0.87 | 0.18 | -1.26 | 6,6,6,6                    | 0     |
| 56  | MG   | 1D    | 309  | 1/1   | 0.98 | 0.16 | -1.26 | 26,26,26,26                | 0     |
| 56  | MG   | 1A    | 8209 | 1/1   | 0.95 | 0.15 | -1.26 | 15,15,15,15                | 0     |
| 56  | MG   | 2B    | 3004 | 1/1   | 0.92 | 0.17 | -1.27 | 63,63,63,63                | 0     |
| 56  | MG   | 1A    | 8437 | 1/1   | 0.88 | 0.15 | -1.27 | 6,6,6,6                    | 0     |
| 56  | MG   | 1l    | 101  | 1/1   | 0.96 | 0.15 | -1.30 | 26,26,26,26                | 0     |
| 56  | MG   | 2A    | 3927 | 1/1   | 0.85 | 0.15 | -1.32 | 30,30,30,30                | 0     |
| 56  | MG   | 2A    | 3973 | 1/1   | 0.96 | 0.17 | -1.34 | 35,35,35,35                | 0     |
| 56  | MG   | 1A    | 8923 | 1/1   | 0.97 | 0.18 | -1.37 | 17,17,17,17                | 0     |
| 56  | MG   | 2A    | 3932 | 1/1   | 0.94 | 0.18 | -1.39 | 31,31,31,31                | 0     |
| 56  | MG   | 1A    | 8749 | 1/1   | 0.97 | 0.14 | -1.40 | 22,22,22,22                | 0     |
| 56  | MG   | 2A    | 3893 | 1/1   | 0.86 | 0.15 | -1.41 | 44,44,44,44                | 0     |
| 56  | MG   | 1D    | 301  | 1/1   | 0.93 | 0.14 | -1.42 | 21,21,21,21                | 0     |
| 56  | MG   | 2A    | 3799 | 1/1   | 0.74 | 0.16 | -1.43 | 54,54,54,54                | 0     |
| 56  | MG   | 2a    | 1616 | 1/1   | 0.92 | 0.15 | -1.45 | 37,37,37,37                | 0     |
| 57  | ZN   | 14    | 501  | 1/1   | 0.85 | 0.13 | -1.45 | 75,75,75,75                | 0     |
| 56  | MG   | 1a    | 1605 | 1/1   | 0.84 | 0.15 | -1.46 | 43,43,43,43                | 0     |
| 56  | MG   | 1A    | 8380 | 1/1   | 0.84 | 0.15 | -1.47 | 16,16,16,16                | 0     |
| 56  | MG   | 1A    | 8491 | 1/1   | 0.91 | 0.15 | -1.48 | 9,9,9,9                    | 0     |
| 56  | MG   | 1A    | 8097 | 1/1   | 0.94 | 0.14 | -1.48 | 18,18,18,18                | 0     |
| 56  | MG   | 1A    | 8348 | 1/1   | 0.89 | 0.13 | -1.48 | 7,7,7,7                    | 0     |
| 56  | MG   | 2a    | 1720 | 1/1   | 0.86 | 0.15 | -1.48 | 43,43,43,43                | 0     |
| 56  | MG   | 1t    | 3001 | 1/1   | 0.99 | 0.21 | -1.48 | 37,37,37,37                | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|----------------------------|-------|
| 56  | MG   | 2G    | 3001 | 1/1   | 0.79 | 0.16 | -1.48 | 67,67,67,67                | 0     |
| 56  | MG   | 2A    | 3012 | 1/1   | 0.96 | 0.15 | -1.49 | 41,41,41,41                | 0     |
| 56  | MG   | 11    | 102  | 1/1   | 0.95 | 0.14 | -1.50 | 23,23,23,23                | 0     |
| 56  | MG   | 1b    | 3001 | 1/1   | 0.96 | 0.13 | -1.51 | 50,50,50,50                | 0     |
| 56  | MG   | 1a    | 1650 | 1/1   | 0.94 | 0.18 | -1.53 | 42,42,42,42                | 0     |
| 56  | MG   | 15    | 101  | 1/1   | 0.95 | 0.10 | -1.59 | 32,32,32,32                | 0     |
| 56  | MG   | 1R    | 201  | 1/1   | 0.92 | 0.16 | -1.59 | 18,18,18,18                | 0     |
| 56  | MG   | 2a    | 1791 | 1/1   | 0.88 | 0.11 | -1.59 | 51,51,51,51                | 0     |
| 56  | MG   | 2A    | 3676 | 1/1   | 0.95 | 0.16 | -1.62 | 31,31,31,31                | 0     |
| 56  | MG   | 1a    | 1838 | 1/1   | 0.93 | 0.13 | -1.63 | 46,46,46,46                | 0     |
| 56  | MG   | 2A    | 3280 | 1/1   | 0.83 | 0.14 | -1.63 | 35,35,35,35                | 0     |
| 56  | MG   | 2a    | 1817 | 1/1   | 0.97 | 0.10 | -1.63 | 49,49,49,49                | 0     |
| 56  | MG   | 1A    | 8288 | 1/1   | 0.97 | 0.15 | -1.64 | 8,8,8,8                    | 0     |
| 56  | MG   | 2D    | 311  | 1/1   | 0.95 | 0.14 | -1.65 | 29,29,29,29                | 0     |
| 56  | MG   | 1a    | 1620 | 1/1   | 0.83 | 0.17 | -1.66 | 46,46,46,46                | 0     |
| 56  | MG   | 1D    | 306  | 1/1   | 0.94 | 0.13 | -1.66 | 21,21,21,21                | 0     |
| 56  | MG   | 1a    | 1753 | 1/1   | 0.57 | 0.17 | -1.68 | 54,54,54,54                | 0     |
| 56  | MG   | 1A    | 8120 | 1/1   | 0.91 | 0.12 | -1.68 | 53,53,53,53                | 0     |
| 56  | MG   | 1A    | 8908 | 1/1   | 0.95 | 0.16 | -1.70 | 9,9,9,9                    | 0     |
| 56  | MG   | 1a    | 1634 | 1/1   | 0.92 | 0.14 | -1.71 | 22,22,22,22                | 0     |
| 56  | MG   | 1A    | 8298 | 1/1   | 0.92 | 0.12 | -1.71 | 12,12,12,12                | 0     |
| 56  | MG   | 1a    | 1785 | 1/1   | 0.65 | 0.15 | -1.72 | 74,74,74,74                | 0     |
| 56  | MG   | 2a    | 1633 | 1/1   | 0.98 | 0.12 | -1.73 | 41,41,41,41                | 0     |
| 56  | MG   | 2A    | 3443 | 1/1   | 0.98 | 0.15 | -1.73 | 31,31,31,31                | 0     |
| 56  | MG   | 1A    | 8581 | 1/1   | 0.98 | 0.14 | -1.73 | 15,15,15,15                | 0     |
| 56  | MG   | 2A    | 3260 | 1/1   | 0.93 | 0.17 | -1.75 | 26,26,26,26                | 0     |
| 56  | MG   | 1a    | 1702 | 1/1   | 0.94 | 0.14 | -1.75 | 48,48,48,48                | 0     |
| 56  | MG   | 2A    | 3007 | 1/1   | 0.93 | 0.14 | -1.76 | 38,38,38,38                | 0     |
| 56  | MG   | 2A    | 3965 | 1/1   | 0.98 | 0.15 | -1.78 | 32,32,32,32                | 0     |
| 56  | MG   | 1E    | 303  | 1/1   | 0.92 | 0.13 | -1.78 | 11,11,11,11                | 0     |
| 56  | MG   | 1A    | 8717 | 1/1   | 0.92 | 0.14 | -1.79 | 16,16,16,16                | 0     |
| 56  | MG   | 2a    | 1786 | 1/1   | 0.69 | 0.14 | -1.80 | 48,48,48,48                | 0     |
| 56  | MG   | 2A    | 3541 | 1/1   | 0.92 | 0.15 | -1.80 | 24,24,24,24                | 0     |
| 56  | MG   | 1a    | 1707 | 1/1   | 0.65 | 0.14 | -1.80 | 51,51,51,51                | 0     |
| 56  | MG   | 1A    | 8474 | 1/1   | 0.97 | 0.16 | -1.81 | 13,13,13,13                | 0     |
| 56  | MG   | 2a    | 1781 | 1/1   | 0.94 | 0.17 | -1.81 | 61,61,61,61                | 0     |
| 56  | MG   | 1A    | 8436 | 1/1   | 0.93 | 0.14 | -1.84 | 7,7,7,7                    | 0     |
| 56  | MG   | 2d    | 503  | 1/1   | 0.91 | 0.09 | -1.85 | 54,54,54,54                | 0     |
| 56  | MG   | 1a    | 1749 | 1/1   | 0.83 | 0.14 | -1.86 | 54,54,54,54                | 0     |
| 56  | MG   | 1Q    | 206  | 1/1   | 0.95 | 0.12 | -1.86 | 17,17,17,17                | 0     |
| 56  | MG   | 1a    | 1617 | 1/1   | 0.93 | 0.15 | -1.89 | 53,53,53,53                | 0     |
| 58  | SF4  | 1d    | 501  | 8/8   | 0.97 | 0.08 | -1.90 | 48,49,54,54                | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|----------------------------|-------|
| 56  | MG   | 1F    | 309  | 1/1   | 0.98 | 0.13 | -1.90 | 14,14,14,14                | 0     |
| 56  | MG   | 2a    | 1675 | 1/1   | 0.91 | 0.18 | -1.90 | 42,42,42,42                | 0     |
| 56  | MG   | 2a    | 1613 | 1/1   | 0.87 | 0.14 | -1.94 | 46,46,46,46                | 0     |
| 56  | MG   | 2A    | 3009 | 1/1   | 0.95 | 0.12 | -1.96 | 42,42,42,42                | 0     |
| 57  | ZN   | 2n    | 501  | 1/1   | 0.96 | 0.08 | -1.97 | 64,64,64,64                | 0     |
| 56  | MG   | 2A    | 3479 | 1/1   | 0.88 | 0.13 | -1.98 | 26,26,26,26                | 0     |
| 56  | MG   | 2A    | 3809 | 1/1   | 0.96 | 0.13 | -1.99 | 20,20,20,20                | 0     |
| 56  | MG   | 2A    | 3274 | 1/1   | 0.97 | 0.17 | -2.01 | 42,42,42,42                | 0     |
| 57  | ZN   | 16    | 101  | 1/1   | 0.99 | 0.09 | -2.02 | 24,24,24,24                | 0     |
| 56  | MG   | 2A    | 3438 | 1/1   | 0.89 | 0.16 | -2.04 | 25,25,25,25                | 0     |
| 56  | MG   | 1A    | 8382 | 1/1   | 0.98 | 0.13 | -2.04 | 8,8,8,8                    | 0     |
| 56  | MG   | 1A    | 8567 | 1/1   | 0.97 | 0.11 | -2.04 | 31,31,31,31                | 0     |
| 56  | MG   | 2A    | 3425 | 1/1   | 0.68 | 0.19 | -2.04 | 25,25,25,25                | 0     |
| 56  | MG   | 2a    | 1612 | 1/1   | 0.90 | 0.11 | -2.09 | 43,43,43,43                | 0     |
| 56  | MG   | 1A    | 8143 | 1/1   | 0.85 | 0.10 | -2.09 | 20,20,20,20                | 0     |
| 56  | MG   | 1a    | 1834 | 1/1   | 0.88 | 0.15 | -2.10 | 46,46,46,46                | 0     |
| 56  | MG   | 1Q    | 203  | 1/1   | 0.97 | 0.12 | -2.13 | 19,19,19,19                | 0     |
| 56  | MG   | 1a    | 1615 | 1/1   | 0.94 | 0.12 | -2.13 | 51,51,51,51                | 0     |
| 56  | MG   | 2a    | 1734 | 1/1   | 0.70 | 0.11 | -2.13 | 59,59,59,59                | 0     |
| 56  | MG   | 2A    | 3711 | 1/1   | 0.88 | 0.12 | -2.15 | 29,29,29,29                | 0     |
| 56  | MG   | 1a    | 1837 | 1/1   | 0.95 | 0.15 | -2.16 | 39,39,39,39                | 0     |
| 56  | MG   | 1A    | 8465 | 1/1   | 0.85 | 0.12 | -2.16 | 24,24,24,24                | 0     |
| 56  | MG   | 1A    | 8761 | 1/1   | 1.00 | 0.12 | -2.18 | 7,7,7,7                    | 0     |
| 56  | MG   | 2A    | 3347 | 1/1   | 0.96 | 0.15 | -2.19 | 34,34,34,34                | 0     |
| 56  | MG   | 2A    | 3919 | 1/1   | 0.98 | 0.14 | -2.20 | 32,32,32,32                | 0     |
| 56  | MG   | 2A    | 3276 | 1/1   | 0.92 | 0.12 | -2.21 | 42,42,42,42                | 0     |
| 56  | MG   | 2A    | 3023 | 1/1   | 0.96 | 0.14 | -2.24 | 43,43,43,43                | 0     |
| 56  | MG   | 2A    | 3025 | 1/1   | 0.92 | 0.13 | -2.25 | 33,33,33,33                | 0     |
| 57  | ZN   | 24    | 501  | 1/1   | 0.89 | 0.14 | -2.27 | 99,99,99,99                | 0     |
| 56  | MG   | 1A    | 8121 | 1/1   | 0.90 | 0.11 | -2.29 | 19,19,19,19                | 0     |
| 56  | MG   | 1a    | 1720 | 1/1   | 0.97 | 0.16 | -2.33 | 49,49,49,49                | 0     |
| 56  | MG   | 2A    | 3119 | 1/1   | 0.93 | 0.13 | -2.36 | 35,35,35,35                | 0     |
| 56  | MG   | 1A    | 8833 | 1/1   | 0.92 | 0.14 | -2.36 | 12,12,12,12                | 0     |
| 56  | MG   | 2A    | 3073 | 1/1   | 0.95 | 0.14 | -2.39 | 32,32,32,32                | 0     |
| 56  | MG   | 2A    | 3129 | 1/1   | 0.96 | 0.14 | -2.41 | 28,28,28,28                | 0     |
| 56  | MG   | 1A    | 8006 | 1/1   | 0.97 | 0.12 | -2.42 | 14,14,14,14                | 0     |
| 56  | MG   | 1A    | 8937 | 1/1   | 0.98 | 0.12 | -2.42 | 11,11,11,11                | 0     |
| 56  | MG   | 2F    | 306  | 1/1   | 0.96 | 0.13 | -2.44 | 30,30,30,30                | 0     |
| 56  | MG   | 1a    | 1603 | 1/1   | 0.91 | 0.11 | -2.44 | 39,39,39,39                | 0     |
| 56  | MG   | 1A    | 8424 | 1/1   | 0.92 | 0.13 | -2.44 | 26,26,26,26                | 0     |
| 57  | ZN   | 1Y    | 501  | 1/1   | 0.98 | 0.07 | -2.45 | 47,47,47,47                | 0     |
| 56  | MG   | 2A    | 3049 | 1/1   | 0.89 | 0.15 | -2.46 | 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    | 3536 | 1/1   | 0.67 | 0.13 | -2.47 | 31,31,31,31                 | 0     |
| 56  | MG   | 1A    | 8919 | 1/1   | 0.91 | 0.14 | -2.48 | 11,11,11,11                 | 0     |
| 56  | MG   | 2A    | 3953 | 1/1   | 0.51 | 0.15 | -2.50 | 37,37,37,37                 | 0     |
| 56  | MG   | 2A    | 3147 | 1/1   | 0.95 | 0.11 | -2.51 | 36,36,36,36                 | 0     |
| 56  | MG   | 2A    | 3042 | 1/1   | 0.94 | 0.13 | -2.53 | 38,38,38,38                 | 0     |
| 56  | MG   | 2A    | 3293 | 1/1   | 0.96 | 0.13 | -2.54 | 24,24,24,24                 | 0     |
| 57  | ZN   | 15    | 102  | 1/1   | 0.99 | 0.08 | -2.54 | 31,31,31,31                 | 0     |
| 56  | MG   | 1A    | 8611 | 1/1   | 0.96 | 0.12 | -2.55 | 17,17,17,17                 | 0     |
| 56  | MG   | 2A    | 3945 | 1/1   | 0.88 | 0.13 | -2.55 | 22,22,22,22                 | 0     |
| 56  | MG   | 2A    | 3941 | 1/1   | 0.98 | 0.12 | -2.55 | 35,35,35,35                 | 0     |
| 56  | MG   | 2A    | 3659 | 1/1   | 0.92 | 0.14 | -2.56 | 30,30,30,30                 | 0     |
| 56  | MG   | 1A    | 8461 | 1/1   | 0.90 | 0.12 | -2.58 | 10,10,10,10                 | 0     |
| 56  | MG   | 1A    | 8186 | 1/1   | 0.94 | 0.12 | -2.59 | 26,26,26,26                 | 0     |
| 56  | MG   | 1Q    | 205  | 1/1   | 0.94 | 0.14 | -2.60 | 26,26,26,26                 | 0     |
| 56  | MG   | 1A    | 8572 | 1/1   | 0.92 | 0.14 | -2.63 | 5,5,5,5                     | 0     |
| 56  | MG   | 2A    | 3868 | 1/1   | 0.90 | 0.15 | -2.63 | 48,48,48,48                 | 0     |
| 56  | MG   | 1A    | 8086 | 1/1   | 0.98 | 0.16 | -2.64 | 18,18,18,18                 | 0     |
| 56  | MG   | 1A    | 8149 | 1/1   | 0.98 | 0.12 | -2.65 | 11,11,11,11                 | 0     |
| 56  | MG   | 2D    | 305  | 1/1   | 0.98 | 0.11 | -2.66 | 33,33,33,33                 | 0     |
| 56  | MG   | 2a    | 1797 | 1/1   | 0.82 | 0.12 | -2.68 | 47,47,47,47                 | 0     |
| 56  | MG   | 1A    | 8588 | 1/1   | 0.97 | 0.12 | -2.68 | 11,11,11,11                 | 0     |
| 56  | MG   | 1G    | 3001 | 1/1   | 0.96 | 0.10 | -2.68 | 52,52,52,52                 | 0     |
| 56  | MG   | 1A    | 8257 | 1/1   | 0.96 | 0.13 | -2.68 | 11,11,11,11                 | 0     |
| 56  | MG   | 2d    | 502  | 1/1   | 0.98 | 0.08 | -2.69 | 53,53,53,53                 | 0     |
| 56  | MG   | 1A    | 8959 | 1/1   | 0.92 | 0.17 | -2.70 | 27,27,27,27                 | 0     |
| 56  | MG   | 1A    | 8569 | 1/1   | 0.93 | 0.14 | -2.70 | 16,16,16,16                 | 0     |
| 56  | MG   | 1A    | 8942 | 1/1   | 0.96 | 0.13 | -2.70 | 11,11,11,11                 | 0     |
| 56  | MG   | 1G    | 3003 | 1/1   | 0.99 | 0.10 | -2.71 | 31,31,31,31                 | 0     |
| 56  | MG   | 1A    | 8940 | 1/1   | 0.97 | 0.16 | -2.74 | 6,6,6,6                     | 0     |
| 56  | MG   | 1a    | 1695 | 1/1   | 0.98 | 0.10 | -2.76 | 27,27,27,27                 | 0     |
| 56  | MG   | 2A    | 3692 | 1/1   | 0.97 | 0.09 | -2.79 | 33,33,33,33                 | 0     |
| 56  | MG   | 1A    | 8890 | 1/1   | 0.94 | 0.13 | -2.80 | 23,23,23,23                 | 0     |
| 56  | MG   | 1A    | 8323 | 1/1   | 0.91 | 0.10 | -2.80 | 20,20,20,20                 | 0     |
| 56  | MG   | 1A    | 8063 | 1/1   | 0.92 | 0.13 | -2.81 | 22,22,22,22                 | 0     |
| 56  | MG   | 1A    | 8373 | 1/1   | 0.93 | 0.12 | -2.82 | 13,13,13,13                 | 0     |
| 56  | MG   | 1A    | 8293 | 1/1   | 0.98 | 0.14 | -2.82 | 12,12,12,12                 | 0     |
| 56  | MG   | 1A    | 8071 | 1/1   | 0.98 | 0.14 | -2.82 | 10,10,10,10                 | 0     |
| 56  | MG   | 1a    | 1776 | 1/1   | 0.77 | 0.16 | -2.83 | 35,35,35,35                 | 0     |
| 56  | MG   | 1A    | 8886 | 1/1   | 0.97 | 0.12 | -2.84 | 24,24,24,24                 | 0     |
| 58  | SF4  | 2d    | 501  | 8/8   | 0.97 | 0.08 | -2.85 | 47,53,59,65                 | 0     |
| 56  | MG   | 1A    | 8954 | 1/1   | 0.98 | 0.15 | -2.86 | 13,13,13,13                 | 0     |
| 56  | MG   | 2a    | 1678 | 1/1   | 0.92 | 0.11 | -2.87 | 37,37,37,37                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|----------------------------|-------|
| 56  | MG   | 2F    | 303  | 1/1   | 0.96 | 0.14 | -2.88 | 29,29,29,29                | 0     |
| 56  | MG   | 2A    | 3298 | 1/1   | 0.89 | 0.11 | -2.89 | 29,29,29,29                | 0     |
| 56  | MG   | 1A    | 8517 | 1/1   | 0.91 | 0.10 | -2.89 | 32,32,32,32                | 0     |
| 56  | MG   | 1A    | 8023 | 1/1   | 0.88 | 0.15 | -2.90 | 21,21,21,21                | 0     |
| 56  | MG   | 2A    | 3071 | 1/1   | 0.96 | 0.10 | -2.90 | 25,25,25,25                | 0     |
| 56  | MG   | 1A    | 8603 | 1/1   | 0.93 | 0.12 | -2.91 | 24,24,24,24                | 0     |
| 56  | MG   | 2A    | 3286 | 1/1   | 0.86 | 0.14 | -2.91 | 21,21,21,21                | 0     |
| 56  | MG   | 1B    | 3014 | 1/1   | 0.97 | 0.10 | -2.91 | 31,31,31,31                | 0     |
| 56  | MG   | 1A    | 8267 | 1/1   | 0.97 | 0.09 | -2.92 | 15,15,15,15                | 0     |
| 56  | MG   | 2A    | 3696 | 1/1   | 0.78 | 0.11 | -2.92 | 54,54,54,54                | 0     |
| 56  | MG   | 28    | 101  | 1/1   | 0.85 | 0.14 | -2.93 | 54,54,54,54                | 0     |
| 56  | MG   | 1A    | 8529 | 1/1   | 0.99 | 0.12 | -2.93 | 21,21,21,21                | 0     |
| 56  | MG   | 2a    | 1693 | 1/1   | 0.75 | 0.12 | -2.93 | 47,47,47,47                | 0     |
| 56  | MG   | 1A    | 8825 | 1/1   | 0.95 | 0.12 | -2.94 | 35,35,35,35                | 0     |
| 56  | MG   | 2a    | 1796 | 1/1   | 0.94 | 0.13 | -2.95 | 53,53,53,53                | 0     |
| 57  | ZN   | 1n    | 102  | 1/1   | 0.96 | 0.10 | -2.96 | 55,55,55,55                | 0     |
| 57  | ZN   | 2Y    | 202  | 1/1   | 0.87 | 0.05 | -2.96 | 66,66,66,66                | 0     |
| 56  | MG   | 1a    | 1631 | 1/1   | 0.94 | 0.14 | -2.96 | 34,34,34,34                | 0     |
| 56  | MG   | 2A    | 3493 | 1/1   | 0.93 | 0.12 | -2.96 | 32,32,32,32                | 0     |
| 56  | MG   | 1F    | 306  | 1/1   | 0.97 | 0.14 | -2.97 | 7,7,7,7                    | 0     |
| 56  | MG   | 2A    | 3463 | 1/1   | 0.64 | 0.13 | -2.98 | 42,42,42,42                | 0     |
| 56  | MG   | 2a    | 1731 | 1/1   | 0.79 | 0.13 | -2.98 | 56,56,56,56                | 0     |
| 56  | MG   | 2a    | 1811 | 1/1   | 0.88 | 0.10 | -2.99 | 59,59,59,59                | 0     |
| 56  | MG   | 1a    | 1638 | 1/1   | 0.91 | 0.13 | -3.01 | 27,27,27,27                | 0     |
| 56  | MG   | 1A    | 8425 | 1/1   | 0.90 | 0.16 | -3.02 | 12,12,12,12                | 0     |
| 56  | MG   | 2D    | 309  | 1/1   | 0.96 | 0.14 | -3.02 | 37,37,37,37                | 0     |
| 56  | MG   | 2a    | 1609 | 1/1   | 0.85 | 0.15 | -3.04 | 45,45,45,45                | 0     |
| 56  | MG   | 2A    | 3134 | 1/1   | 0.98 | 0.14 | -3.06 | 24,24,24,24                | 0     |
| 56  | MG   | 1A    | 8404 | 1/1   | 0.97 | 0.14 | -3.08 | 8,8,8,8                    | 0     |
| 56  | MG   | 2A    | 3836 | 1/1   | 0.96 | 0.16 | -3.09 | 32,32,32,32                | 0     |
| 57  | ZN   | 25    | 102  | 1/1   | 0.98 | 0.05 | -3.10 | 53,53,53,53                | 0     |
| 56  | MG   | 1A    | 8956 | 1/1   | 0.98 | 0.12 | -3.12 | 11,11,11,11                | 0     |
| 57  | ZN   | 26    | 101  | 1/1   | 0.98 | 0.06 | -3.14 | 42,42,42,42                | 0     |
| 56  | MG   | 2A    | 3340 | 1/1   | 0.98 | 0.10 | -3.14 | 32,32,32,32                | 0     |
| 57  | ZN   | 29    | 501  | 1/1   | 0.99 | 0.07 | -3.15 | 52,52,52,52                | 0     |
| 56  | MG   | 1A    | 8321 | 1/1   | 0.98 | 0.14 | -3.15 | 5,5,5,5                    | 0     |
| 56  | MG   | 2a    | 1627 | 1/1   | 0.91 | 0.08 | -3.17 | 45,45,45,45                | 0     |
| 56  | MG   | 2A    | 3543 | 1/1   | 0.97 | 0.04 | -3.19 | 50,50,50,50                | 0     |
| 56  | MG   | 2A    | 3418 | 1/1   | 0.82 | 0.11 | -3.19 | 57,57,57,57                | 0     |
| 56  | MG   | 2A    | 3887 | 1/1   | 0.96 | 0.13 | -3.25 | 41,41,41,41                | 0     |
| 56  | MG   | 1A    | 8646 | 1/1   | 0.85 | 0.12 | -3.27 | 30,30,30,30                | 0     |
| 56  | MG   | 1A    | 8894 | 1/1   | 0.89 | 0.14 | -3.27 | 8,8,8,8                    | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|----------------------------|-------|
| 56  | MG   | 1A    | 8945 | 1/1   | 0.97 | 0.11 | -3.28 | 8,8,8,8                    | 0     |
| 56  | MG   | 1A    | 8950 | 1/1   | 0.98 | 0.09 | -3.30 | 26,26,26,26                | 0     |
| 56  | MG   | 2a    | 1818 | 1/1   | 0.92 | 0.08 | -3.36 | 61,61,61,61                | 0     |
| 56  | MG   | 2A    | 3745 | 1/1   | 0.98 | 0.09 | -3.40 | 39,39,39,39                | 0     |
| 56  | MG   | 1D    | 310  | 1/1   | 0.96 | 0.12 | -3.44 | 12,12,12,12                | 0     |
| 56  | MG   | 1A    | 8274 | 1/1   | 0.93 | 0.10 | -3.46 | 23,23,23,23                | 0     |
| 56  | MG   | 1A    | 8938 | 1/1   | 0.99 | 0.13 | -3.47 | 12,12,12,12                | 0     |
| 56  | MG   | 2F    | 304  | 1/1   | 0.96 | 0.09 | -3.48 | 44,44,44,44                | 0     |
| 56  | MG   | 1a    | 1647 | 1/1   | 0.85 | 0.09 | -3.49 | 53,53,53,53                | 0     |
| 56  | MG   | 2D    | 310  | 1/1   | 0.98 | 0.15 | -3.49 | 37,37,37,37                | 0     |
| 56  | MG   | 2A    | 3163 | 1/1   | 0.97 | 0.14 | -3.49 | 23,23,23,23                | 0     |
| 56  | MG   | 2a    | 1682 | 1/1   | 0.95 | 0.11 | -3.50 | 53,53,53,53                | 0     |
| 56  | MG   | 1P    | 203  | 1/1   | 0.96 | 0.12 | -3.52 | 8,8,8,8                    | 0     |
| 56  | MG   | 2A    | 3321 | 1/1   | 0.95 | 0.14 | -3.55 | 18,18,18,18                | 0     |
| 56  | MG   | 1N    | 201  | 1/1   | 0.97 | 0.12 | -3.56 | 24,24,24,24                | 0     |
| 56  | MG   | 1A    | 8868 | 1/1   | 0.92 | 0.11 | -3.57 | 22,22,22,22                | 0     |
| 56  | MG   | 1A    | 8456 | 1/1   | 0.96 | 0.07 | -3.59 | 25,25,25,25                | 0     |
| 56  | MG   | 1A    | 8710 | 1/1   | 0.96 | 0.10 | -3.61 | 16,16,16,16                | 0     |
| 56  | MG   | 1A    | 8728 | 1/1   | 0.98 | 0.10 | -3.62 | 24,24,24,24                | 0     |
| 56  | MG   | 1A    | 8462 | 1/1   | 0.97 | 0.13 | -3.66 | 8,8,8,8                    | 0     |
| 56  | MG   | 1A    | 8446 | 1/1   | 0.97 | 0.10 | -3.66 | 26,26,26,26                | 0     |
| 56  | MG   | 1a    | 1636 | 1/1   | 0.84 | 0.13 | -3.66 | 56,56,56,56                | 0     |
| 56  | MG   | 1D    | 308  | 1/1   | 0.97 | 0.12 | -3.67 | 8,8,8,8                    | 0     |
| 56  | MG   | 1a    | 1786 | 1/1   | 0.76 | 0.14 | -3.69 | 56,56,56,56                | 0     |
| 56  | MG   | 2U    | 201  | 1/1   | 0.94 | 0.13 | -3.70 | 42,42,42,42                | 0     |
| 57  | ZN   | 19    | 102  | 1/1   | 0.99 | 0.12 | -3.70 | 27,27,27,27                | 0     |
| 56  | MG   | 2X    | 102  | 1/1   | 0.90 | 0.10 | -3.70 | 40,40,40,40                | 0     |
| 56  | MG   | 1A    | 8429 | 1/1   | 0.97 | 0.12 | -3.71 | 12,12,12,12                | 0     |
| 56  | MG   | 1B    | 3004 | 1/1   | 0.84 | 0.11 | -3.72 | 35,35,35,35                | 0     |
| 56  | MG   | 2A    | 3792 | 1/1   | 0.88 | 0.10 | -3.75 | 44,44,44,44                | 0     |
| 56  | MG   | 2A    | 3423 | 1/1   | 0.96 | 0.10 | -3.77 | 37,37,37,37                | 0     |
| 56  | MG   | 1A    | 8582 | 1/1   | 0.88 | 0.10 | -3.79 | 15,15,15,15                | 0     |
| 56  | MG   | 2A    | 3123 | 1/1   | 0.89 | 0.12 | -3.82 | 41,41,41,41                | 0     |
| 56  | MG   | 2A    | 3357 | 1/1   | 0.96 | 0.15 | -3.84 | 20,20,20,20                | 0     |
| 56  | MG   | 1A    | 8435 | 1/1   | 0.97 | 0.12 | -3.87 | 16,16,16,16                | 0     |
| 56  | MG   | 1A    | 8311 | 1/1   | 0.93 | 0.15 | -3.87 | 11,11,11,11                | 0     |
| 56  | MG   | 2A    | 3435 | 1/1   | 0.86 | 0.11 | -3.89 | 33,33,33,33                | 0     |
| 56  | MG   | 1A    | 8810 | 1/1   | 0.95 | 0.11 | -3.89 | 8,8,8,8                    | 0     |
| 56  | MG   | 2A    | 3436 | 1/1   | 0.94 | 0.15 | -3.90 | 29,29,29,29                | 0     |
| 56  | MG   | 2A    | 3373 | 1/1   | 0.73 | 0.12 | -3.91 | 29,29,29,29                | 0     |
| 56  | MG   | 2A    | 3824 | 1/1   | 0.96 | 0.08 | -3.95 | 42,42,42,42                | 0     |
| 56  | MG   | 1A    | 8241 | 1/1   | 0.91 | 0.15 | -3.96 | 10,10,10,10                | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|----------------------------|-------|
| 56  | MG   | 1A    | 8299 | 1/1   | 0.86 | 0.08 | -4.01 | 28,28,28,28                | 0     |
| 56  | MG   | 1A    | 8698 | 1/1   | 0.91 | 0.06 | -4.02 | 30,30,30,30                | 0     |
| 56  | MG   | 2A    | 3359 | 1/1   | 0.98 | 0.12 | -4.04 | 30,30,30,30                | 0     |
| 56  | MG   | 1a    | 1818 | 1/1   | 0.97 | 0.10 | -4.04 | 41,41,41,41                | 0     |
| 56  | MG   | 2A    | 3489 | 1/1   | 0.94 | 0.12 | -4.07 | 27,27,27,27                | 0     |
| 56  | MG   | 2A    | 3496 | 1/1   | 0.91 | 0.11 | -4.08 | 36,36,36,36                | 0     |
| 56  | MG   | 1A    | 8418 | 1/1   | 0.89 | 0.09 | -4.11 | 22,22,22,22                | 0     |
| 56  | MG   | 1a    | 1756 | 1/1   | 0.85 | 0.11 | -4.13 | 51,51,51,51                | 0     |
| 56  | MG   | 1F    | 304  | 1/1   | 0.98 | 0.07 | -4.13 | 9,9,9,9                    | 0     |
| 56  | MG   | 1A    | 8305 | 1/1   | 0.96 | 0.12 | -4.21 | 29,29,29,29                | 0     |
| 56  | MG   | 1A    | 8385 | 1/1   | 0.77 | 0.13 | -4.21 | 15,15,15,15                | 0     |
| 56  | MG   | 2A    | 3455 | 1/1   | 0.97 | 0.08 | -4.23 | 40,40,40,40                | 0     |
| 56  | MG   | 1A    | 8961 | 1/1   | 0.95 | 0.12 | -4.23 | 20,20,20,20                | 0     |
| 56  | MG   | 1A    | 8439 | 1/1   | 0.97 | 0.12 | -4.25 | 6,6,6,6                    | 0     |
| 56  | MG   | 1A    | 8083 | 1/1   | 0.93 | 0.13 | -4.25 | 15,15,15,15                | 0     |
| 56  | MG   | 1a    | 1832 | 1/1   | 0.92 | 0.06 | -4.25 | 44,44,44,44                | 0     |
| 56  | MG   | 1a    | 1799 | 1/1   | 0.91 | 0.10 | -4.26 | 35,35,35,35                | 0     |
| 56  | MG   | 1a    | 1657 | 1/1   | 0.88 | 0.12 | -4.26 | 55,55,55,55                | 0     |
| 56  | MG   | 2A    | 3801 | 1/1   | 0.95 | 0.07 | -4.28 | 41,41,41,41                | 0     |
| 56  | MG   | 1A    | 8947 | 1/1   | 0.95 | 0.08 | -4.28 | 19,19,19,19                | 0     |
| 56  | MG   | 1A    | 8804 | 1/1   | 0.87 | 0.09 | -4.29 | 31,31,31,31                | 0     |
| 56  | MG   | 2A    | 3008 | 1/1   | 0.92 | 0.13 | -4.33 | 27,27,27,27                | 0     |
| 56  | MG   | 2A    | 3122 | 1/1   | 0.90 | 0.09 | -4.33 | 55,55,55,55                | 0     |
| 56  | MG   | 2A    | 3297 | 1/1   | 0.96 | 0.09 | -4.33 | 31,31,31,31                | 0     |
| 56  | MG   | 2A    | 3892 | 1/1   | 0.89 | 0.15 | -4.34 | 34,34,34,34                | 0     |
| 56  | MG   | 2A    | 3474 | 1/1   | 0.91 | 0.07 | -4.35 | 37,37,37,37                | 0     |
| 56  | MG   | 2A    | 3355 | 1/1   | 0.96 | 0.12 | -4.38 | 20,20,20,20                | 0     |
| 56  | MG   | 2A    | 3390 | 1/1   | 0.89 | 0.10 | -4.39 | 45,45,45,45                | 0     |
| 56  | MG   | 1A    | 8492 | 1/1   | 0.98 | 0.07 | -4.39 | 18,18,18,18                | 0     |
| 56  | MG   | 1A    | 8345 | 1/1   | 0.94 | 0.10 | -4.42 | 30,30,30,30                | 0     |
| 56  | MG   | 2A    | 3895 | 1/1   | 0.93 | 0.10 | -4.45 | 27,27,27,27                | 0     |
| 56  | MG   | 1A    | 8444 | 1/1   | 0.95 | 0.12 | -4.47 | 12,12,12,12                | 0     |
| 56  | MG   | 1a    | 1689 | 1/1   | 0.95 | 0.11 | -4.53 | 41,41,41,41                | 0     |
| 56  | MG   | 1A    | 8696 | 1/1   | 0.92 | 0.13 | -4.54 | 20,20,20,20                | 0     |
| 56  | MG   | 2A    | 3515 | 1/1   | 0.95 | 0.10 | -4.57 | 48,48,48,48                | 0     |
| 56  | MG   | 1A    | 8349 | 1/1   | 0.95 | 0.11 | -4.64 | 13,13,13,13                | 0     |
| 56  | MG   | 2A    | 3450 | 1/1   | 0.97 | 0.11 | -4.64 | 27,27,27,27                | 0     |
| 56  | MG   | 1E    | 307  | 1/1   | 0.94 | 0.08 | -4.71 | 28,28,28,28                | 0     |
| 56  | MG   | 1B    | 3025 | 1/1   | 0.95 | 0.12 | -4.72 | 26,26,26,26                | 0     |
| 56  | MG   | 2A    | 3805 | 1/1   | 0.78 | 0.08 | -4.73 | 40,40,40,40                | 0     |
| 56  | MG   | 2A    | 3137 | 1/1   | 0.99 | 0.11 | -4.76 | 26,26,26,26                | 0     |
| 56  | MG   | 1A    | 8391 | 1/1   | 0.95 | 0.13 | -4.76 | 6,6,6,6                    | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|----------------------------|-------|
| 56  | MG   | 2A    | 3430 | 1/1   | 0.94 | 0.10 | -4.78 | 30,30,30,30                | 0     |
| 56  | MG   | 2a    | 1802 | 1/1   | 0.92 | 0.12 | -4.81 | 60,60,60,60                | 0     |
| 56  | MG   | 2A    | 3694 | 1/1   | 0.97 | 0.12 | -4.87 | 35,35,35,35                | 0     |
| 56  | MG   | 1A    | 8339 | 1/1   | 0.94 | 0.07 | -4.90 | 32,32,32,32                | 0     |
| 56  | MG   | 1A    | 8295 | 1/1   | 0.86 | 0.10 | -4.90 | 21,21,21,21                | 0     |
| 56  | MG   | 1A    | 8286 | 1/1   | 0.76 | 0.10 | -4.91 | 11,11,11,11                | 0     |
| 56  | MG   | 1A    | 8574 | 1/1   | 0.94 | 0.08 | -4.91 | 15,15,15,15                | 0     |
| 56  | MG   | 1A    | 8057 | 1/1   | 0.93 | 0.12 | -4.92 | 12,12,12,12                | 0     |
| 56  | MG   | 1A    | 8457 | 1/1   | 0.90 | 0.11 | -4.92 | 9,9,9,9                    | 0     |
| 56  | MG   | 2A    | 3975 | 1/1   | 0.97 | 0.13 | -4.93 | 22,22,22,22                | 0     |
| 56  | MG   | 2A    | 3135 | 1/1   | 0.95 | 0.09 | -4.93 | 24,24,24,24                | 0     |
| 56  | MG   | 1a    | 1819 | 1/1   | 0.92 | 0.11 | -4.93 | 37,37,37,37                | 0     |
| 56  | MG   | 2A    | 3396 | 1/1   | 0.99 | 0.07 | -4.94 | 25,25,25,25                | 0     |
| 56  | MG   | 1A    | 8354 | 1/1   | 0.94 | 0.10 | -4.97 | 9,9,9,9                    | 0     |
| 56  | MG   | 1A    | 8792 | 1/1   | 0.98 | 0.10 | -4.97 | 15,15,15,15                | 0     |
| 56  | MG   | 1A    | 8807 | 1/1   | 0.94 | 0.08 | -4.99 | 18,18,18,18                | 0     |
| 56  | MG   | 2A    | 3687 | 1/1   | 0.92 | 0.10 | -4.99 | 30,30,30,30                | 0     |
| 56  | MG   | 2A    | 3638 | 1/1   | 0.95 | 0.10 | -5.00 | 32,32,32,32                | 0     |
| 56  | MG   | 1X    | 101  | 1/1   | 0.96 | 0.07 | -5.01 | 20,20,20,20                | 0     |
| 56  | MG   | 1D    | 303  | 1/1   | 0.95 | 0.09 | -5.01 | 17,17,17,17                | 0     |
| 56  | MG   | 1A    | 8678 | 1/1   | 0.98 | 0.13 | -5.03 | 21,21,21,21                | 0     |
| 56  | MG   | 2A    | 3773 | 1/1   | 0.94 | 0.09 | -5.03 | 24,24,24,24                | 0     |
| 56  | MG   | 1A    | 8151 | 1/1   | 0.94 | 0.13 | -5.04 | 10,10,10,10                | 0     |
| 56  | MG   | 2A    | 3841 | 1/1   | 0.94 | 0.12 | -5.06 | 40,40,40,40                | 0     |
| 56  | MG   | 1A    | 8313 | 1/1   | 0.87 | 0.13 | -5.09 | 16,16,16,16                | 0     |
| 56  | MG   | 2A    | 3476 | 1/1   | 0.95 | 0.10 | -5.09 | 34,34,34,34                | 0     |
| 56  | MG   | 2a    | 1787 | 1/1   | 0.87 | 0.08 | -5.13 | 49,49,49,49                | 0     |
| 56  | MG   | 2A    | 3363 | 1/1   | 0.91 | 0.12 | -5.16 | 26,26,26,26                | 0     |
| 56  | MG   | 2A    | 3456 | 1/1   | 0.92 | 0.12 | -5.16 | 23,23,23,23                | 0     |
| 56  | MG   | 2A    | 3345 | 1/1   | 0.97 | 0.07 | -5.17 | 39,39,39,39                | 0     |
| 56  | MG   | 2a    | 1699 | 1/1   | 0.94 | 0.12 | -5.17 | 68,68,68,68                | 0     |
| 56  | MG   | 2A    | 3925 | 1/1   | 0.92 | 0.05 | -5.20 | 42,42,42,42                | 0     |
| 56  | MG   | 2A    | 3808 | 1/1   | 0.86 | 0.11 | -5.21 | 31,31,31,31                | 0     |
| 56  | MG   | 2A    | 3578 | 1/1   | 0.85 | 0.08 | -5.32 | 47,47,47,47                | 0     |
| 56  | MG   | 1A    | 8680 | 1/1   | 0.94 | 0.12 | -5.35 | 19,19,19,19                | 0     |
| 56  | MG   | 1a    | 1711 | 1/1   | 0.94 | 0.08 | -5.35 | 45,45,45,45                | 0     |
| 56  | MG   | 2A    | 3370 | 1/1   | 0.77 | 0.13 | -5.36 | 21,21,21,21                | 0     |
| 56  | MG   | 1A    | 8280 | 1/1   | 0.97 | 0.07 | -5.36 | 18,18,18,18                | 0     |
| 56  | MG   | 2A    | 3132 | 1/1   | 0.96 | 0.11 | -5.41 | 32,32,32,32                | 0     |
| 56  | MG   | 1A    | 8786 | 1/1   | 0.94 | 0.08 | -5.42 | 15,15,15,15                | 0     |
| 56  | MG   | 2A    | 3653 | 1/1   | 0.96 | 0.11 | -5.42 | 41,41,41,41                | 0     |
| 56  | MG   | 1A    | 8546 | 1/1   | 0.90 | 0.11 | -5.44 | 21,21,21,21                | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|----------------------------|-------|
| 56  | MG   | 2A    | 3429 | 1/1   | 0.92 | 0.11 | -5.50 | 37,37,37,37                | 0     |
| 56  | MG   | 1A    | 8716 | 1/1   | 0.88 | 0.11 | -5.51 | 39,39,39,39                | 0     |
| 56  | MG   | 1A    | 8472 | 1/1   | 0.95 | 0.11 | -5.54 | 11,11,11,11                | 0     |
| 56  | MG   | 2A    | 3708 | 1/1   | 0.95 | 0.08 | -5.56 | 30,30,30,30                | 0     |
| 56  | MG   | 2A    | 3366 | 1/1   | 0.96 | 0.11 | -5.57 | 29,29,29,29                | 0     |
| 56  | MG   | 1A    | 8633 | 1/1   | 0.96 | 0.09 | -5.57 | 10,10,10,10                | 0     |
| 56  | MG   | 1A    | 8431 | 1/1   | 0.92 | 0.10 | -5.59 | 17,17,17,17                | 0     |
| 56  | MG   | 1A    | 8203 | 1/1   | 0.91 | 0.11 | -5.59 | 15,15,15,15                | 0     |
| 56  | MG   | 2A    | 3983 | 1/1   | 0.87 | 0.10 | -5.65 | 23,23,23,23                | 0     |
| 56  | MG   | 1A    | 8809 | 1/1   | 0.84 | 0.15 | -5.66 | 21,21,21,21                | 0     |
| 56  | MG   | 1A    | 8294 | 1/1   | 0.96 | 0.06 | -5.69 | 29,29,29,29                | 0     |
| 56  | MG   | 2A    | 3759 | 1/1   | 0.92 | 0.13 | -5.71 | 52,52,52,52                | 0     |
| 56  | MG   | 2A    | 3712 | 1/1   | 0.80 | 0.08 | -5.74 | 29,29,29,29                | 0     |
| 56  | MG   | 1A    | 8750 | 1/1   | 0.98 | 0.06 | -5.77 | 31,31,31,31                | 0     |
| 56  | MG   | 1A    | 8396 | 1/1   | 0.95 | 0.07 | -5.77 | 14,14,14,14                | 0     |
| 56  | MG   | 2B    | 3018 | 1/1   | 0.59 | 0.11 | -5.81 | 57,57,57,57                | 0     |
| 56  | MG   | 2A    | 3750 | 1/1   | 0.92 | 0.06 | -5.96 | 24,24,24,24                | 0     |
| 56  | MG   | 1A    | 8166 | 1/1   | 0.99 | 0.10 | -6.09 | 14,14,14,14                | 0     |
| 56  | MG   | 1A    | 8713 | 1/1   | 0.95 | 0.08 | -6.15 | 9,9,9,9                    | 0     |
| 56  | MG   | 1A    | 8297 | 1/1   | 0.97 | 0.09 | -6.22 | 13,13,13,13                | 0     |
| 56  | MG   | 2A    | 3354 | 1/1   | 0.90 | 0.09 | -6.29 | 27,27,27,27                | 0     |
| 56  | MG   | 2A    | 3570 | 1/1   | 0.98 | 0.05 | -6.30 | 35,35,35,35                | 0     |
| 56  | MG   | 1A    | 8752 | 1/1   | 0.97 | 0.10 | -6.34 | 12,12,12,12                | 0     |
| 56  | MG   | 2a    | 1691 | 1/1   | 0.84 | 0.09 | -6.38 | 52,52,52,52                | 0     |
| 56  | MG   | 2D    | 306  | 1/1   | 0.94 | 0.14 | -6.38 | 34,34,34,34                | 0     |
| 56  | MG   | 1A    | 8481 | 1/1   | 0.98 | 0.06 | -6.47 | 20,20,20,20                | 0     |
| 56  | MG   | 2A    | 3288 | 1/1   | 0.97 | 0.11 | -6.49 | 25,25,25,25                | 0     |
| 56  | MG   | 1A    | 8061 | 1/1   | 0.90 | 0.09 | -6.50 | 41,41,41,41                | 0     |
| 56  | MG   | 1A    | 8314 | 1/1   | 0.97 | 0.11 | -6.52 | 12,12,12,12                | 0     |
| 56  | MG   | 1A    | 8869 | 1/1   | 0.98 | 0.09 | -6.52 | 20,20,20,20                | 0     |
| 56  | MG   | 2A    | 3714 | 1/1   | 0.93 | 0.10 | -6.65 | 39,39,39,39                | 0     |
| 56  | MG   | 1A    | 8642 | 1/1   | 0.97 | 0.10 | -6.69 | 18,18,18,18                | 0     |
| 56  | MG   | 1A    | 8837 | 1/1   | 0.96 | 0.07 | -6.71 | 18,18,18,18                | 0     |
| 56  | MG   | 1A    | 8476 | 1/1   | 0.98 | 0.08 | -6.74 | 17,17,17,17                | 0     |
| 56  | MG   | 1A    | 8450 | 1/1   | 0.98 | 0.09 | -6.76 | 14,14,14,14                | 0     |
| 56  | MG   | 1A    | 8801 | 1/1   | 0.85 | 0.10 | -6.79 | 25,25,25,25                | 0     |
| 56  | MG   | 1A    | 8672 | 1/1   | 0.90 | 0.13 | -6.80 | 19,19,19,19                | 0     |
| 56  | MG   | 1B    | 3018 | 1/1   | 0.89 | 0.13 | -6.84 | 41,41,41,41                | 0     |
| 56  | MG   | 2A    | 3141 | 1/1   | 0.91 | 0.12 | -7.12 | 27,27,27,27                | 0     |
| 56  | MG   | 1A    | 8357 | 1/1   | 0.95 | 0.08 | -7.14 | 6,6,6,6                    | 0     |
| 56  | MG   | 1A    | 8430 | 1/1   | 0.93 | 0.08 | -7.15 | 13,13,13,13                | 0     |
| 56  | MG   | 2A    | 3404 | 1/1   | 0.96 | 0.08 | -7.17 | 25,25,25,25                | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF   | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|--------|-----------------------------|-------|
| 56  | MG   | 1A    | 8891 | 1/1   | 0.95 | 0.09 | -7.23  | 15,15,15,15                 | 0     |
| 56  | MG   | 1A    | 8310 | 1/1   | 0.96 | 0.09 | -7.41  | 8,8,8,8                     | 0     |
| 56  | MG   | 2A    | 3788 | 1/1   | 0.95 | 0.10 | -7.46  | 36,36,36,36                 | 0     |
| 56  | MG   | 2a    | 1754 | 1/1   | 0.91 | 0.06 | -7.53  | 42,42,42,42                 | 0     |
| 56  | MG   | 2A    | 3412 | 1/1   | 0.72 | 0.16 | -7.61  | 21,21,21,21                 | 0     |
| 56  | MG   | 1A    | 8842 | 1/1   | 0.99 | 0.05 | -7.64  | 11,11,11,11                 | 0     |
| 56  | MG   | 2A    | 3336 | 1/1   | 0.93 | 0.08 | -7.66  | 44,44,44,44                 | 0     |
| 56  | MG   | 2a    | 1686 | 1/1   | 0.89 | 0.06 | -7.76  | 41,41,41,41                 | 0     |
| 56  | MG   | 25    | 101  | 1/1   | 0.96 | 0.11 | -7.80  | 27,27,27,27                 | 0     |
| 56  | MG   | 1E    | 301  | 1/1   | 0.94 | 0.07 | -7.94  | 22,22,22,22                 | 0     |
| 56  | MG   | 2A    | 3900 | 1/1   | 0.93 | 0.11 | -7.99  | 41,41,41,41                 | 0     |
| 56  | MG   | 1A    | 8366 | 1/1   | 0.94 | 0.07 | -8.05  | 14,14,14,14                 | 0     |
| 56  | MG   | 2a    | 1614 | 1/1   | 0.94 | 0.12 | -8.06  | 49,49,49,49                 | 0     |
| 56  | MG   | 2A    | 3756 | 1/1   | 0.96 | 0.10 | -8.07  | 28,28,28,28                 | 0     |
| 56  | MG   | 1A    | 8369 | 1/1   | 0.97 | 0.12 | -8.12  | 11,11,11,11                 | 0     |
| 56  | MG   | 1A    | 8342 | 1/1   | 0.96 | 0.12 | -8.24  | 9,9,9,9                     | 0     |
| 56  | MG   | 2A    | 3839 | 1/1   | 0.96 | 0.10 | -8.36  | 27,27,27,27                 | 0     |
| 56  | MG   | 1A    | 8794 | 1/1   | 0.88 | 0.12 | -8.45  | 24,24,24,24                 | 0     |
| 56  | MG   | 2A    | 3544 | 1/1   | 0.89 | 0.08 | -8.47  | 38,38,38,38                 | 0     |
| 56  | MG   | 2A    | 3369 | 1/1   | 0.91 | 0.09 | -8.60  | 25,25,25,25                 | 0     |
| 56  | MG   | 2A    | 3349 | 1/1   | 0.85 | 0.10 | -9.13  | 43,43,43,43                 | 0     |
| 56  | MG   | 1a    | 1808 | 1/1   | 0.96 | 0.07 | -9.19  | 35,35,35,35                 | 0     |
| 56  | MG   | 2A    | 3445 | 1/1   | 0.97 | 0.10 | -9.19  | 42,42,42,42                 | 0     |
| 56  | MG   | 2A    | 3439 | 1/1   | 0.94 | 0.06 | -9.59  | 25,25,25,25                 | 0     |
| 56  | MG   | 2A    | 3247 | 1/1   | 0.98 | 0.12 | -9.74  | 25,25,25,25                 | 0     |
| 56  | MG   | 1A    | 8543 | 1/1   | 0.96 | 0.08 | -9.95  | 20,20,20,20                 | 0     |
| 56  | MG   | 2A    | 3313 | 1/1   | 0.97 | 0.12 | -10.09 | 31,31,31,31                 | 0     |
| 56  | MG   | 2A    | 3311 | 1/1   | 0.91 | 0.10 | -10.34 | 29,29,29,29                 | 0     |
| 56  | MG   | 2A    | 3470 | 1/1   | 0.97 | 0.10 | -10.42 | 24,24,24,24                 | 0     |
| 56  | MG   | 2A    | 3278 | 1/1   | 0.92 | 0.11 | -10.67 | 30,30,30,30                 | 0     |
| 56  | MG   | 2D    | 308  | 1/1   | 0.97 | 0.08 | -10.99 | 33,33,33,33                 | 0     |
| 56  | MG   | 2A    | 3431 | 1/1   | 0.79 | 0.09 | -11.17 | 39,39,39,39                 | 0     |
| 56  | MG   | 1A    | 8359 | 1/1   | 0.96 | 0.08 | -11.66 | 24,24,24,24                 | 0     |
| 56  | MG   | 1A    | 8330 | 1/1   | 0.98 | 0.07 | -12.29 | 13,13,13,13                 | 0     |
| 56  | MG   | 1A    | 8775 | 1/1   | 0.95 | 0.06 | -15.46 | 9,9,9,9                     | 0     |
| 56  | MG   | 1a    | 1698 | 1/1   | 0.89 | 0.07 | -16.97 | 29,29,29,29                 | 0     |
| 56  | MG   | 1A    | 8451 | 1/1   | 0.98 | 0.05 | -18.88 | 19,19,19,19                 | 0     |
| 56  | MG   | 2A    | 3820 | 1/1   | 0.93 | 0.07 | -20.88 | 29,29,29,29                 | 0     |
| 56  | MG   | 2A    | 3166 | 1/1   | 0.94 | 0.10 | -      | 42,42,42,42                 | 0     |
| 56  | MG   | 1a    | 1828 | 1/1   | 0.84 | 0.20 | -      | 52,52,52,52                 | 0     |
| 56  | MG   | 2A    | 3686 | 1/1   | 0.73 | 0.44 | -      | 53,53,53,53                 | 0     |
| 56  | MG   | 2A    | 3719 | 1/1   | 0.84 | 0.50 | -      | 37,37,37,37                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|----------------------------|-------|
| 56  | MG   | 2A    | 3884 | 1/1   | 0.93 | 0.16 | -    | 37,37,37,37                | 0     |
| 56  | MG   | 1A    | 8700 | 1/1   | 0.93 | 0.15 | -    | 27,27,27,27                | 0     |
| 56  | MG   | 2A    | 3268 | 1/1   | 0.97 | 0.22 | -    | 42,42,42,42                | 0     |
| 56  | MG   | 2A    | 3587 | 1/1   | 0.91 | 0.80 | -    | 39,39,39,39                | 0     |
| 56  | MG   | 2A    | 3665 | 1/1   | 0.92 | 0.19 | -    | 29,29,29,29                | 0     |
| 56  | MG   | 1A    | 8856 | 1/1   | 0.92 | 0.14 | -    | 18,18,18,18                | 0     |
| 56  | MG   | 1a    | 1717 | 1/1   | 0.98 | 0.10 | -    | 32,32,32,32                | 0     |
| 56  | MG   | 1A    | 8200 | 1/1   | 0.92 | 0.14 | -    | 46,46,46,46                | 0     |
| 56  | MG   | 1A    | 8903 | 1/1   | 0.96 | 0.15 | -    | 19,19,19,19                | 0     |
| 56  | MG   | 1A    | 8039 | 1/1   | 0.81 | 0.17 | -    | 12,12,12,12                | 0     |
| 56  | MG   | 1A    | 8880 | 1/1   | 0.65 | 0.39 | -    | 46,46,46,46                | 0     |
| 56  | MG   | 1A    | 8074 | 1/1   | 0.86 | 0.27 | -    | 18,18,18,18                | 0     |
| 56  | MG   | 1A    | 8568 | 1/1   | 0.93 | 0.15 | -    | 11,11,11,11                | 0     |
| 56  | MG   | 2A    | 3161 | 1/1   | 0.90 | 0.13 | -    | 33,33,33,33                | 0     |
| 56  | MG   | 2a    | 1690 | 1/1   | 0.39 | 0.10 | -    | 57,57,57,57                | 0     |
| 56  | MG   | 2a    | 1724 | 1/1   | 0.89 | 0.22 | -    | 56,56,56,56                | 0     |
| 56  | MG   | 1A    | 8287 | 1/1   | 0.97 | 0.17 | -    | 23,23,23,23                | 0     |
| 56  | MG   | 2A    | 3642 | 1/1   | 0.97 | 0.12 | -    | 37,37,37,37                | 0     |
| 56  | MG   | 1a    | 1761 | 1/1   | 0.97 | 0.14 | -    | 44,44,44,44                | 0     |
| 56  | MG   | 2A    | 3716 | 1/1   | 0.93 | 0.38 | -    | 37,37,37,37                | 0     |
| 56  | MG   | 1A    | 8479 | 1/1   | 0.94 | 0.24 | -    | 38,38,38,38                | 0     |
| 56  | MG   | 2A    | 3114 | 1/1   | 0.82 | 0.16 | -    | 33,33,33,33                | 0     |
| 56  | MG   | 1a    | 1713 | 1/1   | 0.90 | 0.11 | -    | 39,39,39,39                | 0     |
| 56  | MG   | 2A    | 3846 | 1/1   | 0.82 | 0.14 | -    | 38,38,38,38                | 0     |
| 56  | MG   | 2D    | 315  | 1/1   | 0.91 | 0.11 | -    | 24,24,24,24                | 0     |
| 56  | MG   | 2A    | 3040 | 1/1   | 0.87 | 0.07 | -    | 53,53,53,53                | 0     |
| 56  | MG   | 2A    | 3499 | 1/1   | 0.89 | 0.26 | -    | 51,51,51,51                | 0     |
| 56  | MG   | 1A    | 8661 | 1/1   | 0.93 | 0.11 | -    | 7,7,7,7                    | 0     |
| 56  | MG   | 2A    | 3099 | 1/1   | 0.94 | 0.19 | -    | 34,34,34,34                | 0     |
| 56  | MG   | 1A    | 8845 | 1/1   | 0.97 | 0.17 | -    | 28,28,28,28                | 0     |
| 56  | MG   | 2a    | 1812 | 1/1   | 0.92 | 0.12 | -    | 64,64,64,64                | 0     |
| 56  | MG   | 2A    | 3148 | 1/1   | 0.94 | 0.14 | -    | 50,50,50,50                | 0     |
| 56  | MG   | 2A    | 3673 | 1/1   | 0.86 | 0.28 | -    | 41,41,41,41                | 0     |
| 56  | MG   | 2a    | 1617 | 1/1   | 0.90 | 0.11 | -    | 50,50,50,50                | 0     |
| 56  | MG   | 1a    | 1774 | 1/1   | 0.85 | 0.24 | -    | 59,59,59,59                | 0     |
| 56  | MG   | 2A    | 3860 | 1/1   | 0.91 | 0.09 | -    | 46,46,46,46                | 0     |
| 56  | MG   | 2a    | 1745 | 1/1   | 0.91 | 0.05 | -    | 55,55,55,55                | 0     |
| 56  | MG   | 1A    | 8042 | 1/1   | 0.96 | 0.10 | -    | 33,33,33,33                | 0     |
| 56  | MG   | 1A    | 8113 | 1/1   | 0.95 | 0.14 | -    | 16,16,16,16                | 0     |
| 56  | MG   | 2A    | 3838 | 1/1   | 0.94 | 0.41 | -    | 44,44,44,44                | 0     |
| 56  | MG   | 2A    | 3058 | 1/1   | 0.93 | 0.09 | -    | 42,42,42,42                | 0     |
| 56  | MG   | 1A    | 8821 | 1/1   | 0.96 | 0.07 | -    | 9,9,9,9                    | 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   | 0.96 | 0.09 | -    | 48,48,48,48                 | 0     |
| 56  | MG   | 2A    | 3462 | 1/1   | 0.91 | 0.21 | -    | 26,26,26,26                 | 0     |
| 56  | MG   | 2x    | 110  | 1/1   | 0.90 | 0.11 | -    | 42,42,42,42                 | 0     |
| 56  | MG   | 2a    | 1626 | 1/1   | 0.80 | 0.25 | -    | 63,63,63,63                 | 0     |
| 56  | MG   | 2A    | 3283 | 1/1   | 0.83 | 0.16 | -    | 30,30,30,30                 | 0     |
| 56  | MG   | 2A    | 3952 | 1/1   | 0.98 | 0.12 | -    | 36,36,36,36                 | 0     |
| 56  | MG   | 1a    | 1764 | 1/1   | 0.93 | 0.23 | -    | 54,54,54,54                 | 0     |
| 56  | MG   | 1a    | 1782 | 1/1   | 0.87 | 0.10 | -    | 38,38,38,38                 | 0     |
| 56  | MG   | 1A    | 8793 | 1/1   | 0.93 | 0.12 | -    | 27,27,27,27                 | 0     |
| 56  | MG   | 2A    | 3374 | 1/1   | 0.84 | 0.12 | -    | 57,57,57,57                 | 0     |
| 56  | MG   | 1A    | 8066 | 1/1   | 0.97 | 0.16 | -    | 25,25,25,25                 | 0     |
| 56  | MG   | 1A    | 8623 | 1/1   | 0.92 | 0.57 | -    | 18,18,18,18                 | 0     |
| 56  | MG   | 2A    | 3170 | 1/1   | 0.97 | 0.15 | -    | 39,39,39,39                 | 0     |
| 56  | MG   | 1a    | 1681 | 1/1   | 0.89 | 0.16 | -    | 52,52,52,52                 | 0     |
| 56  | MG   | 1A    | 8031 | 1/1   | 0.94 | 0.18 | -    | 12,12,12,12                 | 0     |
| 56  | MG   | 2A    | 3139 | 1/1   | 0.92 | 0.22 | -    | 45,45,45,45                 | 0     |
| 56  | MG   | 2A    | 3844 | 1/1   | 0.92 | 0.15 | -    | 46,46,46,46                 | 0     |
| 56  | MG   | 1A    | 8519 | 1/1   | 0.88 | 0.23 | -    | 29,29,29,29                 | 0     |
| 56  | MG   | 2x    | 112  | 1/1   | 0.98 | 0.15 | -    | 39,39,39,39                 | 0     |
| 56  | MG   | 1A    | 8150 | 1/1   | 0.92 | 0.21 | -    | 36,36,36,36                 | 0     |
| 56  | MG   | 2A    | 3889 | 1/1   | 0.89 | 0.31 | -    | 63,63,63,63                 | 0     |
| 56  | MG   | 2A    | 3083 | 1/1   | 0.87 | 0.19 | -    | 25,25,25,25                 | 0     |
| 56  | MG   | 2A    | 3459 | 1/1   | 0.96 | 0.22 | -    | 33,33,33,33                 | 0     |
| 56  | MG   | 2A    | 3825 | 1/1   | 0.94 | 0.08 | -    | 27,27,27,27                 | 0     |
| 56  | MG   | 2B    | 3011 | 1/1   | 0.87 | 0.08 | -    | 73,73,73,73                 | 0     |
| 56  | MG   | 2a    | 1798 | 1/1   | 0.87 | 0.17 | -    | 49,49,49,49                 | 0     |
| 56  | MG   | 1A    | 8445 | 1/1   | 0.94 | 0.09 | -    | 18,18,18,18                 | 0     |
| 56  | MG   | 1a    | 1630 | 1/1   | 0.96 | 0.26 | -    | 17,17,17,17                 | 0     |
| 56  | MG   | 2A    | 3239 | 1/1   | 0.88 | 0.37 | -    | 51,51,51,51                 | 0     |
| 56  | MG   | 1A    | 8881 | 1/1   | 0.72 | 0.23 | -    | 53,53,53,53                 | 0     |
| 56  | MG   | 1A    | 8027 | 1/1   | 0.92 | 0.13 | -    | 38,38,38,38                 | 0     |
| 56  | MG   | 1A    | 8375 | 1/1   | 0.99 | 0.12 | -    | 11,11,11,11                 | 0     |
| 56  | MG   | 1A    | 8872 | 1/1   | 0.56 | 0.32 | -    | 59,59,59,59                 | 0     |
| 56  | MG   | 1A    | 8594 | 1/1   | 0.84 | 0.15 | -    | 36,36,36,36                 | 0     |
| 56  | MG   | 1A    | 8508 | 1/1   | 0.75 | 0.09 | -    | 34,34,34,34                 | 0     |
| 56  | MG   | 1A    | 8652 | 1/1   | 0.98 | 0.14 | -    | 24,24,24,24                 | 0     |
| 56  | MG   | 1A    | 8634 | 1/1   | 0.88 | 0.20 | -    | 39,39,39,39                 | 0     |
| 56  | MG   | 2a    | 1752 | 1/1   | 0.84 | 0.59 | -    | 71,71,71,71                 | 0     |
| 56  | MG   | 1A    | 8214 | 1/1   | 0.91 | 0.27 | -    | 10,10,10,10                 | 0     |
| 56  | MG   | 1A    | 8835 | 1/1   | 0.86 | 0.10 | -    | 36,36,36,36                 | 0     |
| 56  | MG   | 1A    | 8087 | 1/1   | 0.95 | 0.12 | -    | 45,45,45,45                 | 0     |
| 56  | MG   | 2A    | 3055 | 1/1   | 0.90 | 0.56 | -    | 32,32,32,32                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56  | MG   | 2A    | 3096 | 1/1   | 0.96 | 0.33 | -    | 21,21,21,21                 | 0     |
| 56  | MG   | 2A    | 3898 | 1/1   | 0.96 | 0.18 | -    | 46,46,46,46                 | 0     |
| 56  | MG   | 2A    | 3853 | 1/1   | 0.94 | 0.15 | -    | 54,54,54,54                 | 0     |
| 56  | MG   | 2A    | 3509 | 1/1   | 0.85 | 0.36 | -    | 66,66,66,66                 | 0     |
| 56  | MG   | 1A    | 8426 | 1/1   | 0.93 | 0.06 | -    | 31,31,31,31                 | 0     |
| 56  | MG   | 1A    | 8612 | 1/1   | 0.88 | 0.14 | -    | 8,8,8,8                     | 0     |
| 56  | MG   | 1a    | 1789 | 1/1   | 0.71 | 0.30 | -    | 61,61,61,61                 | 0     |
| 56  | MG   | 2A    | 3789 | 1/1   | 0.95 | 0.08 | -    | 48,48,48,48                 | 0     |
| 56  | MG   | 1A    | 8180 | 1/1   | 0.98 | 0.13 | -    | 17,17,17,17                 | 0     |
| 56  | MG   | 1A    | 8677 | 1/1   | 0.93 | 0.14 | -    | 24,24,24,24                 | 0     |
| 56  | MG   | 2A    | 3731 | 1/1   | 0.83 | 0.46 | -    | 63,63,63,63                 | 0     |
| 56  | MG   | 1B    | 3009 | 1/1   | 0.97 | 0.32 | -    | 37,37,37,37                 | 0     |
| 56  | MG   | 2A    | 3315 | 1/1   | 0.95 | 0.15 | -    | 44,44,44,44                 | 0     |
| 56  | MG   | 1A    | 8724 | 1/1   | 0.89 | 0.12 | -    | 17,17,17,17                 | 0     |
| 56  | MG   | 1A    | 8379 | 1/1   | 0.97 | 0.13 | -    | 19,19,19,19                 | 0     |
| 56  | MG   | 1W    | 3001 | 1/1   | 0.95 | 0.12 | -    | 21,21,21,21                 | 0     |
| 56  | MG   | 1A    | 8758 | 1/1   | 0.99 | 0.10 | -    | 11,11,11,11                 | 0     |
| 56  | MG   | 2A    | 3271 | 1/1   | 0.94 | 0.41 | -    | 42,42,42,42                 | 0     |
| 56  | MG   | 2A    | 3294 | 1/1   | 0.91 | 0.09 | -    | 50,50,50,50                 | 0     |
| 56  | MG   | 2a    | 1713 | 1/1   | 0.36 | 0.23 | -    | 59,59,59,59                 | 0     |
| 56  | MG   | 1A    | 8133 | 1/1   | 0.98 | 0.14 | -    | 15,15,15,15                 | 0     |
| 56  | MG   | 2A    | 3579 | 1/1   | 0.98 | 0.10 | -    | 25,25,25,25                 | 0     |
| 56  | MG   | 1A    | 8818 | 1/1   | 0.93 | 0.39 | -    | 33,33,33,33                 | 0     |
| 56  | MG   | 2A    | 3739 | 1/1   | 0.89 | 0.29 | -    | 46,46,46,46                 | 0     |
| 56  | MG   | 1A    | 8392 | 1/1   | 0.94 | 0.14 | -    | 37,37,37,37                 | 0     |
| 56  | MG   | 1A    | 8812 | 1/1   | 0.94 | 0.11 | -    | 31,31,31,31                 | 0     |
| 56  | MG   | 2A    | 3828 | 1/1   | 0.84 | 0.22 | -    | 58,58,58,58                 | 0     |
| 56  | MG   | 1A    | 8799 | 1/1   | 0.96 | 0.22 | -    | 23,23,23,23                 | 0     |
| 56  | MG   | 1x    | 3014 | 1/1   | 0.95 | 0.16 | -    | 29,29,29,29                 | 0     |
| 56  | MG   | 1A    | 8576 | 1/1   | 0.96 | 0.06 | -    | 29,29,29,29                 | 0     |
| 56  | MG   | 1A    | 8459 | 1/1   | 0.98 | 0.08 | -    | 24,24,24,24                 | 0     |
| 56  | MG   | 1a    | 1814 | 1/1   | 0.87 | 0.16 | -    | 40,40,40,40                 | 0     |
| 56  | MG   | 1A    | 8909 | 1/1   | 0.85 | 0.21 | -    | 15,15,15,15                 | 0     |
| 56  | MG   | 1A    | 8520 | 1/1   | 0.94 | 0.23 | -    | 9,9,9,9                     | 0     |
| 56  | MG   | 1A    | 8533 | 1/1   | 0.91 | 0.13 | -    | 28,28,28,28                 | 0     |
| 56  | MG   | 1H    | 201  | 1/1   | 0.89 | 0.14 | -    | 38,38,38,38                 | 0     |
| 56  | MG   | 2A    | 3879 | 1/1   | 0.91 | 0.22 | -    | 36,36,36,36                 | 0     |
| 56  | MG   | 1A    | 8112 | 1/1   | 0.99 | 0.17 | -    | 13,13,13,13                 | 0     |
| 56  | MG   | 2A    | 3319 | 1/1   | 0.85 | 0.20 | -    | 68,68,68,68                 | 0     |
| 56  | MG   | 2A    | 3419 | 1/1   | 0.87 | 0.08 | -    | 48,48,48,48                 | 0     |
| 56  | MG   | 1A    | 8712 | 1/1   | 0.94 | 0.12 | -    | 24,24,24,24                 | 0     |
| 56  | MG   | 1A    | 8148 | 1/1   | 0.93 | 0.13 | -    | 7,7,7,7                     | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56  | MG   | 2a    | 1706 | 1/1   | 0.75 | 0.15 | -    | 55,55,55,55                 | 0     |
| 56  | MG   | 2A    | 3356 | 1/1   | 0.88 | 0.15 | -    | 30,30,30,30                 | 0     |
| 56  | MG   | 1a    | 1724 | 1/1   | 0.92 | 0.13 | -    | 50,50,50,50                 | 0     |
| 56  | MG   | 1A    | 8883 | 1/1   | 0.95 | 0.08 | -    | 30,30,30,30                 | 0     |
| 56  | MG   | 1A    | 8005 | 1/1   | 0.87 | 0.14 | -    | 20,20,20,20                 | 0     |
| 56  | MG   | 1N    | 203  | 1/1   | 0.91 | 0.14 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | 1A    | 8236 | 1/1   | 0.95 | 0.27 | -    | 22,22,22,22                 | 0     |
| 56  | MG   | 1A    | 8583 | 1/1   | 0.95 | 0.17 | -    | 8,8,8,8                     | 0     |
| 56  | MG   | 1A    | 8141 | 1/1   | 0.97 | 0.21 | -    | 22,22,22,22                 | 0     |
| 56  | MG   | 1A    | 8254 | 1/1   | 0.95 | 0.14 | -    | 15,15,15,15                 | 0     |
| 56  | MG   | 2A    | 3488 | 1/1   | 0.92 | 0.21 | -    | 30,30,30,30                 | 0     |
| 56  | MG   | 1A    | 8830 | 1/1   | 0.96 | 0.09 | -    | 27,27,27,27                 | 0     |
| 56  | MG   | 2A    | 3097 | 1/1   | 0.93 | 0.41 | -    | 38,38,38,38                 | 0     |
| 56  | MG   | 2A    | 3365 | 1/1   | 0.90 | 0.14 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | 2A    | 3819 | 1/1   | 0.97 | 0.07 | -    | 32,32,32,32                 | 0     |
| 56  | MG   | 1A    | 8941 | 1/1   | 0.91 | 0.29 | -    | 45,45,45,45                 | 0     |
| 56  | MG   | 1A    | 8119 | 1/1   | 0.88 | 0.09 | -    | 29,29,29,29                 | 0     |
| 56  | MG   | 2E    | 303  | 1/1   | 0.88 | 0.17 | -    | 64,64,64,64                 | 0     |
| 56  | MG   | 1A    | 8046 | 1/1   | 0.98 | 0.15 | -    | 12,12,12,12                 | 0     |
| 56  | MG   | 1a    | 1737 | 1/1   | 0.96 | 0.13 | -    | 40,40,40,40                 | 0     |
| 56  | MG   | 1A    | 8931 | 1/1   | 0.92 | 0.14 | -    | 18,18,18,18                 | 0     |
| 56  | MG   | 1a    | 1733 | 1/1   | 0.82 | 0.33 | -    | 58,58,58,58                 | 0     |
| 56  | MG   | 2A    | 3075 | 1/1   | 0.94 | 0.15 | -    | 35,35,35,35                 | 0     |
| 56  | MG   | 1V    | 201  | 1/1   | 0.94 | 0.21 | -    | 28,28,28,28                 | 0     |
| 56  | MG   | 2A    | 3791 | 1/1   | 0.95 | 0.11 | -    | 52,52,52,52                 | 0     |
| 56  | MG   | 1A    | 8142 | 1/1   | 0.95 | 0.37 | -    | 11,11,11,11                 | 0     |
| 56  | MG   | 1x    | 3010 | 1/1   | 0.95 | 0.13 | -    | 34,34,34,34                 | 0     |
| 56  | MG   | 1a    | 1775 | 1/1   | 0.80 | 0.19 | -    | 41,41,41,41                 | 0     |
| 56  | MG   | 2a    | 1680 | 1/1   | 0.74 | 0.64 | -    | 59,59,59,59                 | 0     |
| 56  | MG   | 2R    | 202  | 1/1   | 0.89 | 0.19 | -    | 21,21,21,21                 | 0     |
| 56  | MG   | 2a    | 1808 | 1/1   | 0.98 | 0.11 | -    | 53,53,53,53                 | 0     |
| 56  | MG   | 1A    | 8878 | 1/1   | 0.94 | 0.10 | -    | 16,16,16,16                 | 0     |
| 56  | MG   | 1A    | 8787 | 1/1   | 0.92 | 0.12 | -    | 8,8,8,8                     | 0     |
| 56  | MG   | 2A    | 3309 | 1/1   | 0.89 | 0.08 | -    | 38,38,38,38                 | 0     |
| 56  | MG   | 2B    | 3022 | 1/1   | 0.88 | 0.10 | -    | 59,59,59,59                 | 0     |
| 56  | MG   | 1A    | 8596 | 1/1   | 0.97 | 0.08 | -    | 17,17,17,17                 | 0     |
| 56  | MG   | 1A    | 8815 | 1/1   | 0.97 | 0.19 | -    | 21,21,21,21                 | 0     |
| 56  | MG   | 1a    | 1644 | 1/1   | 0.95 | 0.22 | -    | 38,38,38,38                 | 0     |
| 56  | MG   | 1A    | 8653 | 1/1   | 0.81 | 0.17 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | 2A    | 3826 | 1/1   | 0.92 | 0.07 | -    | 33,33,33,33                 | 0     |
| 56  | MG   | 1A    | 8249 | 1/1   | 0.81 | 0.31 | -    | 36,36,36,36                 | 0     |
| 56  | MG   | 1A    | 8157 | 1/1   | 0.90 | 0.21 | -    | 23,23,23,23                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|----------------------------|-------|
| 56  | MG   | 1A    | 8440 | 1/1   | 0.95 | 0.17 | -    | 5,5,5,5                    | 0     |
| 56  | MG   | 2A    | 3732 | 1/1   | 0.95 | 0.20 | -    | 62,62,62,62                | 0     |
| 56  | MG   | 2A    | 3942 | 1/1   | 0.94 | 0.12 | -    | 43,43,43,43                | 0     |
| 56  | MG   | 2A    | 3920 | 1/1   | 0.93 | 0.18 | -    | 43,43,43,43                | 0     |
| 56  | MG   | 1A    | 8290 | 1/1   | 0.93 | 0.10 | -    | 19,19,19,19                | 0     |
| 56  | MG   | 2A    | 3332 | 1/1   | 0.76 | 0.15 | -    | 69,69,69,69                | 0     |
| 56  | MG   | 2a    | 1761 | 1/1   | 0.83 | 0.12 | -    | 42,42,42,42                | 0     |
| 56  | MG   | 1A    | 8324 | 1/1   | 0.87 | 0.12 | -    | 17,17,17,17                | 0     |
| 56  | MG   | 2A    | 3440 | 1/1   | 0.97 | 0.09 | -    | 30,30,30,30                | 0     |
| 56  | MG   | 2j    | 201  | 1/1   | 0.93 | 0.17 | -    | 65,65,65,65                | 0     |
| 56  | MG   | 1a    | 1801 | 1/1   | 0.78 | 0.18 | -    | 60,60,60,60                | 0     |
| 56  | MG   | 2A    | 3559 | 1/1   | 0.83 | 0.26 | -    | 25,25,25,25                | 0     |
| 56  | MG   | 1A    | 8434 | 1/1   | 0.92 | 0.18 | -    | 16,16,16,16                | 0     |
| 56  | MG   | 2A    | 3764 | 1/1   | 0.91 | 0.07 | -    | 62,62,62,62                | 0     |
| 56  | MG   | 2A    | 3914 | 1/1   | 0.90 | 0.15 | -    | 51,51,51,51                | 0     |
| 56  | MG   | 1q    | 201  | 1/1   | 0.94 | 0.10 | -    | 37,37,37,37                | 0     |
| 56  | MG   | 2A    | 3447 | 1/1   | 0.96 | 0.17 | -    | 22,22,22,22                | 0     |
| 56  | MG   | 2A    | 3815 | 1/1   | 0.92 | 0.11 | -    | 33,33,33,33                | 0     |
| 56  | MG   | 2A    | 3245 | 1/1   | 0.81 | 0.28 | -    | 46,46,46,46                | 0     |
| 56  | MG   | 2A    | 3555 | 1/1   | 0.91 | 0.20 | -    | 35,35,35,35                | 0     |
| 56  | MG   | 1A    | 8513 | 1/1   | 0.95 | 0.06 | -    | 27,27,27,27                | 0     |
| 56  | MG   | 2i    | 3001 | 1/1   | 0.95 | 0.13 | -    | 36,36,36,36                | 0     |
| 56  | MG   | 1A    | 8644 | 1/1   | 0.88 | 0.23 | -    | 36,36,36,36                | 0     |
| 56  | MG   | 2A    | 3873 | 1/1   | 0.79 | 0.36 | -    | 74,74,74,74                | 0     |
| 56  | MG   | 1A    | 8507 | 1/1   | 0.94 | 0.20 | -    | 33,33,33,33                | 0     |
| 56  | MG   | 1A    | 8105 | 1/1   | 0.93 | 0.34 | -    | 12,12,12,12                | 0     |
| 56  | MG   | 1D    | 311  | 1/1   | 0.96 | 0.10 | -    | 31,31,31,31                | 0     |
| 56  | MG   | 1A    | 8667 | 1/1   | 0.81 | 0.24 | -    | 40,40,40,40                | 0     |
| 56  | MG   | 2U    | 206  | 1/1   | 0.93 | 0.24 | -    | 38,38,38,38                | 0     |
| 56  | MG   | 1A    | 8028 | 1/1   | 0.94 | 0.17 | -    | 11,11,11,11                | 0     |
| 56  | MG   | 2A    | 3863 | 1/1   | 0.88 | 0.26 | -    | 54,54,54,54                | 0     |
| 56  | MG   | 2A    | 3972 | 1/1   | 0.95 | 0.11 | -    | 31,31,31,31                | 0     |
| 56  | MG   | 1A    | 8201 | 1/1   | 0.87 | 0.32 | -    | 45,45,45,45                | 0     |
| 56  | MG   | 1A    | 8915 | 1/1   | 0.89 | 0.14 | -    | 38,38,38,38                | 0     |
| 56  | MG   | 2a    | 1821 | 1/1   | 0.76 | 0.18 | -    | 71,71,71,71                | 0     |
| 56  | MG   | 2A    | 3524 | 1/1   | 0.71 | 0.22 | -    | 59,59,59,59                | 0     |
| 56  | MG   | 2A    | 3823 | 1/1   | 0.83 | 0.19 | -    | 43,43,43,43                | 0     |
| 56  | MG   | 2B    | 3019 | 1/1   | 0.69 | 0.10 | -    | 62,62,62,62                | 0     |
| 56  | MG   | 1n    | 101  | 1/1   | 0.89 | 0.29 | -    | 51,51,51,51                | 0     |
| 56  | MG   | 2A    | 3021 | 1/1   | 0.94 | 0.18 | -    | 30,30,30,30                | 0     |
| 56  | MG   | 2A    | 3088 | 1/1   | 0.95 | 0.32 | -    | 33,33,33,33                | 0     |
| 56  | MG   | 2a    | 1684 | 1/1   | 0.87 | 0.29 | -    | 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   | 2A    | 3157 | 1/1   | 0.91 | 0.09 | -    | 40,40,40,40                 | 0     |
| 56  | MG   | 2A    | 3821 | 1/1   | 0.87 | 0.11 | -    | 48,48,48,48                 | 0     |
| 56  | MG   | 2A    | 3284 | 1/1   | 0.96 | 0.10 | -    | 41,41,41,41                 | 0     |
| 56  | MG   | 2A    | 3718 | 1/1   | 0.96 | 0.14 | -    | 30,30,30,30                 | 0     |
| 56  | MG   | 2A    | 3218 | 1/1   | 0.94 | 0.33 | -    | 37,37,37,37                 | 0     |
| 56  | MG   | 2A    | 3912 | 1/1   | 0.93 | 0.78 | -    | 49,49,49,49                 | 0     |
| 56  | MG   | 1A    | 8466 | 1/1   | 0.92 | 0.10 | -    | 25,25,25,25                 | 0     |
| 56  | MG   | 1A    | 8566 | 1/1   | 0.94 | 0.16 | -    | 22,22,22,22                 | 0     |
| 56  | MG   | 1A    | 8808 | 1/1   | 0.95 | 0.10 | -    | 17,17,17,17                 | 0     |
| 56  | MG   | 2A    | 3604 | 1/1   | 0.90 | 0.08 | -    | 43,43,43,43                 | 0     |
| 56  | MG   | 1d    | 505  | 1/1   | 0.81 | 0.05 | -    | 56,56,56,56                 | 0     |
| 56  | MG   | 2A    | 3643 | 1/1   | 0.94 | 0.27 | -    | 27,27,27,27                 | 0     |
| 56  | MG   | 1A    | 8525 | 1/1   | 0.92 | 0.18 | -    | 10,10,10,10                 | 0     |
| 56  | MG   | 1A    | 8364 | 1/1   | 0.95 | 0.14 | -    | 26,26,26,26                 | 0     |
| 56  | MG   | 1A    | 8538 | 1/1   | 0.96 | 0.11 | -    | 14,14,14,14                 | 0     |
| 56  | MG   | 2A    | 3469 | 1/1   | 0.92 | 0.24 | -    | 31,31,31,31                 | 0     |
| 56  | MG   | 1A    | 8019 | 1/1   | 0.91 | 0.41 | -    | 12,12,12,12                 | 0     |
| 56  | MG   | 1a    | 1606 | 1/1   | 0.93 | 0.18 | -    | 36,36,36,36                 | 0     |
| 56  | MG   | 2A    | 3725 | 1/1   | 0.95 | 0.11 | -    | 29,29,29,29                 | 0     |
| 56  | MG   | 2A    | 3797 | 1/1   | 0.94 | 0.19 | -    | 38,38,38,38                 | 0     |
| 56  | MG   | 1A    | 8471 | 1/1   | 0.85 | 0.21 | -    | 17,17,17,17                 | 0     |
| 56  | MG   | 2A    | 3698 | 1/1   | 0.87 | 0.13 | -    | 35,35,35,35                 | 0     |
| 56  | MG   | 1a    | 1744 | 1/1   | 0.77 | 0.15 | -    | 59,59,59,59                 | 0     |
| 56  | MG   | 2A    | 3794 | 1/1   | 0.89 | 0.07 | -    | 63,63,63,63                 | 0     |
| 56  | MG   | 2A    | 3886 | 1/1   | 0.96 | 0.15 | -    | 43,43,43,43                 | 0     |
| 56  | MG   | 1A    | 8335 | 1/1   | 0.95 | 0.26 | -    | 38,38,38,38                 | 0     |
| 56  | MG   | 1A    | 8689 | 1/1   | 0.80 | 0.20 | -    | 33,33,33,33                 | 0     |
| 56  | MG   | 1A    | 8488 | 1/1   | 0.83 | 0.21 | -    | 46,46,46,46                 | 0     |
| 56  | MG   | 2A    | 3843 | 1/1   | 0.95 | 0.16 | -    | 43,43,43,43                 | 0     |
| 56  | MG   | 1a    | 1768 | 1/1   | 0.66 | 0.27 | -    | 53,53,53,53                 | 0     |
| 56  | MG   | 2A    | 3888 | 1/1   | 0.92 | 0.15 | -    | 41,41,41,41                 | 0     |
| 56  | MG   | 2A    | 3229 | 1/1   | 0.94 | 0.14 | -    | 30,30,30,30                 | 0     |
| 56  | MG   | 1g    | 3001 | 1/1   | 0.95 | 0.12 | -    | 38,38,38,38                 | 0     |
| 56  | MG   | 1A    | 8771 | 1/1   | 0.95 | 0.09 | -    | 24,24,24,24                 | 0     |
| 56  | MG   | 2A    | 3043 | 1/1   | 0.91 | 0.18 | -    | 42,42,42,42                 | 0     |
| 56  | MG   | 2G    | 3002 | 1/1   | 0.70 | 0.17 | -    | 63,63,63,63                 | 0     |
| 56  | MG   | 2A    | 3812 | 1/1   | 0.94 | 0.11 | -    | 22,22,22,22                 | 0     |
| 56  | MG   | 1B    | 3006 | 1/1   | 0.92 | 0.13 | -    | 25,25,25,25                 | 0     |
| 56  | MG   | 1A    | 8847 | 1/1   | 0.90 | 0.25 | -    | 16,16,16,16                 | 0     |
| 56  | MG   | 1A    | 8755 | 1/1   | 0.99 | 0.28 | -    | 16,16,16,16                 | 0     |
| 56  | MG   | 2a    | 1717 | 1/1   | 0.93 | 0.13 | -    | 54,54,54,54                 | 0     |
| 56  | MG   | 1a    | 1637 | 1/1   | 0.97 | 0.39 | -    | 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    | 3362 | 1/1   | 0.87 | 0.13 | -    | 61,61,61,61                 | 0     |
| 56  | MG   | 1A    | 8124 | 1/1   | 0.89 | 0.14 | -    | 16,16,16,16                 | 0     |
| 56  | MG   | 1a    | 1652 | 1/1   | 0.87 | 0.16 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | 1B    | 3013 | 1/1   | 0.95 | 0.10 | -    | 24,24,24,24                 | 0     |
| 56  | MG   | 2A    | 3522 | 1/1   | 0.92 | 0.33 | -    | 51,51,51,51                 | 0     |
| 56  | MG   | 1a    | 1646 | 1/1   | 0.97 | 0.35 | -    | 34,34,34,34                 | 0     |
| 56  | MG   | 1A    | 8751 | 1/1   | 0.83 | 0.16 | -    | 44,44,44,44                 | 0     |
| 56  | MG   | 1A    | 8307 | 1/1   | 0.94 | 0.05 | -    | 18,18,18,18                 | 0     |
| 56  | MG   | 1A    | 8778 | 1/1   | 0.98 | 0.06 | -    | 21,21,21,21                 | 0     |
| 56  | MG   | 2A    | 3780 | 1/1   | 0.93 | 0.31 | -    | 44,44,44,44                 | 0     |
| 56  | MG   | 1A    | 8563 | 1/1   | 0.96 | 0.13 | -    | 11,11,11,11                 | 0     |
| 56  | MG   | 2A    | 3133 | 1/1   | 0.96 | 0.50 | -    | 39,39,39,39                 | 0     |
| 56  | MG   | 1A    | 8622 | 1/1   | 0.97 | 0.12 | -    | 26,26,26,26                 | 0     |
| 56  | MG   | 2A    | 3861 | 1/1   | 0.95 | 0.06 | -    | 50,50,50,50                 | 0     |
| 56  | MG   | 2A    | 3882 | 1/1   | 0.92 | 0.05 | -    | 46,46,46,46                 | 0     |
| 56  | MG   | 2A    | 3706 | 1/1   | 0.85 | 0.21 | -    | 32,32,32,32                 | 0     |
| 56  | MG   | 1A    | 8744 | 1/1   | 0.91 | 0.13 | -    | 17,17,17,17                 | 0     |
| 56  | MG   | 2A    | 3243 | 1/1   | 0.58 | 0.45 | -    | 31,31,31,31                 | 0     |
| 56  | MG   | 2A    | 3726 | 1/1   | 0.86 | 0.12 | -    | 50,50,50,50                 | 0     |
| 56  | MG   | 1A    | 8383 | 1/1   | 0.88 | 0.09 | -    | 10,10,10,10                 | 0     |
| 56  | MG   | 1A    | 8695 | 1/1   | 0.87 | 0.16 | -    | 11,11,11,11                 | 0     |
| 56  | MG   | 2A    | 3610 | 1/1   | 0.89 | 0.14 | -    | 57,57,57,57                 | 0     |
| 56  | MG   | 1a    | 1700 | 1/1   | 0.88 | 0.23 | -    | 45,45,45,45                 | 0     |
| 56  | MG   | 1A    | 8873 | 1/1   | 0.96 | 0.13 | -    | 10,10,10,10                 | 0     |
| 56  | MG   | 2A    | 3811 | 1/1   | 0.94 | 0.07 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | 1A    | 8159 | 1/1   | 0.92 | 0.15 | -    | 21,21,21,21                 | 0     |
| 56  | MG   | 1A    | 8318 | 1/1   | 0.97 | 0.17 | -    | 6,6,6,6                     | 0     |
| 56  | MG   | 1A    | 8859 | 1/1   | 0.83 | 0.15 | -    | 37,37,37,37                 | 0     |
| 56  | MG   | 2A    | 3504 | 1/1   | 0.87 | 0.25 | -    | 45,45,45,45                 | 0     |
| 56  | MG   | 2A    | 3574 | 1/1   | 0.91 | 0.16 | -    | 31,31,31,31                 | 0     |
| 56  | MG   | 2A    | 3768 | 1/1   | 0.83 | 0.13 | -    | 42,42,42,42                 | 0     |
| 56  | MG   | 1A    | 8171 | 1/1   | 0.89 | 0.13 | -    | 28,28,28,28                 | 0     |
| 56  | MG   | 1A    | 8528 | 1/1   | 0.97 | 0.20 | -    | 18,18,18,18                 | 0     |
| 56  | MG   | 2a    | 1685 | 1/1   | 0.93 | 0.08 | -    | 41,41,41,41                 | 0     |
| 56  | MG   | 1a    | 1604 | 1/1   | 0.79 | 0.33 | -    | 50,50,50,50                 | 0     |
| 56  | MG   | 2A    | 3675 | 1/1   | 0.81 | 0.19 | -    | 44,44,44,44                 | 0     |
| 56  | MG   | 1A    | 8769 | 1/1   | 0.95 | 0.12 | -    | 20,20,20,20                 | 0     |
| 56  | MG   | 2A    | 3845 | 1/1   | 0.92 | 0.38 | -    | 51,51,51,51                 | 0     |
| 56  | MG   | 2A    | 3679 | 1/1   | 0.77 | 0.22 | -    | 60,60,60,60                 | 0     |
| 56  | MG   | 1A    | 8341 | 1/1   | 0.92 | 0.14 | -    | 17,17,17,17                 | 0     |
| 56  | MG   | 2D    | 317  | 1/1   | 0.66 | 0.34 | -    | 59,59,59,59                 | 0     |
| 56  | MG   | 2A    | 3121 | 1/1   | 0.93 | 0.05 | -    | 42,42,42,42                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|----------------------------|-------|
| 56  | MG   | 2A    | 3331 | 1/1   | 0.91 | 0.25 | -    | 48,48,48,48                | 0     |
| 56  | MG   | 1E    | 304  | 1/1   | 0.93 | 0.10 | -    | 27,27,27,27                | 0     |
| 56  | MG   | 1A    | 8648 | 1/1   | 0.89 | 0.16 | -    | 27,27,27,27                | 0     |
| 56  | MG   | 2F    | 305  | 1/1   | 0.94 | 0.15 | -    | 26,26,26,26                | 0     |
| 56  | MG   | 2A    | 3074 | 1/1   | 0.75 | 0.48 | -    | 33,33,33,33                | 0     |
| 56  | MG   | 1A    | 8518 | 1/1   | 0.91 | 0.15 | -    | 35,35,35,35                | 0     |
| 56  | MG   | 1A    | 8844 | 1/1   | 0.97 | 0.23 | -    | 15,15,15,15                | 0     |
| 56  | MG   | 1A    | 8841 | 1/1   | 0.96 | 0.10 | -    | 34,34,34,34                | 0     |
| 56  | MG   | 2a    | 1715 | 1/1   | 0.78 | 0.21 | -    | 50,50,50,50                | 0     |
| 56  | MG   | 1A    | 8081 | 1/1   | 0.98 | 0.13 | -    | 16,16,16,16                | 0     |
| 56  | MG   | 1A    | 8679 | 1/1   | 0.74 | 0.19 | -    | 34,34,34,34                | 0     |
| 56  | MG   | 1A    | 8926 | 1/1   | 0.97 | 0.10 | -    | 35,35,35,35                | 0     |
| 56  | MG   | 2A    | 3894 | 1/1   | 0.94 | 0.09 | -    | 36,36,36,36                | 0     |
| 56  | MG   | 2A    | 3848 | 1/1   | 0.61 | 0.17 | -    | 63,63,63,63                | 0     |
| 56  | MG   | 2A    | 3943 | 1/1   | 0.96 | 0.24 | -    | 40,40,40,40                | 0     |
| 56  | MG   | 1A    | 8604 | 1/1   | 0.83 | 0.25 | -    | 29,29,29,29                | 0     |
| 56  | MG   | 2A    | 3632 | 1/1   | 0.95 | 0.12 | -    | 38,38,38,38                | 0     |
| 56  | MG   | 2a    | 1730 | 1/1   | 0.90 | 0.10 | -    | 71,71,71,71                | 0     |
| 56  | MG   | 1a    | 1662 | 1/1   | 0.94 | 0.12 | -    | 44,44,44,44                | 0     |
| 56  | MG   | 1f    | 8001 | 1/1   | 0.92 | 0.15 | -    | 36,36,36,36                | 0     |
| 56  | MG   | 1D    | 312  | 1/1   | 0.91 | 0.13 | -    | 41,41,41,41                | 0     |
| 56  | MG   | 2A    | 3399 | 1/1   | 0.90 | 0.27 | -    | 46,46,46,46                | 0     |
| 56  | MG   | 1A    | 8674 | 1/1   | 0.85 | 0.26 | -    | 35,35,35,35                | 0     |
| 56  | MG   | 2A    | 3867 | 1/1   | 0.92 | 0.11 | -    | 42,42,42,42                | 0     |
| 56  | MG   | 1A    | 8606 | 1/1   | 0.95 | 0.08 | -    | 26,26,26,26                | 0     |
| 56  | MG   | 2A    | 3859 | 1/1   | 0.94 | 0.10 | -    | 41,41,41,41                | 0     |
| 56  | MG   | 1A    | 8415 | 1/1   | 0.97 | 0.08 | -    | 16,16,16,16                | 0     |
| 56  | MG   | 2D    | 301  | 1/1   | 0.79 | 0.31 | -    | 52,52,52,52                | 0     |
| 56  | MG   | 1a    | 1800 | 1/1   | 0.73 | 0.11 | -    | 31,31,31,31                | 0     |
| 56  | MG   | 1A    | 8389 | 1/1   | 0.89 | 0.07 | -    | 32,32,32,32                | 0     |
| 56  | MG   | 1G    | 3002 | 1/1   | 0.81 | 0.10 | -    | 44,44,44,44                | 0     |
| 56  | MG   | 1A    | 8573 | 1/1   | 0.89 | 0.15 | -    | 18,18,18,18                | 0     |
| 56  | MG   | 2A    | 3790 | 1/1   | 0.91 | 0.15 | -    | 45,45,45,45                | 0     |
| 56  | MG   | 2A    | 3913 | 1/1   | 0.97 | 0.41 | -    | 34,34,34,34                | 0     |
| 56  | MG   | 1A    | 8497 | 1/1   | 0.93 | 0.13 | -    | 20,20,20,20                | 0     |
| 56  | MG   | 2A    | 3658 | 1/1   | 0.74 | 0.10 | -    | 29,29,29,29                | 0     |
| 56  | MG   | 1l    | 201  | 1/1   | 0.88 | 0.14 | -    | 42,42,42,42                | 0     |
| 56  | MG   | 1A    | 8449 | 1/1   | 0.87 | 0.08 | -    | 61,61,61,61                | 0     |
| 56  | MG   | 1A    | 8248 | 1/1   | 0.95 | 0.27 | -    | 17,17,17,17                | 0     |
| 56  | MG   | 2A    | 3551 | 1/1   | 0.80 | 0.27 | -    | 34,34,34,34                | 0     |
| 56  | MG   | 2A    | 3259 | 1/1   | 0.89 | 0.29 | -    | 33,33,33,33                | 0     |
| 56  | MG   | 1a    | 1784 | 1/1   | 0.89 | 0.20 | -    | 54,54,54,54                | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|----------------------------|-------|
| 56  | MG   | 2a    | 1645 | 1/1   | 0.96 | 0.12 | -    | 53,53,53,53                | 0     |
| 56  | MG   | 2A    | 3880 | 1/1   | 0.88 | 0.20 | -    | 32,32,32,32                | 0     |
| 56  | MG   | 2a    | 1768 | 1/1   | 0.92 | 0.21 | -    | 57,57,57,57                | 0     |
| 56  | MG   | 2A    | 3741 | 1/1   | 0.93 | 0.23 | -    | 69,69,69,69                | 0     |
| 56  | MG   | 1A    | 8916 | 1/1   | 0.78 | 0.07 | -    | 75,75,75,75                | 0     |
| 56  | MG   | 1E    | 302  | 1/1   | 0.95 | 0.14 | -    | 9,9,9,9                    | 0     |
| 56  | MG   | 1a    | 1835 | 1/1   | 0.95 | 0.14 | -    | 43,43,43,43                | 0     |
| 56  | MG   | 1A    | 8013 | 1/1   | 0.89 | 0.14 | -    | 20,20,20,20                | 0     |
| 56  | MG   | 2A    | 3746 | 1/1   | 0.97 | 0.22 | -    | 27,27,27,27                | 0     |
| 56  | MG   | 1A    | 8593 | 1/1   | 0.93 | 0.28 | -    | 16,16,16,16                | 0     |
| 56  | MG   | 1A    | 8650 | 1/1   | 0.94 | 0.19 | -    | 39,39,39,39                | 0     |
| 56  | MG   | 2a    | 1737 | 1/1   | 0.93 | 0.08 | -    | 53,53,53,53                | 0     |
| 56  | MG   | 2A    | 3571 | 1/1   | 0.89 | 0.15 | -    | 26,26,26,26                | 0     |
| 56  | MG   | 2D    | 316  | 1/1   | 0.63 | 0.15 | -    | 47,47,47,47                | 0     |
| 56  | MG   | 1A    | 8544 | 1/1   | 0.79 | 0.18 | -    | 27,27,27,27                | 0     |
| 56  | MG   | 2A    | 3038 | 1/1   | 0.96 | 0.26 | -    | 30,30,30,30                | 0     |
| 56  | MG   | 2A    | 3520 | 1/1   | 0.52 | 0.29 | -    | 74,74,74,74                | 0     |
| 56  | MG   | 2A    | 3204 | 1/1   | 0.90 | 0.31 | -    | 31,31,31,31                | 0     |
| 56  | MG   | 1A    | 8610 | 1/1   | 0.83 | 0.29 | -    | 41,41,41,41                | 0     |
| 56  | MG   | 1A    | 8765 | 1/1   | 0.97 | 0.08 | -    | 23,23,23,23                | 0     |
| 56  | MG   | 2A    | 3428 | 1/1   | 0.90 | 0.14 | -    | 30,30,30,30                | 0     |
| 56  | MG   | 1A    | 8802 | 1/1   | 0.88 | 0.11 | -    | 26,26,26,26                | 0     |
| 56  | MG   | 2N    | 202  | 1/1   | 0.89 | 0.21 | -    | 49,49,49,49                | 0     |
| 56  | MG   | 2A    | 3480 | 1/1   | 0.85 | 0.39 | -    | 63,63,63,63                | 0     |
| 56  | MG   | 1A    | 8309 | 1/1   | 0.97 | 0.10 | -    | 19,19,19,19                | 0     |
| 56  | MG   | 2A    | 3377 | 1/1   | 0.91 | 0.19 | -    | 32,32,32,32                | 0     |
| 56  | MG   | 2A    | 3807 | 1/1   | 0.90 | 0.11 | -    | 29,29,29,29                | 0     |
| 56  | MG   | 2A    | 3047 | 1/1   | 0.98 | 0.16 | -    | 18,18,18,18                | 0     |
| 56  | MG   | 2A    | 3503 | 1/1   | 0.86 | 0.21 | -    | 47,47,47,47                | 0     |
| 56  | MG   | 2A    | 3054 | 1/1   | 0.94 | 0.12 | -    | 22,22,22,22                | 0     |
| 56  | MG   | 1W    | 3002 | 1/1   | 0.96 | 0.28 | -    | 28,28,28,28                | 0     |
| 56  | MG   | 1U    | 202  | 1/1   | 0.95 | 0.14 | -    | 17,17,17,17                | 0     |
| 56  | MG   | 2A    | 3343 | 1/1   | 0.87 | 0.15 | -    | 35,35,35,35                | 0     |
| 56  | MG   | 1A    | 8319 | 1/1   | 0.95 | 0.09 | -    | 27,27,27,27                | 0     |
| 56  | MG   | 1A    | 8232 | 1/1   | 0.87 | 0.18 | -    | 34,34,34,34                | 0     |
| 56  | MG   | 2A    | 3822 | 1/1   | 0.96 | 0.04 | -    | 46,46,46,46                | 0     |
| 56  | MG   | 2A    | 3208 | 1/1   | 0.94 | 0.42 | -    | 31,31,31,31                | 0     |
| 56  | MG   | 1A    | 8395 | 1/1   | 0.97 | 0.16 | -    | 34,34,34,34                | 0     |
| 56  | MG   | 1A    | 8725 | 1/1   | 0.95 | 0.14 | -    | 18,18,18,18                | 0     |
| 56  | MG   | 1A    | 8346 | 1/1   | 0.95 | 0.18 | -    | 14,14,14,14                | 0     |
| 56  | MG   | 2A    | 3552 | 1/1   | 0.86 | 0.32 | -    | 47,47,47,47                | 0     |
| 56  | MG   | 2A    | 3325 | 1/1   | 0.95 | 0.23 | -    | 35,35,35,35                | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56  | MG   | 2A    | 3915 | 1/1   | 0.80 | 0.13 | -    | 42,42,42,42                 | 0     |
| 56  | MG   | 2A    | 3735 | 1/1   | 0.93 | 0.08 | -    | 46,46,46,46                 | 0     |
| 56  | MG   | 1A    | 8547 | 1/1   | 0.88 | 0.11 | -    | 21,21,21,21                 | 0     |
| 56  | MG   | 1A    | 8601 | 1/1   | 0.93 | 0.12 | -    | 36,36,36,36                 | 0     |
| 56  | MG   | 1a    | 1612 | 1/1   | 0.90 | 0.09 | -    | 52,52,52,52                 | 0     |
| 56  | MG   | 1A    | 8803 | 1/1   | 0.89 | 0.13 | -    | 59,59,59,59                 | 0     |
| 56  | MG   | 1A    | 8125 | 1/1   | 0.97 | 0.17 | -    | 30,30,30,30                 | 0     |
| 56  | MG   | 2A    | 3228 | 1/1   | 0.92 | 0.40 | -    | 34,34,34,34                 | 0     |
| 56  | MG   | 2A    | 3432 | 1/1   | 0.96 | 0.09 | -    | 45,45,45,45                 | 0     |
| 56  | MG   | 1A    | 8935 | 1/1   | 0.98 | 0.31 | -    | 5,5,5,5                     | 0     |
| 56  | MG   | 2a    | 1784 | 1/1   | 0.81 | 0.25 | -    | 64,64,64,64                 | 0     |
| 56  | MG   | 1A    | 8892 | 1/1   | 0.95 | 0.11 | -    | 28,28,28,28                 | 0     |
| 56  | MG   | 2A    | 3557 | 1/1   | 0.97 | 0.53 | -    | 33,33,33,33                 | 0     |
| 56  | MG   | 1A    | 8843 | 1/1   | 0.95 | 0.13 | -    | 33,33,33,33                 | 0     |
| 56  | MG   | 1A    | 8732 | 1/1   | 0.89 | 0.25 | -    | 33,33,33,33                 | 0     |
| 56  | MG   | 1A    | 8516 | 1/1   | 0.95 | 0.14 | -    | 34,34,34,34                 | 0     |
| 56  | MG   | 1A    | 8625 | 1/1   | 0.84 | 0.20 | -    | 39,39,39,39                 | 0     |
| 56  | MG   | 2A    | 3421 | 1/1   | 0.79 | 0.14 | -    | 49,49,49,49                 | 0     |
| 56  | MG   | 1A    | 8534 | 1/1   | 0.88 | 0.15 | -    | 52,52,52,52                 | 0     |
| 56  | MG   | 1S    | 201  | 1/1   | 0.89 | 0.12 | -    | 23,23,23,23                 | 0     |
| 56  | MG   | 2A    | 3111 | 1/1   | 0.91 | 0.48 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | 1A    | 8649 | 1/1   | 0.86 | 0.32 | -    | 18,18,18,18                 | 0     |
| 56  | MG   | 2E    | 302  | 1/1   | 0.90 | 0.11 | -    | 26,26,26,26                 | 0     |
| 56  | MG   | 29    | 503  | 1/1   | 0.84 | 0.22 | -    | 62,62,62,62                 | 0     |
| 56  | MG   | 1A    | 8617 | 1/1   | 0.72 | 0.17 | -    | 43,43,43,43                 | 0     |
| 56  | MG   | 2A    | 3911 | 1/1   | 0.97 | 0.08 | -    | 53,53,53,53                 | 0     |
| 56  | MG   | 2A    | 3640 | 1/1   | 0.91 | 0.29 | -    | 26,26,26,26                 | 0     |
| 56  | MG   | 1A    | 8185 | 1/1   | 0.90 | 0.24 | -    | 26,26,26,26                 | 0     |
| 56  | MG   | 1a    | 1627 | 1/1   | 0.95 | 0.43 | -    | 37,37,37,37                 | 0     |
| 56  | MG   | 1A    | 8140 | 1/1   | 0.90 | 0.06 | -    | 52,52,52,52                 | 0     |
| 56  | MG   | 1A    | 8230 | 1/1   | 0.94 | 0.36 | -    | 13,13,13,13                 | 0     |
| 56  | MG   | 1A    | 8879 | 1/1   | 0.87 | 0.14 | -    | 25,25,25,25                 | 0     |
| 56  | MG   | 1A    | 8405 | 1/1   | 0.96 | 0.11 | -    | 16,16,16,16                 | 0     |
| 56  | MG   | 1A    | 8455 | 1/1   | 0.95 | 0.09 | -    | 22,22,22,22                 | 0     |
| 56  | MG   | 1A    | 8065 | 1/1   | 0.93 | 0.15 | -    | 11,11,11,11                 | 0     |
| 56  | MG   | 2a    | 1601 | 1/1   | 0.82 | 0.18 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | 1A    | 8109 | 1/1   | 0.98 | 0.09 | -    | 12,12,12,12                 | 0     |
| 56  | MG   | 2A    | 3107 | 1/1   | 0.93 | 0.20 | -    | 34,34,34,34                 | 0     |
| 56  | MG   | 2a    | 1721 | 1/1   | 0.95 | 0.14 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | 2a    | 1732 | 1/1   | 0.74 | 0.19 | -    | 77,77,77,77                 | 0     |
| 56  | MG   | 2A    | 3907 | 1/1   | 0.93 | 0.14 | -    | 23,23,23,23                 | 0     |
| 56  | MG   | 1A    | 8783 | 1/1   | 0.96 | 0.13 | -    | 15,15,15,15                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56  | MG   | 2a    | 1813 | 1/1   | 0.91 | 0.15 | -    | 42,42,42,42                 | 0     |
| 56  | MG   | 1A    | 8779 | 1/1   | 0.95 | 0.09 | -    | 29,29,29,29                 | 0     |
| 56  | MG   | 1A    | 8464 | 1/1   | 0.88 | 0.21 | -    | 7,7,7,7                     | 0     |
| 56  | MG   | 2B    | 3017 | 1/1   | 0.75 | 0.42 | -    | 74,74,74,74                 | 0     |
| 56  | MG   | 2D    | 307  | 1/1   | 0.97 | 0.14 | -    | 33,33,33,33                 | 0     |
| 56  | MG   | 1A    | 8628 | 1/1   | 0.56 | 0.21 | -    | 62,62,62,62                 | 0     |
| 56  | MG   | 2A    | 3618 | 1/1   | 0.91 | 0.16 | -    | 43,43,43,43                 | 0     |
| 56  | MG   | 2a    | 1643 | 1/1   | 0.91 | 0.28 | -    | 57,57,57,57                 | 0     |
| 56  | MG   | 1A    | 8828 | 1/1   | 0.90 | 0.06 | -    | 40,40,40,40                 | 0     |
| 56  | MG   | 1a    | 1712 | 1/1   | 0.96 | 0.04 | -    | 39,39,39,39                 | 0     |
| 56  | MG   | 2A    | 3905 | 1/1   | 0.64 | 0.24 | -    | 56,56,56,56                 | 0     |
| 56  | MG   | 1a    | 1777 | 1/1   | 0.84 | 0.41 | -    | 56,56,56,56                 | 0     |
| 56  | MG   | 1a    | 1824 | 1/1   | 0.82 | 0.11 | -    | 54,54,54,54                 | 0     |
| 56  | MG   | 1A    | 8730 | 1/1   | 0.84 | 0.12 | -    | 62,62,62,62                 | 0     |
| 56  | MG   | 1A    | 8745 | 1/1   | 0.93 | 0.19 | -    | 17,17,17,17                 | 0     |
| 56  | MG   | 2A    | 3178 | 1/1   | 0.94 | 0.28 | -    | 31,31,31,31                 | 0     |
| 56  | MG   | 1B    | 3022 | 1/1   | 0.80 | 0.14 | -    | 41,41,41,41                 | 0     |
| 56  | MG   | 2A    | 3883 | 1/1   | 0.92 | 0.09 | -    | 60,60,60,60                 | 0     |
| 56  | MG   | 1A    | 8708 | 1/1   | 0.96 | 0.18 | -    | 17,17,17,17                 | 0     |
| 56  | MG   | 1A    | 8629 | 1/1   | 0.92 | 0.17 | -    | 45,45,45,45                 | 0     |
| 56  | MG   | 2A    | 3246 | 1/1   | 0.96 | 0.07 | -    | 26,26,26,26                 | 0     |
| 56  | MG   | 2A    | 3755 | 1/1   | 0.87 | 0.27 | -    | 50,50,50,50                 | 0     |
| 56  | MG   | 1A    | 8176 | 1/1   | 0.88 | 0.10 | -    | 28,28,28,28                 | 0     |
| 56  | MG   | 2A    | 3491 | 1/1   | 0.97 | 0.20 | -    | 27,27,27,27                 | 0     |
| 56  | MG   | 1a    | 1780 | 1/1   | 0.89 | 0.13 | -    | 61,61,61,61                 | 0     |
| 56  | MG   | 1A    | 8009 | 1/1   | 0.94 | 0.24 | -    | 20,20,20,20                 | 0     |
| 56  | MG   | 1A    | 8060 | 1/1   | 0.91 | 0.14 | -    | 31,31,31,31                 | 0     |
| 56  | MG   | 2A    | 3036 | 1/1   | 0.90 | 0.14 | -    | 34,34,34,34                 | 0     |
| 56  | MG   | 2A    | 3003 | 1/1   | 0.93 | 0.13 | -    | 42,42,42,42                 | 0     |
| 56  | MG   | 1A    | 8671 | 1/1   | 0.97 | 0.11 | -    | 17,17,17,17                 | 0     |
| 56  | MG   | 2A    | 3535 | 1/1   | 0.76 | 0.21 | -    | 55,55,55,55                 | 0     |
| 56  | MG   | 1A    | 8863 | 1/1   | 0.82 | 0.23 | -    | 24,24,24,24                 | 0     |
| 56  | MG   | 1a    | 1691 | 1/1   | 0.98 | 0.09 | -    | 30,30,30,30                 | 0     |
| 56  | MG   | 2A    | 3174 | 1/1   | 0.86 | 0.10 | -    | 40,40,40,40                 | 0     |
| 56  | MG   | 1x    | 3013 | 1/1   | 0.93 | 0.14 | -    | 53,53,53,53                 | 0     |
| 56  | MG   | 1B    | 3020 | 1/1   | 0.89 | 0.14 | -    | 23,23,23,23                 | 0     |
| 56  | MG   | 2V    | 201  | 1/1   | 0.94 | 0.08 | -    | 32,32,32,32                 | 0     |
| 56  | MG   | 2A    | 3382 | 1/1   | 0.90 | 0.10 | -    | 38,38,38,38                 | 0     |
| 56  | MG   | 2A    | 3707 | 1/1   | 0.93 | 0.06 | -    | 31,31,31,31                 | 0     |
| 56  | MG   | 2A    | 3483 | 1/1   | 0.94 | 0.17 | -    | 48,48,48,48                 | 0     |
| 56  | MG   | 1A    | 8782 | 1/1   | 0.94 | 0.14 | -    | 24,24,24,24                 | 0     |
| 56  | MG   | 1A    | 8397 | 1/1   | 0.95 | 0.12 | -    | 18,18,18,18                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56  | MG   | 1Q    | 202  | 1/1   | 0.82 | 0.10 | -    | 53,53,53,53                 | 0     |
| 56  | MG   | 1A    | 8191 | 1/1   | 0.95 | 0.21 | -    | 17,17,17,17                 | 0     |
| 56  | MG   | 1A    | 8864 | 1/1   | 0.84 | 0.15 | -    | 26,26,26,26                 | 0     |
| 56  | MG   | 2A    | 3513 | 1/1   | 0.92 | 0.19 | -    | 38,38,38,38                 | 0     |
| 56  | MG   | 1A    | 8136 | 1/1   | 0.97 | 0.12 | -    | 10,10,10,10                 | 0     |
| 56  | MG   | 1H    | 202  | 1/1   | 0.76 | 0.12 | -    | 39,39,39,39                 | 0     |
| 56  | MG   | 2A    | 3501 | 1/1   | 0.87 | 0.12 | -    | 41,41,41,41                 | 0     |
| 56  | MG   | 2a    | 1774 | 1/1   | 0.90 | 0.14 | -    | 54,54,54,54                 | 0     |
| 56  | MG   | 1A    | 8899 | 1/1   | 0.86 | 0.12 | -    | 37,37,37,37                 | 0     |
| 56  | MG   | 2A    | 3699 | 1/1   | 0.68 | 0.43 | -    | 46,46,46,46                 | 0     |
| 56  | MG   | 2a    | 1764 | 1/1   | 0.88 | 0.22 | -    | 55,55,55,55                 | 0     |
| 56  | MG   | 1a    | 1607 | 1/1   | 0.93 | 0.10 | -    | 49,49,49,49                 | 0     |
| 56  | MG   | 2A    | 3928 | 1/1   | 0.89 | 0.28 | -    | 31,31,31,31                 | 0     |
| 56  | MG   | 1a    | 1680 | 1/1   | 0.87 | 0.24 | -    | 27,27,27,27                 | 0     |
| 56  | MG   | 2A    | 3648 | 1/1   | 0.95 | 0.09 | -    | 34,34,34,34                 | 0     |
| 56  | MG   | 2a    | 1747 | 1/1   | 0.95 | 0.23 | -    | 39,39,39,39                 | 0     |
| 56  | MG   | 1A    | 8668 | 1/1   | 0.92 | 0.25 | -    | 32,32,32,32                 | 0     |
| 56  | MG   | 2A    | 3620 | 1/1   | 0.67 | 0.23 | -    | 61,61,61,61                 | 0     |
| 56  | MG   | 1A    | 8233 | 1/1   | 0.93 | 0.26 | -    | 21,21,21,21                 | 0     |
| 56  | MG   | 2A    | 3341 | 1/1   | 0.77 | 0.14 | -    | 43,43,43,43                 | 0     |
| 56  | MG   | 1A    | 8811 | 1/1   | 0.98 | 0.16 | -    | 35,35,35,35                 | 0     |
| 56  | MG   | 2A    | 3908 | 1/1   | 0.87 | 0.81 | -    | 57,57,57,57                 | 0     |
| 56  | MG   | 1A    | 8714 | 1/1   | 0.95 | 0.12 | -    | 9,9,9,9                     | 0     |
| 56  | MG   | 1A    | 8337 | 1/1   | 0.97 | 0.14 | -    | 34,34,34,34                 | 0     |
| 56  | MG   | 1A    | 8408 | 1/1   | 0.94 | 0.08 | -    | 19,19,19,19                 | 0     |
| 56  | MG   | 1A    | 8522 | 1/1   | 0.94 | 0.13 | -    | 34,34,34,34                 | 0     |
| 56  | MG   | 2A    | 3181 | 1/1   | 0.90 | 0.35 | -    | 31,31,31,31                 | 0     |
| 56  | MG   | 1A    | 8077 | 1/1   | 0.95 | 0.16 | -    | 15,15,15,15                 | 0     |
| 56  | MG   | 1B    | 3026 | 1/1   | 0.94 | 0.29 | -    | 35,35,35,35                 | 0     |
| 56  | MG   | 2A    | 3507 | 1/1   | 0.94 | 0.14 | -    | 43,43,43,43                 | 0     |
| 56  | MG   | 1R    | 204  | 1/1   | 0.90 | 0.15 | -    | 26,26,26,26                 | 0     |
| 56  | MG   | 2A    | 3305 | 1/1   | 0.86 | 0.08 | -    | 41,41,41,41                 | 0     |
| 56  | MG   | 1A    | 8550 | 1/1   | 0.90 | 0.17 | -    | 35,35,35,35                 | 0     |
| 56  | MG   | 1a    | 1763 | 1/1   | 0.91 | 0.06 | -    | 55,55,55,55                 | 0     |
| 56  | MG   | 2a    | 1683 | 1/1   | 0.93 | 0.17 | -    | 61,61,61,61                 | 0     |
| 56  | MG   | 1A    | 8189 | 1/1   | 0.98 | 0.22 | -    | 11,11,11,11                 | 0     |
| 56  | MG   | 2A    | 3152 | 1/1   | 0.94 | 0.13 | -    | 32,32,32,32                 | 0     |
| 56  | MG   | 1A    | 8402 | 1/1   | 0.90 | 0.11 | -    | 29,29,29,29                 | 0     |
| 56  | MG   | 1A    | 8670 | 1/1   | 0.85 | 0.46 | -    | 41,41,41,41                 | 0     |
| 56  | MG   | 1a    | 1831 | 1/1   | 0.97 | 0.37 | -    | 14,14,14,14                 | 0     |
| 56  | MG   | 1N    | 204  | 1/1   | 0.73 | 0.26 | -    | 68,68,68,68                 | 0     |
| 56  | MG   | 2A    | 3186 | 1/1   | 0.98 | 0.26 | -    | 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   | 2a    | 1701 | 1/1   | 0.68 | 0.21 | -    | 82,82,82,82                 | 0     |
| 56  | MG   | 1A    | 8247 | 1/1   | 0.84 | 0.17 | -    | 25,25,25,25                 | 0     |
| 56  | MG   | 1a    | 1633 | 1/1   | 0.98 | 0.09 | -    | 27,27,27,27                 | 0     |
| 56  | MG   | 2A    | 3279 | 1/1   | 0.80 | 0.17 | -    | 49,49,49,49                 | 0     |
| 56  | MG   | 1A    | 8242 | 1/1   | 0.90 | 0.23 | -    | 44,44,44,44                 | 0     |
| 56  | MG   | 2A    | 3682 | 1/1   | 0.97 | 0.08 | -    | 40,40,40,40                 | 0     |
| 56  | MG   | 1a    | 1699 | 1/1   | 0.94 | 0.09 | -    | 26,26,26,26                 | 0     |
| 56  | MG   | 1A    | 8222 | 1/1   | 0.93 | 0.23 | -    | 18,18,18,18                 | 0     |
| 56  | MG   | 1F    | 305  | 1/1   | 0.92 | 0.15 | -    | 15,15,15,15                 | 0     |
| 56  | MG   | 2A    | 3724 | 1/1   | 0.92 | 0.56 | -    | 50,50,50,50                 | 0     |
| 56  | MG   | 1A    | 8480 | 1/1   | 0.94 | 0.10 | -    | 34,34,34,34                 | 0     |
| 56  | MG   | 2A    | 3242 | 1/1   | 0.97 | 0.24 | -    | 30,30,30,30                 | 0     |
| 56  | MG   | 2A    | 3852 | 1/1   | 0.97 | 0.21 | -    | 40,40,40,40                 | 0     |
| 56  | MG   | 2A    | 3695 | 1/1   | 0.97 | 0.07 | -    | 33,33,33,33                 | 0     |
| 56  | MG   | 1V    | 203  | 1/1   | 0.96 | 0.10 | -    | 40,40,40,40                 | 0     |
| 56  | MG   | 1A    | 8188 | 1/1   | 0.96 | 0.43 | -    | 16,16,16,16                 | 0     |
| 56  | MG   | 2A    | 3375 | 1/1   | 0.91 | 0.19 | -    | 24,24,24,24                 | 0     |
| 56  | MG   | 2A    | 3662 | 1/1   | 0.81 | 0.11 | -    | 43,43,43,43                 | 0     |
| 56  | MG   | 1A    | 8691 | 1/1   | 0.83 | 0.17 | -    | 14,14,14,14                 | 0     |
| 56  | MG   | 1A    | 8129 | 1/1   | 0.89 | 0.19 | -    | 19,19,19,19                 | 0     |
| 56  | MG   | 2A    | 3192 | 1/1   | 0.93 | 0.21 | -    | 29,29,29,29                 | 0     |
| 56  | MG   | 2A    | 3128 | 1/1   | 0.98 | 0.09 | -    | 48,48,48,48                 | 0     |
| 56  | MG   | 2l    | 202  | 1/1   | 0.96 | 0.09 | -    | 50,50,50,50                 | 0     |
| 56  | MG   | 2a    | 1723 | 1/1   | 0.95 | 0.14 | -    | 50,50,50,50                 | 0     |
| 56  | MG   | 1A    | 8851 | 1/1   | 0.96 | 0.09 | -    | 33,33,33,33                 | 0     |
| 56  | MG   | 2A    | 3664 | 1/1   | 0.84 | 0.20 | -    | 25,25,25,25                 | 0     |
| 56  | MG   | 1A    | 8564 | 1/1   | 0.96 | 0.27 | -    | 11,11,11,11                 | 0     |
| 56  | MG   | 2a    | 1708 | 1/1   | 0.97 | 0.08 | -    | 29,29,29,29                 | 0     |
| 56  | MG   | 1A    | 8897 | 1/1   | 0.93 | 0.10 | -    | 48,48,48,48                 | 0     |
| 56  | MG   | 1A    | 8270 | 1/1   | 0.90 | 0.23 | -    | 20,20,20,20                 | 0     |
| 56  | MG   | 1a    | 1827 | 1/1   | 0.76 | 0.17 | -    | 62,62,62,62                 | 0     |
| 56  | MG   | 2A    | 3337 | 1/1   | 0.94 | 0.14 | -    | 28,28,28,28                 | 0     |
| 56  | MG   | 2U    | 203  | 1/1   | 0.97 | 0.19 | -    | 35,35,35,35                 | 0     |
| 56  | MG   | 2A    | 3704 | 1/1   | 0.87 | 0.23 | -    | 53,53,53,53                 | 0     |
| 56  | MG   | 2A    | 3189 | 1/1   | 0.98 | 0.26 | -    | 32,32,32,32                 | 0     |
| 56  | MG   | 1a    | 1614 | 1/1   | 0.90 | 0.24 | -    | 52,52,52,52                 | 0     |
| 56  | MG   | 2a    | 1816 | 1/1   | 0.95 | 0.16 | -    | 56,56,56,56                 | 0     |
| 56  | MG   | 1A    | 8216 | 1/1   | 0.96 | 0.37 | -    | 15,15,15,15                 | 0     |
| 56  | MG   | 2A    | 3006 | 1/1   | 0.91 | 0.22 | -    | 45,45,45,45                 | 0     |
| 56  | MG   | 2A    | 3533 | 1/1   | 0.98 | 0.08 | -    | 50,50,50,50                 | 0     |
| 56  | MG   | 2A    | 3101 | 1/1   | 0.94 | 0.36 | -    | 48,48,48,48                 | 0     |
| 56  | MG   | 2A    | 3874 | 1/1   | 0.93 | 0.18 | -    | 32,32,32,32                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56  | MG   | 1A    | 8509 | 1/1   | 0.96 | 0.19 | -    | 42,42,42,42                 | 0     |
| 56  | MG   | 1a    | 1726 | 1/1   | 0.81 | 0.36 | -    | 56,56,56,56                 | 0     |
| 56  | MG   | 1A    | 8183 | 1/1   | 0.92 | 0.13 | -    | 24,24,24,24                 | 0     |
| 56  | MG   | 1A    | 8475 | 1/1   | 0.97 | 0.15 | -    | 28,28,28,28                 | 0     |
| 56  | MG   | 1a    | 1641 | 1/1   | 0.92 | 0.20 | -    | 33,33,33,33                 | 0     |
| 56  | MG   | 2A    | 3775 | 1/1   | 0.80 | 0.58 | -    | 51,51,51,51                 | 0     |
| 56  | MG   | 1A    | 8401 | 1/1   | 0.91 | 0.22 | -    | 28,28,28,28                 | 0     |
| 56  | MG   | 1o    | 102  | 1/1   | 0.91 | 0.09 | -    | 26,26,26,26                 | 0     |
| 56  | MG   | 1A    | 8676 | 1/1   | 0.84 | 0.06 | -    | 26,26,26,26                 | 0     |
| 56  | MG   | 1A    | 8239 | 1/1   | 0.94 | 0.17 | -    | 13,13,13,13                 | 0     |
| 56  | MG   | 2A    | 3634 | 1/1   | 0.99 | 0.03 | -    | 43,43,43,43                 | 0     |
| 56  | MG   | 1N    | 202  | 1/1   | 0.98 | 0.09 | -    | 28,28,28,28                 | 0     |
| 56  | MG   | 1A    | 8069 | 1/1   | 0.88 | 0.19 | -    | 18,18,18,18                 | 0     |
| 56  | MG   | 2A    | 3159 | 1/1   | 0.92 | 0.14 | -    | 36,36,36,36                 | 0     |
| 56  | MG   | 1A    | 8512 | 1/1   | 0.97 | 0.11 | -    | 28,28,28,28                 | 0     |
| 56  | MG   | 2A    | 3832 | 1/1   | 0.79 | 0.24 | -    | 31,31,31,31                 | 0     |
| 56  | MG   | 1A    | 8641 | 1/1   | 0.91 | 0.13 | -    | 20,20,20,20                 | 0     |
| 56  | MG   | 2h    | 3002 | 1/1   | 0.76 | 0.55 | -    | 64,64,64,64                 | 0     |
| 56  | MG   | 1a    | 1665 | 1/1   | 0.97 | 0.23 | -    | 51,51,51,51                 | 0     |
| 56  | MG   | 2A    | 3289 | 1/1   | 0.97 | 0.13 | -    | 22,22,22,22                 | 0     |
| 56  | MG   | 2A    | 3525 | 1/1   | 0.84 | 0.14 | -    | 25,25,25,25                 | 0     |
| 56  | MG   | 2A    | 3281 | 1/1   | 0.91 | 0.17 | -    | 52,52,52,52                 | 0     |
| 56  | MG   | 1A    | 8010 | 1/1   | 0.88 | 0.22 | -    | 7,7,7,7                     | 0     |
| 56  | MG   | 2a    | 1714 | 1/1   | 0.64 | 0.23 | -    | 60,60,60,60                 | 0     |
| 56  | MG   | 1A    | 8438 | 1/1   | 0.86 | 0.12 | -    | 34,34,34,34                 | 0     |
| 56  | MG   | 2a    | 1758 | 1/1   | 0.64 | 0.81 | -    | 83,83,83,83                 | 0     |
| 56  | MG   | 2A    | 3451 | 1/1   | 0.98 | 0.16 | -    | 46,46,46,46                 | 0     |
| 56  | MG   | 2A    | 3328 | 1/1   | 0.92 | 0.33 | -    | 31,31,31,31                 | 0     |
| 56  | MG   | 2a    | 1629 | 1/1   | 0.89 | 0.54 | -    | 53,53,53,53                 | 0     |
| 56  | MG   | 1A    | 8064 | 1/1   | 0.96 | 0.14 | -    | 23,23,23,23                 | 0     |
| 56  | MG   | 2a    | 1700 | 1/1   | 0.84 | 0.17 | -    | 51,51,51,51                 | 0     |
| 56  | MG   | 2A    | 3197 | 1/1   | 0.93 | 0.08 | -    | 37,37,37,37                 | 0     |
| 56  | MG   | 2A    | 3017 | 1/1   | 0.93 | 0.22 | -    | 46,46,46,46                 | 0     |
| 56  | MG   | 2H    | 8002 | 1/1   | 0.55 | 0.69 | -    | 79,79,79,79                 | 0     |
| 56  | MG   | 2A    | 3855 | 1/1   | 0.93 | 0.14 | -    | 32,32,32,32                 | 0     |
| 56  | MG   | 1A    | 8645 | 1/1   | 0.95 | 0.16 | -    | 11,11,11,11                 | 0     |
| 56  | MG   | 1A    | 8220 | 1/1   | 0.85 | 0.12 | -    | 52,52,52,52                 | 0     |
| 56  | MG   | 1a    | 1715 | 1/1   | 0.98 | 0.07 | -    | 32,32,32,32                 | 0     |
| 56  | MG   | 2A    | 3039 | 1/1   | 0.94 | 0.20 | -    | 38,38,38,38                 | 0     |
| 56  | MG   | 2A    | 3053 | 1/1   | 0.92 | 0.42 | -    | 27,27,27,27                 | 0     |
| 56  | MG   | 1A    | 8184 | 1/1   | 0.99 | 0.22 | -    | 17,17,17,17                 | 0     |
| 56  | MG   | 1A    | 8813 | 1/1   | 0.95 | 0.10 | -    | 11,11,11,11                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56  | MG   | 2A    | 3849 | 1/1   | 0.71 | 0.22 | -    | 56,56,56,56                 | 0     |
| 56  | MG   | 15    | 104  | 1/1   | 0.95 | 0.24 | -    | 16,16,16,16                 | 0     |
| 56  | MG   | 1A    | 8122 | 1/1   | 0.93 | 0.10 | -    | 18,18,18,18                 | 0     |
| 56  | MG   | 2A    | 3967 | 1/1   | 0.67 | 0.59 | -    | 55,55,55,55                 | 0     |
| 56  | MG   | 1a    | 1757 | 1/1   | 0.90 | 0.12 | -    | 44,44,44,44                 | 0     |
| 56  | MG   | 1A    | 8910 | 1/1   | 0.98 | 0.09 | -    | 19,19,19,19                 | 0     |
| 56  | MG   | 1a    | 1705 | 1/1   | 0.96 | 0.14 | -    | 25,25,25,25                 | 0     |
| 56  | MG   | 1A    | 8422 | 1/1   | 0.98 | 0.05 | -    | 33,33,33,33                 | 0     |
| 56  | MG   | 1x    | 3003 | 1/1   | 0.90 | 0.14 | -    | 31,31,31,31                 | 0     |
| 56  | MG   | 2a    | 1631 | 1/1   | 0.96 | 0.22 | -    | 42,42,42,42                 | 0     |
| 56  | MG   | 2A    | 3929 | 1/1   | 0.89 | 0.15 | -    | 48,48,48,48                 | 0     |
| 56  | MG   | 2A    | 3765 | 1/1   | 0.79 | 0.08 | -    | 48,48,48,48                 | 0     |
| 56  | MG   | 1a    | 1718 | 1/1   | 0.88 | 0.09 | -    | 44,44,44,44                 | 0     |
| 56  | MG   | 1A    | 8496 | 1/1   | 0.97 | 0.11 | -    | 21,21,21,21                 | 0     |
| 56  | MG   | 2a    | 1719 | 1/1   | 0.77 | 0.39 | -    | 39,39,39,39                 | 0     |
| 56  | MG   | 1A    | 8059 | 1/1   | 0.93 | 0.16 | -    | 7,7,7,7                     | 0     |
| 56  | MG   | 10    | 106  | 1/1   | 0.90 | 0.08 | -    | 46,46,46,46                 | 0     |
| 56  | MG   | 1a    | 1675 | 1/1   | 0.97 | 0.11 | -    | 19,19,19,19                 | 0     |
| 56  | MG   | 2A    | 3233 | 1/1   | 0.93 | 0.45 | -    | 28,28,28,28                 | 0     |
| 56  | MG   | 1a    | 1661 | 1/1   | 0.87 | 0.19 | -    | 48,48,48,48                 | 0     |
| 56  | MG   | 1A    | 8839 | 1/1   | 0.90 | 0.31 | -    | 31,31,31,31                 | 0     |
| 56  | MG   | 1B    | 3002 | 1/1   | 0.95 | 0.09 | -    | 33,33,33,33                 | 0     |
| 56  | MG   | 2a    | 1651 | 1/1   | 0.94 | 0.13 | -    | 48,48,48,48                 | 0     |
| 56  | MG   | 1A    | 8367 | 1/1   | 0.84 | 0.14 | -    | 33,33,33,33                 | 0     |
| 56  | MG   | 1A    | 8511 | 1/1   | 0.95 | 0.16 | -    | 32,32,32,32                 | 0     |
| 56  | MG   | 2A    | 3666 | 1/1   | 0.78 | 0.25 | -    | 48,48,48,48                 | 0     |
| 56  | MG   | 1A    | 8187 | 1/1   | 0.85 | 0.22 | -    | 20,20,20,20                 | 0     |
| 56  | MG   | 1A    | 8805 | 1/1   | 0.93 | 0.10 | -    | 34,34,34,34                 | 0     |
| 56  | MG   | 1A    | 8246 | 1/1   | 0.90 | 0.13 | -    | 45,45,45,45                 | 0     |
| 56  | MG   | 1a    | 1628 | 1/1   | 0.92 | 0.12 | -    | 39,39,39,39                 | 0     |
| 56  | MG   | 2h    | 3001 | 1/1   | 0.89 | 0.34 | -    | 30,30,30,30                 | 0     |
| 56  | MG   | 1A    | 8904 | 1/1   | 0.88 | 0.09 | -    | 41,41,41,41                 | 0     |
| 56  | MG   | 2A    | 3800 | 1/1   | 0.91 | 0.14 | -    | 34,34,34,34                 | 0     |
| 56  | MG   | 1a    | 1829 | 1/1   | 0.93 | 0.12 | -    | 36,36,36,36                 | 0     |
| 56  | MG   | 1A    | 8368 | 1/1   | 0.94 | 0.19 | -    | 14,14,14,14                 | 0     |
| 56  | MG   | 1a    | 1678 | 1/1   | 0.81 | 0.24 | -    | 43,43,43,43                 | 0     |
| 56  | MG   | 2A    | 3013 | 1/1   | 0.79 | 0.23 | -    | 29,29,29,29                 | 0     |
| 56  | MG   | 1A    | 8705 | 1/1   | 0.96 | 0.09 | -    | 10,10,10,10                 | 0     |
| 56  | MG   | 2A    | 3267 | 1/1   | 0.77 | 0.21 | -    | 58,58,58,58                 | 0     |
| 56  | MG   | 1A    | 8016 | 1/1   | 0.95 | 0.12 | -    | 18,18,18,18                 | 0     |
| 56  | MG   | 2A    | 3713 | 1/1   | 0.92 | 0.12 | -    | 24,24,24,24                 | 0     |
| 56  | MG   | 2A    | 3004 | 1/1   | 0.95 | 0.13 | -    | 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   | 2A    | 3866 | 1/1   | 0.50 | 0.42 | -    | 84,84,84,84                 | 0     |
| 56  | MG   | 2x    | 102  | 1/1   | 0.95 | 0.27 | -    | 51,51,51,51                 | 0     |
| 56  | MG   | 1A    | 8664 | 1/1   | 0.96 | 0.12 | -    | 26,26,26,26                 | 0     |
| 56  | MG   | 1a    | 1710 | 1/1   | 0.82 | 0.09 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | 2A    | 3145 | 1/1   | 0.96 | 0.15 | -    | 32,32,32,32                 | 0     |
| 56  | MG   | 2A    | 3275 | 1/1   | 0.95 | 0.18 | -    | 42,42,42,42                 | 0     |
| 56  | MG   | 2A    | 3778 | 1/1   | 0.78 | 0.32 | -    | 46,46,46,46                 | 0     |
| 56  | MG   | 1A    | 8777 | 1/1   | 0.94 | 0.19 | -    | 31,31,31,31                 | 0     |
| 56  | MG   | 2A    | 3540 | 1/1   | 0.93 | 0.16 | -    | 48,48,48,48                 | 0     |
| 56  | MG   | 1A    | 8549 | 1/1   | 0.83 | 0.19 | -    | 38,38,38,38                 | 0     |
| 56  | MG   | 1A    | 8660 | 1/1   | 0.96 | 0.11 | -    | 16,16,16,16                 | 0     |
| 56  | MG   | 1A    | 8876 | 1/1   | 0.93 | 0.14 | -    | 10,10,10,10                 | 0     |
| 56  | MG   | 1a    | 1752 | 1/1   | 0.90 | 0.14 | -    | 45,45,45,45                 | 0     |
| 56  | MG   | 1B    | 3012 | 1/1   | 0.96 | 0.10 | -    | 25,25,25,25                 | 0     |
| 56  | MG   | 2a    | 1658 | 1/1   | 0.94 | 0.17 | -    | 63,63,63,63                 | 0     |
| 56  | MG   | 1A    | 8536 | 1/1   | 0.85 | 0.17 | -    | 54,54,54,54                 | 0     |
| 56  | MG   | 1a    | 1731 | 1/1   | 0.82 | 0.41 | -    | 64,64,64,64                 | 0     |
| 56  | MG   | 2E    | 301  | 1/1   | 0.91 | 0.19 | -    | 37,37,37,37                 | 0     |
| 56  | MG   | 2A    | 3076 | 1/1   | 0.83 | 1.04 | -    | 44,44,44,44                 | 0     |
| 56  | MG   | 1A    | 8420 | 1/1   | 0.91 | 0.10 | -    | 28,28,28,28                 | 0     |
| 56  | MG   | 1a    | 1727 | 1/1   | 0.93 | 0.09 | -    | 32,32,32,32                 | 0     |
| 56  | MG   | 1A    | 8234 | 1/1   | 0.83 | 0.15 | -    | 32,32,32,32                 | 0     |
| 56  | MG   | 2a    | 1687 | 1/1   | 0.67 | 0.12 | -    | 58,58,58,58                 | 0     |
| 56  | MG   | 2a    | 1801 | 1/1   | 0.82 | 0.14 | -    | 61,61,61,61                 | 0     |
| 56  | MG   | 2a    | 1820 | 1/1   | 0.86 | 0.31 | -    | 60,60,60,60                 | 0     |
| 56  | MG   | 23    | 102  | 1/1   | 0.94 | 0.25 | -    | 41,41,41,41                 | 0     |
| 56  | MG   | 1A    | 8115 | 1/1   | 0.92 | 0.18 | -    | 13,13,13,13                 | 0     |
| 56  | MG   | 2A    | 3368 | 1/1   | 0.91 | 0.50 | -    | 54,54,54,54                 | 0     |
| 56  | MG   | 1A    | 8827 | 1/1   | 0.89 | 0.07 | -    | 12,12,12,12                 | 0     |
| 56  | MG   | 2A    | 3410 | 1/1   | 0.91 | 0.04 | -    | 45,45,45,45                 | 0     |
| 56  | MG   | 2a    | 1733 | 1/1   | 0.86 | 0.20 | -    | 69,69,69,69                 | 0     |
| 56  | MG   | 1d    | 502  | 1/1   | 0.85 | 0.21 | -    | 56,56,56,56                 | 0     |
| 56  | MG   | 2A    | 3230 | 1/1   | 0.92 | 0.27 | -    | 33,33,33,33                 | 0     |
| 56  | MG   | 1A    | 8135 | 1/1   | 0.98 | 0.11 | -    | 26,26,26,26                 | 0     |
| 56  | MG   | 1a    | 1672 | 1/1   | 0.95 | 0.21 | -    | 38,38,38,38                 | 0     |
| 56  | MG   | 1A    | 8225 | 1/1   | 0.96 | 0.20 | -    | 10,10,10,10                 | 0     |
| 56  | MG   | 1A    | 8887 | 1/1   | 0.98 | 0.34 | -    | 24,24,24,24                 | 0     |
| 56  | MG   | 2A    | 3875 | 1/1   | 0.93 | 0.15 | -    | 23,23,23,23                 | 0     |
| 56  | MG   | 1A    | 8102 | 1/1   | 0.88 | 0.24 | -    | 16,16,16,16                 | 0     |
| 56  | MG   | 2A    | 3639 | 1/1   | 0.90 | 0.47 | -    | 41,41,41,41                 | 0     |
| 56  | MG   | 2P    | 203  | 1/1   | 0.61 | 0.23 | -    | 63,63,63,63                 | 0     |
| 56  | MG   | 2A    | 3526 | 1/1   | 0.85 | 0.13 | -    | 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    | 1750 | 1/1   | 0.93 | 0.14 | -    | 67,67,67,67                 | 0     |
| 56  | MG   | 2A    | 3444 | 1/1   | 0.92 | 0.12 | -    | 32,32,32,32                 | 0     |
| 56  | MG   | 2A    | 3498 | 1/1   | 0.88 | 0.18 | -    | 45,45,45,45                 | 0     |
| 56  | MG   | 2A    | 3717 | 1/1   | 0.92 | 0.24 | -    | 24,24,24,24                 | 0     |
| 56  | MG   | 1A    | 8296 | 1/1   | 0.97 | 0.10 | -    | 21,21,21,21                 | 0     |
| 56  | MG   | 2a    | 1815 | 1/1   | 0.85 | 0.44 | -    | 58,58,58,58                 | 0     |
| 56  | MG   | 2A    | 3806 | 1/1   | 0.73 | 0.36 | -    | 65,65,65,65                 | 0     |
| 56  | MG   | 2a    | 1705 | 1/1   | 0.84 | 0.26 | -    | 63,63,63,63                 | 0     |
| 56  | MG   | 1a    | 1632 | 1/1   | 0.97 | 0.44 | -    | 41,41,41,41                 | 0     |
| 56  | MG   | 1A    | 8138 | 1/1   | 0.92 | 0.14 | -    | 14,14,14,14                 | 0     |
| 56  | MG   | 1A    | 8912 | 1/1   | 0.95 | 0.14 | -    | 15,15,15,15                 | 0     |
| 56  | MG   | 1B    | 3019 | 1/1   | 0.96 | 0.07 | -    | 23,23,23,23                 | 0     |
| 56  | MG   | 1A    | 8626 | 1/1   | 0.95 | 0.19 | -    | 22,22,22,22                 | 0     |
| 56  | MG   | 1A    | 8785 | 1/1   | 0.94 | 0.07 | -    | 23,23,23,23                 | 0     |
| 56  | MG   | 2a    | 1793 | 1/1   | 0.85 | 0.10 | -    | 52,52,52,52                 | 0     |
| 56  | MG   | 1A    | 8033 | 1/1   | 0.88 | 0.21 | -    | 27,27,27,27                 | 0     |
| 56  | MG   | 1a    | 1616 | 1/1   | 0.94 | 0.20 | -    | 45,45,45,45                 | 0     |
| 56  | MG   | 25    | 104  | 1/1   | 0.80 | 0.27 | -    | 53,53,53,53                 | 0     |
| 56  | MG   | 1a    | 1805 | 1/1   | 0.89 | 0.07 | -    | 55,55,55,55                 | 0     |
| 56  | MG   | 2A    | 3144 | 1/1   | 0.94 | 0.10 | -    | 63,63,63,63                 | 0     |
| 56  | MG   | 2F    | 309  | 1/1   | 0.84 | 0.14 | -    | 58,58,58,58                 | 0     |
| 56  | MG   | 17    | 102  | 1/1   | 0.91 | 0.14 | -    | 34,34,34,34                 | 0     |
| 56  | MG   | 2A    | 3308 | 1/1   | 0.96 | 0.17 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | 2A    | 3183 | 1/1   | 0.93 | 0.17 | -    | 36,36,36,36                 | 0     |
| 56  | MG   | 2A    | 3417 | 1/1   | 0.93 | 0.17 | -    | 51,51,51,51                 | 0     |
| 56  | MG   | 2a    | 1697 | 1/1   | 0.80 | 0.08 | -    | 54,54,54,54                 | 0     |
| 56  | MG   | 1l    | 202  | 1/1   | 0.93 | 0.05 | -    | 38,38,38,38                 | 0     |
| 56  | MG   | 1A    | 8542 | 1/1   | 0.87 | 0.26 | -    | 40,40,40,40                 | 0     |
| 56  | MG   | 1a    | 1666 | 1/1   | 0.93 | 0.27 | -    | 31,31,31,31                 | 0     |
| 56  | MG   | 2B    | 3013 | 1/1   | 0.79 | 0.12 | -    | 51,51,51,51                 | 0     |
| 56  | MG   | 1a    | 1654 | 1/1   | 0.96 | 0.19 | -    | 43,43,43,43                 | 0     |
| 56  | MG   | 1A    | 8056 | 1/1   | 0.97 | 0.07 | -    | 12,12,12,12                 | 0     |
| 56  | MG   | 2A    | 3387 | 1/1   | 0.99 | 0.15 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | 1A    | 8103 | 1/1   | 0.84 | 0.23 | -    | 13,13,13,13                 | 0     |
| 56  | MG   | 1a    | 1732 | 1/1   | 0.98 | 0.08 | -    | 38,38,38,38                 | 0     |
| 56  | MG   | 1A    | 8800 | 1/1   | 0.85 | 0.29 | -    | 44,44,44,44                 | 0     |
| 56  | MG   | 2A    | 3613 | 1/1   | 0.73 | 0.09 | -    | 62,62,62,62                 | 0     |
| 56  | MG   | 1a    | 1825 | 1/1   | 0.80 | 0.14 | -    | 43,43,43,43                 | 0     |
| 56  | MG   | 1a    | 1766 | 1/1   | 0.97 | 0.14 | -    | 34,34,34,34                 | 0     |
| 56  | MG   | 2a    | 1646 | 1/1   | 0.66 | 0.57 | -    | 48,48,48,48                 | 0     |
| 56  | MG   | 1A    | 8452 | 1/1   | 0.95 | 0.06 | -    | 26,26,26,26                 | 0     |
| 56  | MG   | 1A    | 8332 | 1/1   | 0.95 | 0.12 | -    | 48,48,48,48                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|----------------------------|-------|
| 56  | MG   | 2A    | 3060 | 1/1   | 0.97 | 0.17 | -    | 51,51,51,51                | 0     |
| 56  | MG   | 2A    | 3517 | 1/1   | 0.93 | 0.21 | -    | 47,47,47,47                | 0     |
| 56  | MG   | 1x    | 3011 | 1/1   | 0.78 | 0.15 | -    | 34,34,34,34                | 0     |
| 56  | MG   | 2A    | 3803 | 1/1   | 0.73 | 0.46 | -    | 71,71,71,71                | 0     |
| 56  | MG   | 1A    | 8613 | 1/1   | 0.90 | 0.10 | -    | 36,36,36,36                | 0     |
| 56  | MG   | 1A    | 8416 | 1/1   | 0.96 | 0.08 | -    | 36,36,36,36                | 0     |
| 56  | MG   | 2A    | 3461 | 1/1   | 0.88 | 0.13 | -    | 30,30,30,30                | 0     |
| 56  | MG   | 2a    | 1663 | 1/1   | 0.94 | 0.17 | -    | 43,43,43,43                | 0     |
| 56  | MG   | 1A    | 8301 | 1/1   | 0.97 | 0.12 | -    | 27,27,27,27                | 0     |
| 56  | MG   | 2A    | 3179 | 1/1   | 0.96 | 0.10 | -    | 35,35,35,35                | 0     |
| 56  | MG   | 2A    | 3545 | 1/1   | 0.85 | 0.12 | -    | 47,47,47,47                | 0     |
| 56  | MG   | 15    | 103  | 1/1   | 0.90 | 0.19 | -    | 20,20,20,20                | 0     |
| 56  | MG   | 1A    | 8746 | 1/1   | 0.95 | 0.20 | -    | 22,22,22,22                | 0     |
| 56  | MG   | 2A    | 3681 | 1/1   | 0.98 | 0.21 | -    | 57,57,57,57                | 0     |
| 56  | MG   | 2A    | 3376 | 1/1   | 0.88 | 0.12 | -    | 23,23,23,23                | 0     |
| 56  | MG   | 1A    | 8015 | 1/1   | 0.84 | 0.14 | -    | 28,28,28,28                | 0     |
| 56  | MG   | 1a    | 1667 | 1/1   | 0.76 | 0.31 | -    | 59,59,59,59                | 0     |
| 56  | MG   | 2A    | 3529 | 1/1   | 0.91 | 0.14 | -    | 44,44,44,44                | 0     |
| 56  | MG   | 2A    | 3052 | 1/1   | 0.96 | 0.31 | -    | 37,37,37,37                | 0     |
| 56  | MG   | 2A    | 3262 | 1/1   | 0.84 | 0.15 | -    | 38,38,38,38                | 0     |
| 56  | MG   | 2A    | 3621 | 1/1   | 0.90 | 0.13 | -    | 44,44,44,44                | 0     |
| 56  | MG   | 1A    | 8866 | 1/1   | 0.82 | 0.09 | -    | 32,32,32,32                | 0     |
| 56  | MG   | 2A    | 3475 | 1/1   | 0.90 | 0.09 | -    | 23,23,23,23                | 0     |
| 56  | MG   | 2A    | 3441 | 1/1   | 0.97 | 0.09 | -    | 38,38,38,38                | 0     |
| 56  | MG   | 1A    | 8699 | 1/1   | 0.96 | 0.12 | -    | 17,17,17,17                | 0     |
| 56  | MG   | 2A    | 3633 | 1/1   | 0.92 | 0.32 | -    | 44,44,44,44                | 0     |
| 56  | MG   | 1B    | 3017 | 1/1   | 0.78 | 0.12 | -    | 44,44,44,44                | 0     |
| 56  | MG   | 2a    | 1608 | 1/1   | 0.90 | 0.12 | -    | 36,36,36,36                | 0     |
| 56  | MG   | 2A    | 3497 | 1/1   | 0.98 | 0.07 | -    | 28,28,28,28                | 0     |
| 56  | MG   | 2A    | 3690 | 1/1   | 0.72 | 0.59 | -    | 67,67,67,67                | 0     |
| 56  | MG   | 2A    | 3255 | 1/1   | 0.89 | 0.17 | -    | 45,45,45,45                | 0     |
| 56  | MG   | 2A    | 3588 | 1/1   | 0.87 | 0.24 | -    | 44,44,44,44                | 0     |
| 56  | MG   | 2A    | 3614 | 1/1   | 0.73 | 0.12 | -    | 42,42,42,42                | 0     |
| 56  | MG   | 2A    | 3890 | 1/1   | 0.92 | 0.39 | -    | 60,60,60,60                | 0     |
| 56  | MG   | 1A    | 8499 | 1/1   | 0.96 | 0.15 | -    | 18,18,18,18                | 0     |
| 56  | MG   | 1A    | 8638 | 1/1   | 0.94 | 0.07 | -    | 18,18,18,18                | 0     |
| 56  | MG   | 1A    | 8654 | 1/1   | 0.92 | 0.29 | -    | 32,32,32,32                | 0     |
| 56  | MG   | 2a    | 1773 | 1/1   | 0.94 | 0.06 | -    | 52,52,52,52                | 0     |
| 56  | MG   | 2A    | 3292 | 1/1   | 0.94 | 0.16 | -    | 51,51,51,51                | 0     |
| 56  | MG   | 2A    | 3077 | 1/1   | 0.91 | 0.36 | -    | 30,30,30,30                | 0     |
| 56  | MG   | 2A    | 3346 | 1/1   | 0.81 | 0.12 | -    | 29,29,29,29                | 0     |
| 56  | MG   | 1A    | 8877 | 1/1   | 0.92 | 0.10 | -    | 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    | 1830 | 1/1   | 0.92 | 0.10 | -    | 45,45,45,45                 | 0     |
| 56  | MG   | 2a    | 1602 | 1/1   | 0.97 | 0.11 | -    | 48,48,48,48                 | 0     |
| 56  | MG   | 2A    | 3630 | 1/1   | 0.87 | 0.20 | -    | 57,57,57,57                 | 0     |
| 56  | MG   | 1A    | 8721 | 1/1   | 0.96 | 0.14 | -    | 11,11,11,11                 | 0     |
| 56  | MG   | 1A    | 8893 | 1/1   | 0.99 | 0.10 | -    | 21,21,21,21                 | 0     |
| 56  | MG   | 2A    | 3871 | 1/1   | 0.91 | 0.15 | -    | 56,56,56,56                 | 0     |
| 56  | MG   | 2A    | 3173 | 1/1   | 0.94 | 0.15 | -    | 37,37,37,37                 | 0     |
| 56  | MG   | 1A    | 8259 | 1/1   | 0.93 | 0.12 | -    | 28,28,28,28                 | 0     |
| 56  | MG   | 2A    | 3212 | 1/1   | 0.94 | 0.31 | -    | 27,27,27,27                 | 0     |
| 56  | MG   | 1A    | 8007 | 1/1   | 0.96 | 0.14 | -    | 8,8,8,8                     | 0     |
| 56  | MG   | 2A    | 3583 | 1/1   | 0.95 | 0.11 | -    | 25,25,25,25                 | 0     |
| 56  | MG   | 1A    | 8134 | 1/1   | 0.96 | 0.13 | -    | 12,12,12,12                 | 0     |
| 56  | MG   | 2A    | 3752 | 1/1   | 0.84 | 0.42 | -    | 39,39,39,39                 | 0     |
| 56  | MG   | 2A    | 3067 | 1/1   | 0.95 | 0.18 | -    | 20,20,20,20                 | 0     |
| 56  | MG   | 2A    | 3232 | 1/1   | 0.87 | 0.28 | -    | 46,46,46,46                 | 0     |
| 56  | MG   | 1A    | 8386 | 1/1   | 0.95 | 0.09 | -    | 16,16,16,16                 | 0     |
| 56  | MG   | 2A    | 3078 | 1/1   | 0.94 | 0.32 | -    | 24,24,24,24                 | 0     |
| 56  | MG   | 2A    | 3221 | 1/1   | 0.88 | 0.62 | -    | 29,29,29,29                 | 0     |
| 56  | MG   | 1A    | 8034 | 1/1   | 0.90 | 0.14 | -    | 24,24,24,24                 | 0     |
| 56  | MG   | 1A    | 8898 | 1/1   | 0.95 | 0.16 | -    | 39,39,39,39                 | 0     |
| 56  | MG   | 1a    | 1621 | 1/1   | 0.95 | 0.25 | -    | 26,26,26,26                 | 0     |
| 56  | MG   | 1A    | 8570 | 1/1   | 0.93 | 0.19 | -    | 34,34,34,34                 | 0     |
| 56  | MG   | 1P    | 204  | 1/1   | 0.66 | 0.18 | -    | 62,62,62,62                 | 0     |
| 56  | MG   | 2A    | 3532 | 1/1   | 0.76 | 0.17 | -    | 54,54,54,54                 | 0     |
| 56  | MG   | 1A    | 8399 | 1/1   | 0.97 | 0.04 | -    | 34,34,34,34                 | 0     |
| 56  | MG   | 2B    | 3021 | 1/1   | 0.74 | 0.25 | -    | 50,50,50,50                 | 0     |
| 56  | MG   | 2o    | 3001 | 1/1   | 0.85 | 0.15 | -    | 32,32,32,32                 | 0     |
| 56  | MG   | 1a    | 1671 | 1/1   | 0.88 | 0.15 | -    | 39,39,39,39                 | 0     |
| 56  | MG   | 2A    | 3931 | 1/1   | 0.87 | 0.15 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | 2A    | 3528 | 1/1   | 0.88 | 0.08 | -    | 40,40,40,40                 | 0     |
| 56  | MG   | 2A    | 3878 | 1/1   | 0.94 | 0.10 | -    | 45,45,45,45                 | 0     |
| 56  | MG   | 1A    | 8853 | 1/1   | 0.84 | 0.21 | -    | 50,50,50,50                 | 0     |
| 56  | MG   | 1A    | 8733 | 1/1   | 0.92 | 0.18 | -    | 54,54,54,54                 | 0     |
| 56  | MG   | 2A    | 3398 | 1/1   | 0.89 | 0.22 | -    | 39,39,39,39                 | 0     |
| 56  | MG   | 2A    | 3553 | 1/1   | 0.92 | 0.10 | -    | 52,52,52,52                 | 0     |
| 56  | MG   | 2A    | 3923 | 1/1   | 0.75 | 0.25 | -    | 39,39,39,39                 | 0     |
| 56  | MG   | 1a    | 1778 | 1/1   | 0.91 | 0.10 | -    | 33,33,33,33                 | 0     |
| 56  | MG   | 2A    | 3437 | 1/1   | 0.88 | 0.07 | -    | 59,59,59,59                 | 0     |
| 56  | MG   | 1A    | 8179 | 1/1   | 0.93 | 0.39 | -    | 16,16,16,16                 | 0     |
| 56  | MG   | 1A    | 8960 | 1/1   | 0.95 | 0.10 | -    | 20,20,20,20                 | 0     |
| 56  | MG   | 1A    | 8384 | 1/1   | 0.92 | 0.27 | -    | 36,36,36,36                 | 0     |
| 56  | MG   | 2A    | 3494 | 1/1   | 0.94 | 0.19 | -    | 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   | 1A    | 8504 | 1/1   | 0.88 | 0.17 | -    | 30,30,30,30                 | 0     |
| 56  | MG   | 1A    | 8338 | 1/1   | 0.95 | 0.15 | -    | 13,13,13,13                 | 0     |
| 56  | MG   | 2A    | 3041 | 1/1   | 0.87 | 0.18 | -    | 39,39,39,39                 | 0     |
| 56  | MG   | 1D    | 304  | 1/1   | 0.91 | 0.20 | -    | 14,14,14,14                 | 0     |
| 56  | MG   | 2A    | 3466 | 1/1   | 0.98 | 0.08 | -    | 46,46,46,46                 | 0     |
| 56  | MG   | 1A    | 8502 | 1/1   | 0.97 | 0.18 | -    | 18,18,18,18                 | 0     |
| 56  | MG   | 1A    | 8586 | 1/1   | 0.92 | 0.23 | -    | 27,27,27,27                 | 0     |
| 56  | MG   | 1B    | 3023 | 1/1   | 0.77 | 0.11 | -    | 46,46,46,46                 | 0     |
| 56  | MG   | 2E    | 306  | 1/1   | 0.93 | 0.07 | -    | 44,44,44,44                 | 0     |
| 56  | MG   | 1A    | 8614 | 1/1   | 0.85 | 0.21 | -    | 41,41,41,41                 | 0     |
| 56  | MG   | 1A    | 8748 | 1/1   | 0.98 | 0.16 | -    | 18,18,18,18                 | 0     |
| 56  | MG   | 2a    | 1800 | 1/1   | 0.87 | 0.14 | -    | 39,39,39,39                 | 0     |
| 56  | MG   | 1A    | 8849 | 1/1   | 0.84 | 0.13 | -    | 39,39,39,39                 | 0     |
| 56  | MG   | 1a    | 1759 | 1/1   | 0.82 | 0.11 | -    | 63,63,63,63                 | 0     |
| 56  | MG   | 1A    | 8889 | 1/1   | 0.99 | 0.15 | -    | 17,17,17,17                 | 0     |
| 56  | MG   | 1A    | 8192 | 1/1   | 0.88 | 0.29 | -    | 22,22,22,22                 | 0     |
| 56  | MG   | 1A    | 8145 | 1/1   | 0.83 | 0.23 | -    | 15,15,15,15                 | 0     |
| 56  | MG   | 2A    | 3761 | 1/1   | 0.92 | 0.38 | -    | 43,43,43,43                 | 0     |
| 56  | MG   | 2A    | 3950 | 1/1   | 0.94 | 0.12 | -    | 41,41,41,41                 | 0     |
| 56  | MG   | 1A    | 8924 | 1/1   | 0.96 | 0.13 | -    | 12,12,12,12                 | 0     |
| 56  | MG   | 1A    | 8037 | 1/1   | 0.92 | 0.11 | -    | 14,14,14,14                 | 0     |
| 56  | MG   | 2v    | 101  | 1/1   | 0.77 | 0.19 | -    | 61,61,61,61                 | 0     |
| 56  | MG   | 1A    | 8643 | 1/1   | 0.94 | 0.30 | -    | 28,28,28,28                 | 0     |
| 56  | MG   | 2A    | 3554 | 1/1   | 0.93 | 0.41 | -    | 37,37,37,37                 | 0     |
| 56  | MG   | 2a    | 1674 | 1/1   | 0.84 | 0.09 | -    | 37,37,37,37                 | 0     |
| 56  | MG   | 2A    | 3477 | 1/1   | 0.49 | 0.37 | -    | 62,62,62,62                 | 0     |
| 56  | MG   | 2A    | 3550 | 1/1   | 0.94 | 0.33 | -    | 50,50,50,50                 | 0     |
| 56  | MG   | 2a    | 1632 | 1/1   | 0.94 | 0.21 | -    | 51,51,51,51                 | 0     |
| 56  | MG   | 1A    | 8526 | 1/1   | 0.88 | 0.08 | -    | 42,42,42,42                 | 0     |
| 56  | MG   | 1A    | 8473 | 1/1   | 0.85 | 0.25 | -    | 35,35,35,35                 | 0     |
| 56  | MG   | 2A    | 3250 | 1/1   | 0.90 | 0.71 | -    | 40,40,40,40                 | 0     |
| 56  | MG   | 2A    | 3516 | 1/1   | 0.94 | 0.10 | -    | 48,48,48,48                 | 0     |
| 56  | MG   | 2A    | 3296 | 1/1   | 0.82 | 0.11 | -    | 49,49,49,49                 | 0     |
| 56  | MG   | 2a    | 1605 | 1/1   | 0.95 | 0.13 | -    | 40,40,40,40                 | 0     |
| 56  | MG   | 1B    | 3027 | 1/1   | 0.82 | 0.32 | -    | 66,66,66,66                 | 0     |
| 56  | MG   | 2A    | 3371 | 1/1   | 0.92 | 0.13 | -    | 18,18,18,18                 | 0     |
| 56  | MG   | 2A    | 3960 | 1/1   | 0.91 | 0.73 | -    | 45,45,45,45                 | 0     |
| 56  | MG   | 2a    | 1652 | 1/1   | 0.90 | 0.16 | -    | 28,28,28,28                 | 0     |
| 56  | MG   | 2a    | 1806 | 1/1   | 0.90 | 0.19 | -    | 65,65,65,65                 | 0     |
| 56  | MG   | 2A    | 3393 | 1/1   | 0.95 | 0.17 | -    | 27,27,27,27                 | 0     |
| 56  | MG   | 2A    | 3782 | 1/1   | 0.95 | 0.33 | -    | 60,60,60,60                 | 0     |
| 56  | MG   | 1a    | 1659 | 1/1   | 0.78 | 0.21 | -    | 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    | 3402 | 1/1   | 0.87 | 0.09 | -    | 39,39,39,39                 | 0     |
| 56  | MG   | 1A    | 8458 | 1/1   | 0.97 | 0.18 | -    | 53,53,53,53                 | 0     |
| 56  | MG   | 1a    | 1794 | 1/1   | 0.95 | 0.44 | -    | 43,43,43,43                 | 0     |
| 56  | MG   | 1a    | 1683 | 1/1   | 0.89 | 0.14 | -    | 39,39,39,39                 | 0     |
| 56  | MG   | 2A    | 3548 | 1/1   | 0.60 | 0.17 | -    | 52,52,52,52                 | 0     |
| 56  | MG   | 2A    | 3091 | 1/1   | 0.88 | 0.18 | -    | 50,50,50,50                 | 0     |
| 56  | MG   | 1A    | 8336 | 1/1   | 0.80 | 0.14 | -    | 32,32,32,32                 | 0     |
| 56  | MG   | 2A    | 3851 | 1/1   | 0.90 | 0.10 | -    | 37,37,37,37                 | 0     |
| 56  | MG   | 19    | 104  | 1/1   | 0.88 | 0.18 | -    | 34,34,34,34                 | 0     |
| 56  | MG   | 2A    | 3510 | 1/1   | 0.96 | 0.15 | -    | 54,54,54,54                 | 0     |
| 56  | MG   | 1A    | 8398 | 1/1   | 0.92 | 0.21 | -    | 41,41,41,41                 | 0     |
| 56  | MG   | 1A    | 8944 | 1/1   | 0.96 | 0.14 | -    | 24,24,24,24                 | 0     |
| 56  | MG   | 2A    | 3624 | 1/1   | 0.90 | 0.14 | -    | 52,52,52,52                 | 0     |
| 56  | MG   | 2A    | 3982 | 1/1   | 0.78 | 0.35 | -    | 26,26,26,26                 | 0     |
| 56  | MG   | 2a    | 1751 | 1/1   | 0.76 | 0.14 | -    | 50,50,50,50                 | 0     |
| 56  | MG   | 19    | 103  | 1/1   | 0.95 | 0.23 | -    | 23,23,23,23                 | 0     |
| 56  | MG   | 2A    | 3146 | 1/1   | 0.97 | 0.35 | -    | 28,28,28,28                 | 0     |
| 56  | MG   | 2a    | 1603 | 1/1   | 0.94 | 0.16 | -    | 45,45,45,45                 | 0     |
| 56  | MG   | 2A    | 3381 | 1/1   | 0.97 | 0.09 | -    | 31,31,31,31                 | 0     |
| 56  | MG   | 2a    | 1607 | 1/1   | 0.89 | 0.34 | -    | 55,55,55,55                 | 0     |
| 56  | MG   | 17    | 101  | 1/1   | 0.98 | 0.13 | -    | 21,21,21,21                 | 0     |
| 56  | MG   | 2a    | 1809 | 1/1   | 0.64 | 0.32 | -    | 81,81,81,81                 | 0     |
| 56  | MG   | 2A    | 3862 | 1/1   | 0.87 | 0.26 | -    | 32,32,32,32                 | 0     |
| 56  | MG   | 1A    | 8002 | 1/1   | 0.91 | 0.17 | -    | 21,21,21,21                 | 0     |
| 56  | MG   | 2A    | 3771 | 1/1   | 0.99 | 0.21 | -    | 41,41,41,41                 | 0     |
| 56  | MG   | 2A    | 3069 | 1/1   | 0.91 | 0.45 | -    | 36,36,36,36                 | 0     |
| 56  | MG   | 1A    | 8781 | 1/1   | 0.93 | 0.15 | -    | 14,14,14,14                 | 0     |
| 56  | MG   | 2A    | 3877 | 1/1   | 0.98 | 0.12 | -    | 20,20,20,20                 | 0     |
| 56  | MG   | 2a    | 1742 | 1/1   | 0.69 | 0.22 | -    | 62,62,62,62                 | 0     |
| 56  | MG   | 1A    | 8707 | 1/1   | 0.96 | 0.06 | -    | 45,45,45,45                 | 0     |
| 56  | MG   | 2A    | 3590 | 1/1   | 0.88 | 0.15 | -    | 65,65,65,65                 | 0     |
| 56  | MG   | 1a    | 1696 | 1/1   | 0.97 | 0.05 | -    | 54,54,54,54                 | 0     |
| 56  | MG   | 2A    | 3689 | 1/1   | 0.83 | 0.13 | -    | 32,32,32,32                 | 0     |
| 56  | MG   | 1A    | 8278 | 1/1   | 0.95 | 0.12 | -    | 8,8,8,8                     | 0     |
| 56  | MG   | 1A    | 8377 | 1/1   | 0.78 | 0.21 | -    | 20,20,20,20                 | 0     |
| 56  | MG   | 2A    | 3140 | 1/1   | 0.92 | 0.17 | -    | 25,25,25,25                 | 0     |
| 56  | MG   | 1a    | 1816 | 1/1   | 0.84 | 0.15 | -    | 49,49,49,49                 | 0     |
| 56  | MG   | 2A    | 3781 | 1/1   | 0.81 | 0.26 | -    | 51,51,51,51                 | 0     |
| 56  | MG   | 1A    | 8194 | 1/1   | 0.96 | 0.31 | -    | 17,17,17,17                 | 0     |
| 56  | MG   | 2A    | 3646 | 1/1   | 0.91 | 0.14 | -    | 51,51,51,51                 | 0     |
| 56  | MG   | 2A    | 3776 | 1/1   | 0.91 | 0.07 | -    | 51,51,51,51                 | 0     |
| 56  | MG   | 2x    | 109  | 1/1   | 0.89 | 0.25 | -    | 56,56,56,56                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56  | MG   | 2A    | 3969 | 1/1   | 0.95 | 0.21 | -    | 55,55,55,55                 | 0     |
| 56  | MG   | 1A    | 8693 | 1/1   | 0.98 | 0.07 | -    | 28,28,28,28                 | 0     |
| 56  | MG   | 1A    | 8448 | 1/1   | 0.91 | 0.19 | -    | 8,8,8,8                     | 0     |
| 56  | MG   | 1A    | 8485 | 1/1   | 0.92 | 0.11 | -    | 30,30,30,30                 | 0     |
| 56  | MG   | 1A    | 8854 | 1/1   | 0.95 | 0.09 | -    | 22,22,22,22                 | 0     |
| 56  | MG   | 2A    | 3864 | 1/1   | 0.78 | 0.21 | -    | 39,39,39,39                 | 0     |
| 56  | MG   | 1A    | 8885 | 1/1   | 0.94 | 0.10 | -    | 31,31,31,31                 | 0     |
| 56  | MG   | 1A    | 8640 | 1/1   | 0.98 | 0.16 | -    | 40,40,40,40                 | 0     |
| 56  | MG   | 2A    | 3360 | 1/1   | 0.97 | 0.12 | -    | 33,33,33,33                 | 0     |
| 56  | MG   | 2a    | 1740 | 1/1   | 0.67 | 0.15 | -    | 62,62,62,62                 | 0     |
| 56  | MG   | 1A    | 8609 | 1/1   | 0.92 | 0.13 | -    | 18,18,18,18                 | 0     |
| 56  | MG   | 1A    | 8181 | 1/1   | 0.96 | 0.12 | -    | 18,18,18,18                 | 0     |
| 56  | MG   | 1A    | 8017 | 1/1   | 0.98 | 0.12 | -    | 13,13,13,13                 | 0     |
| 56  | MG   | 1a    | 1734 | 1/1   | 0.94 | 0.11 | -    | 42,42,42,42                 | 0     |
| 56  | MG   | 2A    | 3930 | 1/1   | 0.92 | 0.42 | -    | 48,48,48,48                 | 0     |
| 56  | MG   | 1a    | 1797 | 1/1   | 0.84 | 0.29 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | 1a    | 1673 | 1/1   | 0.92 | 0.17 | -    | 35,35,35,35                 | 0     |
| 56  | MG   | 2A    | 3389 | 1/1   | 0.91 | 0.07 | -    | 45,45,45,45                 | 0     |
| 56  | MG   | 1A    | 8453 | 1/1   | 0.97 | 0.08 | -    | 24,24,24,24                 | 0     |
| 56  | MG   | 1A    | 8204 | 1/1   | 0.96 | 0.37 | -    | 20,20,20,20                 | 0     |
| 56  | MG   | 1A    | 8585 | 1/1   | 0.87 | 0.15 | -    | 29,29,29,29                 | 0     |
| 56  | MG   | 2A    | 3547 | 1/1   | 0.86 | 0.18 | -    | 43,43,43,43                 | 0     |
| 56  | MG   | 1a    | 1787 | 1/1   | 0.95 | 0.43 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | 1A    | 8284 | 1/1   | 0.94 | 0.21 | -    | 50,50,50,50                 | 0     |
| 56  | MG   | 1A    | 8100 | 1/1   | 0.95 | 0.23 | -    | 28,28,28,28                 | 0     |
| 56  | MG   | 1A    | 8521 | 1/1   | 0.98 | 0.13 | -    | 12,12,12,12                 | 0     |
| 56  | MG   | 1A    | 8776 | 1/1   | 0.92 | 0.26 | -    | 35,35,35,35                 | 0     |
| 56  | MG   | 1A    | 8968 | 1/1   | 0.95 | 0.11 | -    | 34,34,34,34                 | 0     |
| 56  | MG   | 10    | 105  | 1/1   | 0.91 | 0.11 | -    | 27,27,27,27                 | 0     |
| 56  | MG   | 2A    | 3597 | 1/1   | 0.98 | 0.28 | -    | 44,44,44,44                 | 0     |
| 56  | MG   | 1A    | 8548 | 1/1   | 0.91 | 0.08 | -    | 27,27,27,27                 | 0     |
| 56  | MG   | 2A    | 3252 | 1/1   | 0.60 | 0.32 | -    | 53,53,53,53                 | 0     |
| 56  | MG   | 1A    | 8637 | 1/1   | 0.98 | 0.10 | -    | 11,11,11,11                 | 0     |
| 56  | MG   | 1A    | 8822 | 1/1   | 0.95 | 0.04 | -    | 44,44,44,44                 | 0     |
| 56  | MG   | 1a    | 1721 | 1/1   | 0.94 | 0.10 | -    | 49,49,49,49                 | 0     |
| 56  | MG   | 1a    | 1701 | 1/1   | 0.95 | 0.16 | -    | 44,44,44,44                 | 0     |
| 56  | MG   | 2A    | 3595 | 1/1   | 0.95 | 0.10 | -    | 32,32,32,32                 | 0     |
| 56  | MG   | 2A    | 3601 | 1/1   | 0.92 | 0.29 | -    | 44,44,44,44                 | 0     |
| 56  | MG   | 1A    | 8018 | 1/1   | 0.97 | 0.18 | -    | 10,10,10,10                 | 0     |
| 56  | MG   | 2A    | 3100 | 1/1   | 0.94 | 0.17 | -    | 37,37,37,37                 | 0     |
| 56  | MG   | 2A    | 3318 | 1/1   | 0.96 | 0.10 | -    | 30,30,30,30                 | 0     |
| 56  | MG   | 2A    | 3495 | 1/1   | 0.89 | 0.33 | -    | 57,57,57,57                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|----------------------------|-------|
| 56  | MG   | 1A    | 8498 | 1/1   | 0.77 | 0.12 | -    | 34,34,34,34                | 0     |
| 56  | MG   | 1A    | 8817 | 1/1   | 0.84 | 0.06 | -    | 31,31,31,31                | 0     |
| 56  | MG   | 1A    | 8824 | 1/1   | 0.93 | 0.14 | -    | 37,37,37,37                | 0     |
| 56  | MG   | 2A    | 3856 | 1/1   | 0.66 | 0.41 | -    | 53,53,53,53                | 0     |
| 56  | MG   | 1A    | 8163 | 1/1   | 0.96 | 0.22 | -    | 17,17,17,17                | 0     |
| 56  | MG   | 1A    | 8118 | 1/1   | 0.96 | 0.17 | -    | 10,10,10,10                | 0     |
| 56  | MG   | 1A    | 8487 | 1/1   | 0.93 | 0.15 | -    | 31,31,31,31                | 0     |
| 56  | MG   | 1d    | 504  | 1/1   | 0.86 | 0.12 | -    | 45,45,45,45                | 0     |
| 56  | MG   | 1a    | 1602 | 1/1   | 0.97 | 0.12 | -    | 54,54,54,54                | 0     |
| 56  | MG   | 1A    | 8245 | 1/1   | 0.97 | 0.14 | -    | 8,8,8,8                    | 0     |
| 56  | MG   | 2A    | 3426 | 1/1   | 0.79 | 0.10 | -    | 55,55,55,55                | 0     |
| 56  | MG   | 1A    | 8636 | 1/1   | 0.81 | 0.20 | -    | 45,45,45,45                | 0     |
| 56  | MG   | 2A    | 3703 | 1/1   | 0.89 | 0.15 | -    | 26,26,26,26                | 0     |
| 56  | MG   | 2a    | 1642 | 1/1   | 0.75 | 0.32 | -    | 51,51,51,51                | 0     |
| 56  | MG   | 1A    | 8530 | 1/1   | 0.98 | 0.14 | -    | 27,27,27,27                | 0     |
| 56  | MG   | 2A    | 3560 | 1/1   | 0.87 | 0.59 | -    | 43,43,43,43                | 0     |
| 56  | MG   | 1A    | 8739 | 1/1   | 0.96 | 0.19 | -    | 28,28,28,28                | 0     |
| 56  | MG   | 1A    | 8490 | 1/1   | 0.92 | 0.25 | -    | 18,18,18,18                | 0     |
| 56  | MG   | 1A    | 8860 | 1/1   | 0.94 | 0.06 | -    | 22,22,22,22                | 0     |
| 56  | MG   | 1A    | 8673 | 1/1   | 0.98 | 0.24 | -    | 32,32,32,32                | 0     |
| 56  | MG   | 2a    | 1620 | 1/1   | 0.92 | 0.27 | -    | 69,69,69,69                | 0     |
| 56  | MG   | 1A    | 8169 | 1/1   | 0.88 | 0.63 | -    | 16,16,16,16                | 0     |
| 56  | MG   | 1A    | 8553 | 1/1   | 0.97 | 0.13 | -    | 18,18,18,18                | 0     |
| 56  | MG   | 2A    | 3446 | 1/1   | 0.84 | 0.25 | -    | 29,29,29,29                | 0     |
| 56  | MG   | 2x    | 105  | 1/1   | 0.94 | 0.21 | -    | 59,59,59,59                | 0     |
| 56  | MG   | 2A    | 3816 | 1/1   | 0.56 | 0.13 | -    | 62,62,62,62                | 0     |
| 56  | MG   | 2A    | 3906 | 1/1   | 0.94 | 0.10 | -    | 39,39,39,39                | 0     |
| 56  | MG   | 2A    | 3342 | 1/1   | 0.82 | 0.19 | -    | 25,25,25,25                | 0     |
| 56  | MG   | 2A    | 3304 | 1/1   | 0.80 | 0.14 | -    | 47,47,47,47                | 0     |
| 56  | MG   | 1A    | 8390 | 1/1   | 0.91 | 0.11 | -    | 41,41,41,41                | 0     |
| 56  | MG   | 1A    | 8602 | 1/1   | 0.88 | 0.11 | -    | 47,47,47,47                | 0     |
| 56  | MG   | 2a    | 1778 | 1/1   | 0.82 | 0.16 | -    | 42,42,42,42                | 0     |
| 56  | MG   | 1A    | 8826 | 1/1   | 0.97 | 0.07 | -    | 14,14,14,14                | 0     |
| 56  | MG   | 1A    | 8326 | 1/1   | 0.97 | 0.21 | -    | 20,20,20,20                | 0     |
| 56  | MG   | 1a    | 1684 | 1/1   | 0.96 | 0.18 | -    | 35,35,35,35                | 0     |
| 56  | MG   | 1A    | 8552 | 1/1   | 0.84 | 0.20 | -    | 23,23,23,23                | 0     |
| 56  | MG   | 2A    | 3650 | 1/1   | 0.87 | 0.18 | -    | 36,36,36,36                | 0     |
| 56  | MG   | 2A    | 3344 | 1/1   | 0.91 | 0.12 | -    | 41,41,41,41                | 0     |
| 56  | MG   | 1A    | 8279 | 1/1   | 0.80 | 0.10 | -    | 30,30,30,30                | 0     |
| 56  | MG   | 1A    | 8099 | 1/1   | 0.97 | 0.18 | -    | 12,12,12,12                | 0     |
| 56  | MG   | 2a    | 1650 | 1/1   | 0.88 | 0.20 | -    | 46,46,46,46                | 0     |
| 56  | MG   | 2A    | 3026 | 1/1   | 0.98 | 0.33 | -    | 28,28,28,28                | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56  | MG   | 2A    | 3143 | 1/1   | 0.84 | 0.16 | -    | 33,33,33,33                 | 0     |
| 56  | MG   | 2A    | 3636 | 1/1   | 0.86 | 0.33 | -    | 48,48,48,48                 | 0     |
| 56  | MG   | 1a    | 1788 | 1/1   | 0.86 | 0.20 | -    | 42,42,42,42                 | 0     |
| 56  | MG   | 1a    | 1686 | 1/1   | 0.83 | 0.20 | -    | 46,46,46,46                 | 0     |
| 56  | MG   | 2A    | 3254 | 1/1   | 0.94 | 0.24 | -    | 38,38,38,38                 | 0     |
| 56  | MG   | 2A    | 3384 | 1/1   | 0.93 | 0.17 | -    | 40,40,40,40                 | 0     |
| 56  | MG   | 1A    | 8834 | 1/1   | 0.89 | 0.09 | -    | 18,18,18,18                 | 0     |
| 56  | MG   | 1A    | 8934 | 1/1   | 0.89 | 0.11 | -    | 48,48,48,48                 | 0     |
| 56  | MG   | 2A    | 3118 | 1/1   | 0.90 | 0.36 | -    | 48,48,48,48                 | 0     |
| 56  | MG   | 2A    | 3251 | 1/1   | 0.97 | 0.11 | -    | 43,43,43,43                 | 0     |
| 56  | MG   | 1x    | 3006 | 1/1   | 0.82 | 0.19 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | 2A    | 3194 | 1/1   | 0.96 | 0.14 | -    | 24,24,24,24                 | 0     |
| 56  | MG   | 1A    | 8537 | 1/1   | 0.94 | 0.10 | -    | 21,21,21,21                 | 0     |
| 56  | MG   | 2A    | 3505 | 1/1   | 0.93 | 0.32 | -    | 43,43,43,43                 | 0     |
| 56  | MG   | 2A    | 3760 | 1/1   | 0.95 | 0.13 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | 1A    | 8766 | 1/1   | 0.96 | 0.05 | -    | 37,37,37,37                 | 0     |
| 56  | MG   | 2A    | 3240 | 1/1   | 0.98 | 0.08 | -    | 57,57,57,57                 | 0     |
| 56  | MG   | 2a    | 1615 | 1/1   | 0.84 | 0.57 | -    | 50,50,50,50                 | 0     |
| 56  | MG   | 2A    | 3518 | 1/1   | 0.86 | 0.18 | -    | 24,24,24,24                 | 0     |
| 56  | MG   | 2a    | 1703 | 1/1   | 0.82 | 0.09 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | 2a    | 1776 | 1/1   | 0.97 | 0.07 | -    | 51,51,51,51                 | 0     |
| 56  | MG   | 2A    | 3857 | 1/1   | 0.87 | 0.20 | -    | 40,40,40,40                 | 0     |
| 56  | MG   | 2A    | 3095 | 1/1   | 0.97 | 0.15 | -    | 29,29,29,29                 | 0     |
| 56  | MG   | 2A    | 3155 | 1/1   | 0.97 | 0.12 | -    | 24,24,24,24                 | 0     |
| 56  | MG   | 1A    | 8393 | 1/1   | 0.94 | 0.16 | -    | 20,20,20,20                 | 0     |
| 56  | MG   | 2A    | 3586 | 1/1   | 0.90 | 0.16 | -    | 33,33,33,33                 | 0     |
| 56  | MG   | 2A    | 3709 | 1/1   | 0.86 | 0.21 | -    | 40,40,40,40                 | 0     |
| 56  | MG   | 1a    | 1736 | 1/1   | 0.92 | 0.07 | -    | 40,40,40,40                 | 0     |
| 56  | MG   | 2A    | 3453 | 1/1   | 0.97 | 0.14 | -    | 44,44,44,44                 | 0     |
| 56  | MG   | 2A    | 3030 | 1/1   | 0.90 | 0.14 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | 1a    | 1820 | 1/1   | 0.97 | 0.05 | -    | 51,51,51,51                 | 0     |
| 56  | MG   | 2A    | 3326 | 1/1   | 0.71 | 0.22 | -    | 55,55,55,55                 | 0     |
| 56  | MG   | 1A    | 8774 | 1/1   | 0.94 | 0.12 | -    | 25,25,25,25                 | 0     |
| 56  | MG   | 2A    | 3729 | 1/1   | 0.82 | 0.39 | -    | 76,76,76,76                 | 0     |
| 56  | MG   | 1a    | 1658 | 1/1   | 0.91 | 0.40 | -    | 29,29,29,29                 | 0     |
| 56  | MG   | 2A    | 3721 | 1/1   | 0.76 | 0.26 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | 1a    | 1735 | 1/1   | 0.86 | 0.24 | -    | 54,54,54,54                 | 0     |
| 56  | MG   | 2A    | 3448 | 1/1   | 0.65 | 0.16 | -    | 65,65,65,65                 | 0     |
| 56  | MG   | 2e    | 201  | 1/1   | 0.68 | 0.16 | -    | 56,56,56,56                 | 0     |
| 56  | MG   | 1A    | 8770 | 1/1   | 0.94 | 0.14 | -    | 21,21,21,21                 | 0     |
| 56  | MG   | 1A    | 8914 | 1/1   | 0.94 | 0.12 | -    | 46,46,46,46                 | 0     |
| 56  | MG   | 2A    | 3302 | 1/1   | 0.92 | 0.18 | -    | 48,48,48,48                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|----------------------------|-------|
| 56  | MG   | 1A    | 8182 | 1/1   | 0.95 | 0.11 | -    | 12,12,12,12                | 0     |
| 56  | MG   | 1A    | 8562 | 1/1   | 0.97 | 0.14 | -    | 9,9,9,9                    | 0     |
| 56  | MG   | 10    | 104  | 1/1   | 0.69 | 0.15 | -    | 41,41,41,41                | 0     |
| 56  | MG   | 2a    | 1638 | 1/1   | 0.86 | 0.33 | -    | 54,54,54,54                | 0     |
| 56  | MG   | 1P    | 202  | 1/1   | 0.98 | 0.11 | -    | 39,39,39,39                | 0     |
| 56  | MG   | 1A    | 8551 | 1/1   | 0.95 | 0.04 | -    | 32,32,32,32                | 0     |
| 56  | MG   | 1A    | 8900 | 1/1   | 0.83 | 0.14 | -    | 13,13,13,13                | 0     |
| 56  | MG   | 1a    | 1793 | 1/1   | 0.94 | 0.12 | -    | 45,45,45,45                | 0     |
| 56  | MG   | 1A    | 8791 | 1/1   | 0.95 | 0.10 | -    | 39,39,39,39                | 0     |
| 56  | MG   | 2a    | 1669 | 1/1   | 0.94 | 0.12 | -    | 40,40,40,40                | 0     |
| 56  | MG   | 2A    | 3171 | 1/1   | 0.98 | 0.18 | -    | 33,33,33,33                | 0     |
| 56  | MG   | 1A    | 8004 | 1/1   | 0.96 | 0.16 | -    | 18,18,18,18                | 0     |
| 56  | MG   | 1A    | 8951 | 1/1   | 0.96 | 0.11 | -    | 20,20,20,20                | 0     |
| 56  | MG   | 1A    | 8482 | 1/1   | 0.90 | 0.14 | -    | 31,31,31,31                | 0     |
| 56  | MG   | 2a    | 1819 | 1/1   | 0.90 | 0.33 | -    | 59,59,59,59                | 0     |
| 56  | MG   | 2A    | 3195 | 1/1   | 0.90 | 0.29 | -    | 31,31,31,31                | 0     |
| 56  | MG   | 2a    | 1668 | 1/1   | 0.97 | 0.21 | -    | 46,46,46,46                | 0     |
| 56  | MG   | 1A    | 8662 | 1/1   | 0.87 | 0.18 | -    | 29,29,29,29                | 0     |
| 56  | MG   | 2a    | 1709 | 1/1   | 0.98 | 0.07 | -    | 33,33,33,33                | 0     |
| 56  | MG   | 1A    | 8737 | 1/1   | 0.90 | 0.08 | -    | 24,24,24,24                | 0     |
| 56  | MG   | 1a    | 1690 | 1/1   | 0.98 | 0.24 | -    | 36,36,36,36                | 0     |
| 56  | MG   | 1A    | 8768 | 1/1   | 0.96 | 0.14 | -    | 12,12,12,12                | 0     |
| 56  | MG   | 1A    | 8428 | 1/1   | 0.94 | 0.11 | -    | 14,14,14,14                | 0     |
| 56  | MG   | 1A    | 8365 | 1/1   | 0.97 | 0.22 | -    | 24,24,24,24                | 0     |
| 56  | MG   | 2A    | 3870 | 1/1   | 0.78 | 0.34 | -    | 63,63,63,63                | 0     |
| 56  | MG   | 2a    | 1749 | 1/1   | 0.95 | 0.18 | -    | 57,57,57,57                | 0     |
| 56  | MG   | 2a    | 1654 | 1/1   | 0.85 | 0.11 | -    | 62,62,62,62                | 0     |
| 56  | MG   | 1A    | 8722 | 1/1   | 0.88 | 0.10 | -    | 22,22,22,22                | 0     |
| 56  | MG   | 1A    | 8756 | 1/1   | 0.95 | 0.26 | -    | 14,14,14,14                | 0     |
| 56  | MG   | 1a    | 1811 | 1/1   | 0.96 | 0.07 | -    | 58,58,58,58                | 0     |
| 56  | MG   | 1A    | 8193 | 1/1   | 0.86 | 0.19 | -    | 28,28,28,28                | 0     |
| 56  | MG   | 2A    | 3367 | 1/1   | 0.93 | 0.37 | -    | 55,55,55,55                | 0     |
| 56  | MG   | 1A    | 8403 | 1/1   | 0.93 | 0.17 | -    | 13,13,13,13                | 0     |
| 56  | MG   | 1A    | 8164 | 1/1   | 0.94 | 0.10 | -    | 31,31,31,31                | 0     |
| 56  | MG   | 1A    | 8619 | 1/1   | 0.98 | 0.32 | -    | 20,20,20,20                | 0     |
| 56  | MG   | 1a    | 1660 | 1/1   | 0.76 | 0.40 | -    | 39,39,39,39                | 0     |
| 56  | MG   | 1A    | 8686 | 1/1   | 0.86 | 0.20 | -    | 38,38,38,38                | 0     |
| 56  | MG   | 1a    | 1687 | 1/1   | 0.97 | 0.15 | -    | 39,39,39,39                | 0     |
| 56  | MG   | 1A    | 8264 | 1/1   | 0.87 | 0.23 | -    | 37,37,37,37                | 0     |
| 56  | MG   | 1a    | 1822 | 1/1   | 0.96 | 0.05 | -    | 25,25,25,25                | 0     |
| 56  | MG   | 1A    | 8130 | 1/1   | 0.89 | 0.18 | -    | 20,20,20,20                | 0     |
| 56  | MG   | 2A    | 3414 | 1/1   | 0.90 | 0.07 | -    | 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    | 3600 | 1/1   | 0.91 | 0.28 | -    | 40,40,40,40                 | 0     |
| 56  | MG   | 1A    | 8560 | 1/1   | 0.94 | 0.19 | -    | 18,18,18,18                 | 0     |
| 56  | MG   | 1A    | 8331 | 1/1   | 0.94 | 0.17 | -    | 19,19,19,19                 | 0     |
| 56  | MG   | 1A    | 8082 | 1/1   | 0.83 | 0.23 | -    | 27,27,27,27                 | 0     |
| 56  | MG   | 2A    | 3020 | 1/1   | 0.92 | 0.22 | -    | 26,26,26,26                 | 0     |
| 56  | MG   | 2A    | 3979 | 1/1   | 0.93 | 0.16 | -    | 57,57,57,57                 | 0     |
| 56  | MG   | 2A    | 3087 | 1/1   | 0.60 | 0.20 | -    | 54,54,54,54                 | 0     |
| 56  | MG   | 1a    | 1624 | 1/1   | 0.91 | 0.20 | -    | 34,34,34,34                 | 0     |
| 56  | MG   | 2A    | 3209 | 1/1   | 0.95 | 0.28 | -    | 37,37,37,37                 | 0     |
| 56  | MG   | 2A    | 3397 | 1/1   | 0.95 | 0.18 | -    | 21,21,21,21                 | 0     |
| 56  | MG   | 1A    | 8352 | 1/1   | 0.96 | 0.08 | -    | 21,21,21,21                 | 0     |
| 56  | MG   | 1A    | 8590 | 1/1   | 0.94 | 0.21 | -    | 29,29,29,29                 | 0     |
| 56  | MG   | 2A    | 3743 | 1/1   | 0.84 | 0.38 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | 1A    | 8036 | 1/1   | 0.96 | 0.12 | -    | 17,17,17,17                 | 0     |
| 56  | MG   | 1A    | 8360 | 1/1   | 0.97 | 0.07 | -    | 25,25,25,25                 | 0     |
| 56  | MG   | 2A    | 3176 | 1/1   | 0.93 | 0.22 | -    | 42,42,42,42                 | 0     |
| 56  | MG   | 1A    | 8104 | 1/1   | 0.94 | 0.27 | -    | 44,44,44,44                 | 0     |
| 56  | MG   | 1A    | 8202 | 1/1   | 0.88 | 0.27 | -    | 11,11,11,11                 | 0     |
| 56  | MG   | 1A    | 8621 | 1/1   | 0.78 | 0.16 | -    | 24,24,24,24                 | 0     |
| 56  | MG   | 1A    | 8784 | 1/1   | 0.80 | 0.20 | -    | 38,38,38,38                 | 0     |
| 56  | MG   | 1A    | 8861 | 1/1   | 0.93 | 0.16 | -    | 39,39,39,39                 | 0     |
| 56  | MG   | 1A    | 8575 | 1/1   | 0.97 | 0.15 | -    | 14,14,14,14                 | 0     |
| 56  | MG   | 1A    | 8213 | 1/1   | 0.95 | 0.17 | -    | 14,14,14,14                 | 0     |
| 56  | MG   | 1U    | 201  | 1/1   | 0.86 | 0.13 | -    | 26,26,26,26                 | 0     |
| 56  | MG   | 2B    | 3007 | 1/1   | 0.86 | 0.12 | -    | 42,42,42,42                 | 0     |
| 56  | MG   | 2A    | 3127 | 1/1   | 0.95 | 0.44 | -    | 27,27,27,27                 | 0     |
| 56  | MG   | 1a    | 1779 | 1/1   | 0.82 | 0.13 | -    | 50,50,50,50                 | 0     |
| 56  | MG   | 2a    | 1807 | 1/1   | 0.36 | 0.45 | -    | 58,58,58,58                 | 0     |
| 56  | MG   | 1A    | 8624 | 1/1   | 0.97 | 0.07 | -    | 34,34,34,34                 | 0     |
| 56  | MG   | 1A    | 8281 | 1/1   | 0.95 | 0.10 | -    | 28,28,28,28                 | 0     |
| 56  | MG   | 1A    | 8921 | 1/1   | 0.90 | 0.14 | -    | 52,52,52,52                 | 0     |
| 56  | MG   | 1A    | 8302 | 1/1   | 0.98 | 0.17 | -    | 21,21,21,21                 | 0     |
| 56  | MG   | 1E    | 306  | 1/1   | 0.90 | 0.10 | -    | 41,41,41,41                 | 0     |
| 56  | MG   | 2A    | 3733 | 1/1   | 0.86 | 0.08 | -    | 33,33,33,33                 | 0     |
| 56  | MG   | 2A    | 3182 | 1/1   | 0.89 | 0.25 | -    | 34,34,34,34                 | 0     |
| 56  | MG   | 1A    | 8413 | 1/1   | 0.70 | 0.17 | -    | 44,44,44,44                 | 0     |
| 56  | MG   | 2a    | 1621 | 1/1   | 0.87 | 0.19 | -    | 49,49,49,49                 | 0     |
| 56  | MG   | 1A    | 8285 | 1/1   | 0.93 | 0.13 | -    | 10,10,10,10                 | 0     |
| 56  | MG   | 1A    | 8635 | 1/1   | 0.95 | 0.20 | -    | 34,34,34,34                 | 0     |
| 56  | MG   | 1A    | 8797 | 1/1   | 0.89 | 0.11 | -    | 20,20,20,20                 | 0     |
| 56  | MG   | 2A    | 3514 | 1/1   | 0.94 | 0.10 | -    | 36,36,36,36                 | 0     |
| 56  | MG   | 1A    | 8723 | 1/1   | 0.98 | 0.14 | -    | 20,20,20,20                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|----------------------------|-------|
| 56  | MG   | 2A    | 3264 | 1/1   | 0.97 | 0.67 | -    | 65,65,65,65                | 0     |
| 56  | MG   | 2A    | 3407 | 1/1   | 0.94 | 0.11 | -    | 29,29,29,29                | 0     |
| 56  | MG   | 1A    | 8381 | 1/1   | 0.96 | 0.15 | -    | 10,10,10,10                | 0     |
| 56  | MG   | 1A    | 8729 | 1/1   | 0.95 | 0.14 | -    | 43,43,43,43                | 0     |
| 56  | MG   | 1A    | 8592 | 1/1   | 0.93 | 0.15 | -    | 24,24,24,24                | 0     |
| 56  | MG   | 2a    | 1711 | 1/1   | 0.81 | 0.19 | -    | 64,64,64,64                | 0     |
| 56  | MG   | 2B    | 3025 | 1/1   | 0.92 | 0.40 | -    | 52,52,52,52                | 0     |
| 56  | MG   | 2A    | 3089 | 1/1   | 0.94 | 0.28 | -    | 34,34,34,34                | 0     |
| 56  | MG   | 1A    | 8058 | 1/1   | 0.76 | 0.14 | -    | 44,44,44,44                | 0     |
| 56  | MG   | 2a    | 1665 | 1/1   | 0.95 | 0.13 | -    | 53,53,53,53                | 0     |
| 56  | MG   | 1A    | 8477 | 1/1   | 0.94 | 0.08 | -    | 14,14,14,14                | 0     |
| 56  | MG   | 1F    | 310  | 1/1   | 0.97 | 0.10 | -    | 29,29,29,29                | 0     |
| 56  | MG   | 2A    | 3285 | 1/1   | 0.72 | 0.14 | -    | 30,30,30,30                | 0     |
| 56  | MG   | 1A    | 8421 | 1/1   | 0.96 | 0.07 | -    | 26,26,26,26                | 0     |
| 56  | MG   | 2A    | 3910 | 1/1   | 0.89 | 0.24 | -    | 60,60,60,60                | 0     |
| 56  | MG   | 2a    | 1766 | 1/1   | 0.87 | 0.51 | -    | 67,67,67,67                | 0     |
| 56  | MG   | 1A    | 8554 | 1/1   | 0.84 | 0.30 | -    | 34,34,34,34                | 0     |
| 56  | MG   | 2A    | 3010 | 1/1   | 0.91 | 0.32 | -    | 28,28,28,28                | 0     |
| 56  | MG   | 1a    | 1810 | 1/1   | 0.96 | 0.07 | -    | 52,52,52,52                | 0     |
| 56  | MG   | 1A    | 8631 | 1/1   | 0.74 | 0.09 | -    | 53,53,53,53                | 0     |
| 56  | MG   | 1A    | 8092 | 1/1   | 0.96 | 0.55 | -    | 17,17,17,17                | 0     |
| 56  | MG   | 2A    | 3668 | 1/1   | 0.83 | 0.49 | -    | 57,57,57,57                | 0     |
| 56  | MG   | 23    | 101  | 1/1   | 0.88 | 0.30 | -    | 51,51,51,51                | 0     |
| 56  | MG   | 1a    | 1643 | 1/1   | 0.92 | 0.16 | -    | 53,53,53,53                | 0     |
| 56  | MG   | 2A    | 3901 | 1/1   | 0.98 | 0.07 | -    | 29,29,29,29                | 0     |
| 56  | MG   | 1A    | 8315 | 1/1   | 0.91 | 0.24 | -    | 28,28,28,28                | 0     |
| 56  | MG   | 2A    | 3104 | 1/1   | 0.96 | 0.23 | -    | 25,25,25,25                | 0     |
| 56  | MG   | 2A    | 3485 | 1/1   | 0.88 | 0.07 | -    | 44,44,44,44                | 0     |
| 56  | MG   | 2A    | 3082 | 1/1   | 0.91 | 0.26 | -    | 35,35,35,35                | 0     |
| 56  | MG   | 1a    | 1745 | 1/1   | 0.96 | 0.11 | -    | 41,41,41,41                | 0     |
| 56  | MG   | 1A    | 8967 | 1/1   | 0.92 | 0.36 | -    | 27,27,27,27                | 0     |
| 56  | MG   | 1A    | 8639 | 1/1   | 0.95 | 0.11 | -    | 24,24,24,24                | 0     |
| 56  | MG   | 2a    | 1736 | 1/1   | 0.90 | 0.15 | -    | 68,68,68,68                | 0     |
| 56  | MG   | 1A    | 8226 | 1/1   | 0.94 | 0.18 | -    | 17,17,17,17                | 0     |
| 56  | MG   | 1a    | 1796 | 1/1   | 0.80 | 0.19 | -    | 58,58,58,58                | 0     |
| 56  | MG   | 2A    | 3394 | 1/1   | 0.78 | 0.35 | -    | 65,65,65,65                | 0     |
| 56  | MG   | 1A    | 8095 | 1/1   | 0.99 | 0.19 | -    | 6,6,6,6                    | 0     |
| 56  | MG   | 1a    | 1813 | 1/1   | 0.78 | 0.11 | -    | 49,49,49,49                | 0     |
| 56  | MG   | 2a    | 1772 | 1/1   | 0.94 | 0.33 | -    | 57,57,57,57                | 0     |
| 56  | MG   | 1A    | 8702 | 1/1   | 0.97 | 0.07 | -    | 30,30,30,30                | 0     |
| 56  | MG   | 1A    | 8685 | 1/1   | 0.89 | 0.10 | -    | 51,51,51,51                | 0     |
| 56  | MG   | 1A    | 8557 | 1/1   | 0.97 | 0.28 | -    | 16,16,16,16                | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56  | MG   | 2A    | 3933 | 1/1   | 0.79 | 0.12 | -    | 51,51,51,51                 | 0     |
| 56  | MG   | 1A    | 8577 | 1/1   | 0.93 | 0.12 | -    | 21,21,21,21                 | 0     |
| 56  | MG   | 2a    | 1788 | 1/1   | 0.82 | 0.12 | -    | 50,50,50,50                 | 0     |
| 56  | MG   | 1a    | 1601 | 1/1   | 0.96 | 0.07 | -    | 43,43,43,43                 | 0     |
| 56  | MG   | 1a    | 1748 | 1/1   | 0.65 | 0.18 | -    | 65,65,65,65                 | 0     |
| 56  | MG   | 1A    | 8598 | 1/1   | 0.97 | 0.13 | -    | 43,43,43,43                 | 0     |
| 56  | MG   | 1A    | 8632 | 1/1   | 0.95 | 0.09 | -    | 55,55,55,55                 | 0     |
| 56  | MG   | 2a    | 1805 | 1/1   | 0.47 | 0.78 | -    | 94,94,94,94                 | 0     |
| 56  | MG   | 2A    | 3180 | 1/1   | 0.78 | 0.34 | -    | 46,46,46,46                 | 0     |
| 56  | MG   | 1A    | 8558 | 1/1   | 0.89 | 0.09 | -    | 42,42,42,42                 | 0     |
| 56  | MG   | 2A    | 3671 | 1/1   | 0.86 | 0.32 | -    | 45,45,45,45                 | 0     |
| 56  | MG   | 1A    | 8158 | 1/1   | 0.95 | 0.19 | -    | 27,27,27,27                 | 0     |
| 56  | MG   | 2U    | 207  | 1/1   | 0.89 | 0.14 | -    | 29,29,29,29                 | 0     |
| 56  | MG   | 2a    | 1611 | 1/1   | 0.87 | 0.42 | -    | 61,61,61,61                 | 0     |
| 56  | MG   | 2a    | 1619 | 1/1   | 0.97 | 0.45 | -    | 50,50,50,50                 | 0     |
| 56  | MG   | 1A    | 8823 | 1/1   | 0.95 | 0.09 | -    | 23,23,23,23                 | 0     |
| 56  | MG   | 2B    | 3016 | 1/1   | 0.91 | 0.19 | -    | 55,55,55,55                 | 0     |
| 56  | MG   | 1A    | 8687 | 1/1   | 0.76 | 0.16 | -    | 46,46,46,46                 | 0     |
| 56  | MG   | 2A    | 3324 | 1/1   | 0.77 | 0.12 | -    | 33,33,33,33                 | 0     |
| 56  | MG   | 1A    | 8101 | 1/1   | 0.98 | 0.29 | -    | 11,11,11,11                 | 0     |
| 56  | MG   | 2A    | 3814 | 1/1   | 0.75 | 0.10 | -    | 33,33,33,33                 | 0     |
| 56  | MG   | 1A    | 8001 | 1/1   | 0.90 | 0.14 | -    | 37,37,37,37                 | 0     |
| 56  | MG   | 2A    | 3002 | 1/1   | 0.97 | 0.17 | -    | 28,28,28,28                 | 0     |
| 56  | MG   | 1B    | 3021 | 1/1   | 0.96 | 0.09 | -    | 28,28,28,28                 | 0     |
| 56  | MG   | 2A    | 3617 | 1/1   | 0.89 | 0.09 | -    | 43,43,43,43                 | 0     |
| 56  | MG   | 1A    | 8742 | 1/1   | 0.90 | 0.09 | -    | 50,50,50,50                 | 0     |
| 56  | MG   | 2W    | 3001 | 1/1   | 0.85 | 0.11 | -    | 45,45,45,45                 | 0     |
| 56  | MG   | 2A    | 3185 | 1/1   | 0.89 | 0.22 | -    | 45,45,45,45                 | 0     |
| 56  | MG   | 1A    | 8665 | 1/1   | 0.83 | 0.27 | -    | 63,63,63,63                 | 0     |
| 56  | MG   | 1A    | 8946 | 1/1   | 0.90 | 0.20 | -    | 11,11,11,11                 | 0     |
| 56  | MG   | 1A    | 8966 | 1/1   | 0.87 | 0.11 | -    | 22,22,22,22                 | 0     |
| 56  | MG   | 2N    | 203  | 1/1   | 0.85 | 0.13 | -    | 49,49,49,49                 | 0     |
| 56  | MG   | 1A    | 8727 | 1/1   | 0.88 | 0.09 | -    | 36,36,36,36                 | 0     |
| 56  | MG   | 2A    | 3361 | 1/1   | 0.96 | 0.07 | -    | 42,42,42,42                 | 0     |
| 56  | MG   | 2a    | 1738 | 1/1   | 0.98 | 0.09 | -    | 43,43,43,43                 | 0     |
| 56  | MG   | 2A    | 3669 | 1/1   | 0.96 | 0.09 | -    | 34,34,34,34                 | 0     |
| 56  | MG   | 1A    | 8510 | 1/1   | 0.96 | 0.15 | -    | 29,29,29,29                 | 0     |
| 56  | MG   | 1A    | 8505 | 1/1   | 0.92 | 0.15 | -    | 24,24,24,24                 | 0     |
| 56  | MG   | 2A    | 3202 | 1/1   | 0.82 | 0.74 | -    | 42,42,42,42                 | 0     |
| 56  | MG   | 2A    | 3263 | 1/1   | 0.81 | 0.41 | -    | 46,46,46,46                 | 0     |
| 56  | MG   | 1A    | 8469 | 1/1   | 0.88 | 0.08 | -    | 29,29,29,29                 | 0     |
| 56  | MG   | 1A    | 8388 | 1/1   | 0.97 | 0.09 | -    | 11,11,11,11                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|----------------------------|-------|
| 56  | MG   | 2A    | 3256 | 1/1   | 0.98 | 0.20 | -    | 33,33,33,33                | 0     |
| 56  | MG   | 2B    | 3023 | 1/1   | 0.85 | 0.14 | -    | 41,41,41,41                | 0     |
| 56  | MG   | 2A    | 3406 | 1/1   | 0.81 | 0.16 | -    | 51,51,51,51                | 0     |
| 56  | MG   | 1A    | 8317 | 1/1   | 0.66 | 0.09 | -    | 35,35,35,35                | 0     |
| 56  | MG   | 1A    | 8055 | 1/1   | 0.88 | 0.26 | -    | 10,10,10,10                | 0     |
| 56  | MG   | 1a    | 1685 | 1/1   | 0.83 | 0.12 | -    | 51,51,51,51                | 0     |
| 56  | MG   | 2a    | 1628 | 1/1   | 0.95 | 0.69 | -    | 58,58,58,58                | 0     |
| 56  | MG   | 2A    | 3785 | 1/1   | 0.80 | 0.17 | -    | 29,29,29,29                | 0     |
| 56  | MG   | 2A    | 3400 | 1/1   | 0.86 | 0.08 | -    | 41,41,41,41                | 0     |
| 56  | MG   | 1A    | 8470 | 1/1   | 0.92 | 0.21 | -    | 39,39,39,39                | 0     |
| 56  | MG   | 1A    | 8531 | 1/1   | 0.99 | 0.10 | -    | 26,26,26,26                | 0     |
| 56  | MG   | 2A    | 3683 | 1/1   | 0.88 | 0.23 | -    | 73,73,73,73                | 0     |
| 56  | MG   | 1A    | 8501 | 1/1   | 0.98 | 0.11 | -    | 29,29,29,29                | 0     |
| 56  | MG   | 2A    | 3840 | 1/1   | 0.86 | 0.19 | -    | 42,42,42,42                | 0     |
| 56  | MG   | 1A    | 8870 | 1/1   | 0.98 | 0.08 | -    | 20,20,20,20                | 0     |
| 56  | MG   | 1A    | 8789 | 1/1   | 0.91 | 0.16 | -    | 22,22,22,22                | 0     |
| 56  | MG   | 2a    | 1763 | 1/1   | 0.55 | 0.24 | -    | 81,81,81,81                | 0     |
| 56  | MG   | 1A    | 8697 | 1/1   | 0.93 | 0.14 | -    | 32,32,32,32                | 0     |
| 56  | MG   | 1a    | 1725 | 1/1   | 0.98 | 0.09 | -    | 35,35,35,35                | 0     |
| 56  | MG   | 1a    | 1802 | 1/1   | 0.99 | 0.13 | -    | 30,30,30,30                | 0     |
| 56  | MG   | 2a    | 1748 | 1/1   | 0.97 | 0.12 | -    | 50,50,50,50                | 0     |
| 56  | MG   | 1A    | 8760 | 1/1   | 0.93 | 0.10 | -    | 12,12,12,12                | 0     |
| 56  | MG   | 2A    | 3700 | 1/1   | 0.87 | 0.10 | -    | 42,42,42,42                | 0     |
| 56  | MG   | 1A    | 8411 | 1/1   | 0.98 | 0.10 | -    | 12,12,12,12                | 0     |
| 56  | MG   | 2A    | 3827 | 1/1   | 0.59 | 0.20 | -    | 66,66,66,66                | 0     |
| 56  | MG   | 1A    | 8483 | 1/1   | 0.93 | 0.12 | -    | 30,30,30,30                | 0     |
| 56  | MG   | 2A    | 3962 | 1/1   | 0.81 | 0.54 | -    | 54,54,54,54                | 0     |
| 56  | MG   | 2A    | 3637 | 1/1   | 0.78 | 0.22 | -    | 48,48,48,48                | 0     |
| 56  | MG   | 1A    | 8253 | 1/1   | 0.94 | 0.28 | -    | 23,23,23,23                | 0     |
| 56  | MG   | 2Y    | 201  | 1/1   | 0.87 | 0.71 | -    | 85,85,85,85                | 0     |
| 56  | MG   | 1B    | 3016 | 1/1   | 0.91 | 0.13 | -    | 51,51,51,51                | 0     |
| 56  | MG   | 2A    | 3282 | 1/1   | 0.89 | 0.24 | -    | 63,63,63,63                | 0     |
| 56  | MG   | 2a    | 1785 | 1/1   | 0.82 | 0.28 | -    | 70,70,70,70                | 0     |
| 56  | MG   | 1A    | 8591 | 1/1   | 0.93 | 0.28 | -    | 10,10,10,10                | 0     |
| 56  | MG   | 1a    | 1679 | 1/1   | 0.91 | 0.26 | -    | 36,36,36,36                | 0     |
| 56  | MG   | 2A    | 3899 | 1/1   | 0.80 | 0.42 | -    | 62,62,62,62                | 0     |
| 56  | MG   | 2A    | 3191 | 1/1   | 0.93 | 0.26 | -    | 35,35,35,35                | 0     |
| 56  | MG   | 1A    | 8358 | 1/1   | 0.94 | 0.08 | -    | 7,7,7,7                    | 0     |
| 56  | MG   | 1A    | 8540 | 1/1   | 0.93 | 0.10 | -    | 21,21,21,21                | 0     |
| 56  | MG   | 1A    | 8684 | 1/1   | 0.98 | 0.07 | -    | 35,35,35,35                | 0     |
| 56  | MG   | 1A    | 8740 | 1/1   | 0.97 | 0.14 | -    | 27,27,27,27                | 0     |
| 56  | MG   | 2A    | 3758 | 1/1   | 0.90 | 0.21 | -    | 28,28,28,28                | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56  | MG   | 2A    | 3502 | 1/1   | 0.83 | 0.10 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | 2A    | 3651 | 1/1   | 0.97 | 0.23 | -    | 35,35,35,35                 | 0     |
| 56  | MG   | 1i    | 3001 | 1/1   | 0.84 | 0.17 | -    | 46,46,46,46                 | 0     |
| 56  | MG   | 20    | 104  | 1/1   | 0.85 | 0.20 | -    | 55,55,55,55                 | 0     |
| 56  | MG   | 1A    | 8584 | 1/1   | 0.98 | 0.20 | -    | 35,35,35,35                 | 0     |
| 56  | MG   | 2A    | 3549 | 1/1   | 0.83 | 0.10 | -    | 39,39,39,39                 | 0     |
| 56  | MG   | 1a    | 1791 | 1/1   | 0.72 | 0.23 | -    | 56,56,56,56                 | 0     |
| 56  | MG   | 2A    | 3512 | 1/1   | 0.92 | 0.05 | -    | 53,53,53,53                 | 0     |
| 56  | MG   | 2A    | 3566 | 1/1   | 0.90 | 0.13 | -    | 43,43,43,43                 | 0     |
| 56  | MG   | 2A    | 3837 | 1/1   | 0.89 | 0.20 | -    | 21,21,21,21                 | 0     |
| 56  | MG   | 1a    | 1642 | 1/1   | 0.82 | 0.20 | -    | 57,57,57,57                 | 0     |
| 56  | MG   | 1A    | 8846 | 1/1   | 0.88 | 0.17 | -    | 37,37,37,37                 | 0     |
| 56  | MG   | 2A    | 3005 | 1/1   | 0.96 | 0.31 | -    | 32,32,32,32                 | 0     |
| 56  | MG   | 2A    | 3207 | 1/1   | 0.86 | 0.69 | -    | 44,44,44,44                 | 0     |
| 56  | MG   | 1a    | 1670 | 1/1   | 0.84 | 0.16 | -    | 44,44,44,44                 | 0     |
| 56  | MG   | 2x    | 103  | 1/1   | 0.94 | 0.14 | -    | 49,49,49,49                 | 0     |
| 56  | MG   | 2A    | 3484 | 1/1   | 0.90 | 0.22 | -    | 57,57,57,57                 | 0     |
| 56  | MG   | 1A    | 8709 | 1/1   | 0.96 | 0.11 | -    | 23,23,23,23                 | 0     |
| 56  | MG   | 2A    | 3622 | 1/1   | 0.89 | 0.16 | -    | 44,44,44,44                 | 0     |
| 56  | MG   | 27    | 102  | 1/1   | 0.88 | 0.11 | -    | 56,56,56,56                 | 0     |
| 56  | MG   | 2a    | 1770 | 1/1   | 0.82 | 0.13 | -    | 52,52,52,52                 | 0     |
| 56  | MG   | 1a    | 1639 | 1/1   | 0.61 | 0.20 | -    | 50,50,50,50                 | 0     |
| 56  | MG   | 2a    | 1662 | 1/1   | 0.84 | 0.15 | -    | 48,48,48,48                 | 0     |
| 56  | MG   | 2A    | 3506 | 1/1   | 0.98 | 0.05 | -    | 33,33,33,33                 | 0     |
| 56  | MG   | 1A    | 8718 | 1/1   | 0.83 | 0.29 | -    | 27,27,27,27                 | 0     |
| 56  | MG   | 1a    | 1611 | 1/1   | 0.96 | 0.08 | -    | 38,38,38,38                 | 0     |
| 56  | MG   | 1A    | 8875 | 1/1   | 0.96 | 0.27 | -    | 10,10,10,10                 | 0     |
| 56  | MG   | 1A    | 8541 | 1/1   | 0.93 | 0.16 | -    | 31,31,31,31                 | 0     |
| 56  | MG   | 1A    | 8539 | 1/1   | 0.93 | 0.16 | -    | 26,26,26,26                 | 0     |
| 56  | MG   | 2a    | 1722 | 1/1   | 0.61 | 0.08 | -    | 61,61,61,61                 | 0     |
| 56  | MG   | 2A    | 3829 | 1/1   | 0.90 | 0.25 | -    | 53,53,53,53                 | 0     |
| 56  | MG   | 1A    | 8094 | 1/1   | 0.93 | 0.19 | -    | 12,12,12,12                 | 0     |
| 56  | MG   | 2A    | 3918 | 1/1   | 0.98 | 0.06 | -    | 43,43,43,43                 | 0     |
| 56  | MG   | 2A    | 3847 | 1/1   | 0.87 | 0.40 | -    | 53,53,53,53                 | 0     |
| 56  | MG   | 2a    | 1710 | 1/1   | 0.87 | 0.19 | -    | 55,55,55,55                 | 0     |
| 56  | MG   | 2A    | 3897 | 1/1   | 0.94 | 0.14 | -    | 59,59,59,59                 | 0     |
| 56  | MG   | 1B    | 3010 | 1/1   | 0.83 | 0.14 | -    | 44,44,44,44                 | 0     |
| 56  | MG   | 1A    | 8106 | 1/1   | 0.91 | 0.16 | -    | 22,22,22,22                 | 0     |
| 56  | MG   | 1a    | 1708 | 1/1   | 0.96 | 0.24 | -    | 43,43,43,43                 | 0     |
| 56  | MG   | 2A    | 3602 | 1/1   | 0.88 | 0.13 | -    | 53,53,53,53                 | 0     |
| 56  | MG   | 1A    | 8088 | 1/1   | 0.93 | 0.15 | -    | 16,16,16,16                 | 0     |
| 56  | MG   | 1A    | 8820 | 1/1   | 0.96 | 0.12 | -    | 24,24,24,24                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56  | MG   | 1A    | 8003 | 1/1   | 0.96 | 0.17 | -    | 29,29,29,29                 | 0     |
| 56  | MG   | 1A    | 8374 | 1/1   | 0.84 | 0.12 | -    | 41,41,41,41                 | 0     |
| 56  | MG   | 1A    | 8580 | 1/1   | 0.98 | 0.06 | -    | 27,27,27,27                 | 0     |
| 56  | MG   | 2A    | 3742 | 1/1   | 0.58 | 0.86 | -    | 35,35,35,35                 | 0     |
| 56  | MG   | 2A    | 3378 | 1/1   | 0.93 | 0.14 | -    | 41,41,41,41                 | 0     |
| 56  | MG   | 2A    | 3564 | 1/1   | 0.86 | 0.27 | -    | 51,51,51,51                 | 0     |
| 56  | MG   | 1A    | 8196 | 1/1   | 0.87 | 0.18 | -    | 49,49,49,49                 | 0     |
| 56  | MG   | 2A    | 3647 | 1/1   | 0.98 | 0.11 | -    | 28,28,28,28                 | 0     |
| 56  | MG   | 1A    | 8255 | 1/1   | 0.89 | 0.57 | -    | 33,33,33,33                 | 0     |
| 56  | MG   | 1A    | 8172 | 1/1   | 0.80 | 0.13 | -    | 53,53,53,53                 | 0     |
| 56  | MG   | 2A    | 3237 | 1/1   | 0.84 | 0.17 | -    | 45,45,45,45                 | 0     |
| 56  | MG   | 1a    | 1651 | 1/1   | 0.97 | 0.15 | -    | 26,26,26,26                 | 0     |
| 56  | MG   | 1a    | 1656 | 1/1   | 0.88 | 0.15 | -    | 51,51,51,51                 | 0     |
| 56  | MG   | 1A    | 8050 | 1/1   | 0.92 | 0.19 | -    | 23,23,23,23                 | 0     |
| 56  | MG   | 1A    | 8312 | 1/1   | 0.88 | 0.10 | -    | 7,7,7,7                     | 0     |
| 56  | MG   | 1A    | 8836 | 1/1   | 0.93 | 0.08 | -    | 17,17,17,17                 | 0     |
| 56  | MG   | 1A    | 8747 | 1/1   | 0.82 | 0.09 | -    | 27,27,27,27                 | 0     |
| 56  | MG   | 2a    | 1735 | 1/1   | 0.90 | 0.26 | -    | 51,51,51,51                 | 0     |
| 56  | MG   | 2A    | 3935 | 1/1   | 0.95 | 0.11 | -    | 68,68,68,68                 | 0     |
| 56  | MG   | 2A    | 3596 | 1/1   | 0.75 | 0.22 | -    | 35,35,35,35                 | 0     |
| 56  | MG   | 2A    | 3467 | 1/1   | 0.80 | 0.12 | -    | 52,52,52,52                 | 0     |
| 56  | MG   | 1a    | 1765 | 1/1   | 0.93 | 0.13 | -    | 44,44,44,44                 | 0     |
| 56  | MG   | 1A    | 8308 | 1/1   | 0.85 | 0.10 | -    | 41,41,41,41                 | 0     |
| 56  | MG   | 1A    | 8848 | 1/1   | 0.92 | 0.08 | -    | 13,13,13,13                 | 0     |
| 56  | MG   | 1A    | 8340 | 1/1   | 0.94 | 0.13 | -    | 19,19,19,19                 | 0     |
| 56  | MG   | 2A    | 3062 | 1/1   | 0.88 | 0.26 | -    | 37,37,37,37                 | 0     |
| 56  | MG   | 1A    | 8736 | 1/1   | 0.85 | 0.36 | -    | 38,38,38,38                 | 0     |
| 56  | MG   | 2A    | 3538 | 1/1   | 0.94 | 0.09 | -    | 32,32,32,32                 | 0     |
| 56  | MG   | 2A    | 3903 | 1/1   | 0.84 | 0.30 | -    | 49,49,49,49                 | 0     |
| 56  | MG   | 1A    | 8432 | 1/1   | 0.97 | 0.07 | -    | 26,26,26,26                 | 0     |
| 56  | MG   | 1P    | 201  | 1/1   | 0.70 | 0.15 | -    | 18,18,18,18                 | 0     |
| 56  | MG   | 1A    | 8757 | 1/1   | 0.94 | 0.28 | -    | 42,42,42,42                 | 0     |
| 56  | MG   | 2A    | 3253 | 1/1   | 0.94 | 0.37 | -    | 39,39,39,39                 | 0     |
| 56  | MG   | 2A    | 3403 | 1/1   | 0.79 | 0.10 | -    | 40,40,40,40                 | 0     |
| 56  | MG   | 2l    | 201  | 1/1   | 0.56 | 0.53 | -    | 65,65,65,65                 | 0     |
| 56  | MG   | 2A    | 3458 | 1/1   | 0.92 | 0.12 | -    | 37,37,37,37                 | 0     |
| 56  | MG   | 1A    | 8328 | 1/1   | 0.85 | 0.25 | -    | 38,38,38,38                 | 0     |
| 56  | MG   | 2Y    | 203  | 1/1   | 0.87 | 0.07 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | 2A    | 3594 | 1/1   | 0.95 | 0.09 | -    | 44,44,44,44                 | 0     |
| 56  | MG   | 1A    | 8738 | 1/1   | 0.89 | 0.08 | -    | 38,38,38,38                 | 0     |
| 56  | MG   | 2A    | 3249 | 1/1   | 0.92 | 0.19 | -    | 31,31,31,31                 | 0     |
| 56  | MG   | 2A    | 3351 | 1/1   | 0.95 | 0.10 | -    | 40,40,40,40                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|----------------------------|-------|
| 56  | MG   | 1A    | 8579 | 1/1   | 0.91 | 0.23 | -    | 27,27,27,27                | 0     |
| 56  | MG   | 1A    | 8282 | 1/1   | 0.91 | 0.10 | -    | 45,45,45,45                | 0     |
| 56  | MG   | 2a    | 1762 | 1/1   | 0.78 | 0.13 | -    | 58,58,58,58                | 0     |
| 56  | MG   | 1A    | 8035 | 1/1   | 0.95 | 0.18 | -    | 30,30,30,30                | 0     |
| 56  | MG   | 1A    | 8085 | 1/1   | 0.95 | 0.19 | -    | 15,15,15,15                | 0     |
| 56  | MG   | 1A    | 8858 | 1/1   | 0.91 | 0.15 | -    | 28,28,28,28                | 0     |
| 56  | MG   | 1A    | 8093 | 1/1   | 0.87 | 0.21 | -    | 20,20,20,20                | 0     |
| 56  | MG   | 2a    | 1694 | 1/1   | 0.95 | 0.12 | -    | 28,28,28,28                | 0     |
| 56  | MG   | 2A    | 3767 | 1/1   | 0.88 | 0.15 | -    | 52,52,52,52                | 0     |
| 56  | MG   | 1A    | 8688 | 1/1   | 0.90 | 0.10 | -    | 20,20,20,20                | 0     |
| 56  | MG   | 2A    | 3963 | 1/1   | 0.93 | 0.29 | -    | 53,53,53,53                | 0     |
| 56  | MG   | 2A    | 3019 | 1/1   | 0.98 | 0.27 | -    | 33,33,33,33                | 0     |
| 56  | MG   | 1h    | 8001 | 1/1   | 0.93 | 0.08 | -    | 52,52,52,52                | 0     |
| 56  | MG   | 2A    | 3117 | 1/1   | 0.90 | 0.40 | -    | 45,45,45,45                | 0     |
| 56  | MG   | 20    | 102  | 1/1   | 0.94 | 0.06 | -    | 43,43,43,43                | 0     |
| 56  | MG   | 1A    | 8608 | 1/1   | 0.81 | 0.23 | -    | 29,29,29,29                | 0     |
| 56  | MG   | 2a    | 1630 | 1/1   | 0.83 | 0.15 | -    | 50,50,50,50                | 0     |
| 56  | MG   | 2A    | 3872 | 1/1   | 0.28 | 0.34 | -    | 69,69,69,69                | 0     |
| 56  | MG   | 2A    | 3048 | 1/1   | 0.91 | 0.40 | -    | 40,40,40,40                | 0     |
| 56  | MG   | 1a    | 1767 | 1/1   | 0.93 | 0.15 | -    | 55,55,55,55                | 0     |
| 56  | MG   | 1A    | 8316 | 1/1   | 0.88 | 0.17 | -    | 14,14,14,14                | 0     |
| 56  | MG   | 2A    | 3922 | 1/1   | 0.86 | 0.28 | -    | 65,65,65,65                | 0     |
| 56  | MG   | 2A    | 3112 | 1/1   | 0.80 | 0.30 | -    | 29,29,29,29                | 0     |
| 56  | MG   | 1B    | 3015 | 1/1   | 0.98 | 0.14 | -    | 18,18,18,18                | 0     |
| 56  | MG   | 1A    | 8958 | 1/1   | 0.90 | 0.21 | -    | 28,28,28,28                | 0     |
| 56  | MG   | 1a    | 1772 | 1/1   | 0.76 | 0.13 | -    | 53,53,53,53                | 0     |
| 56  | MG   | 1x    | 3008 | 1/1   | 0.99 | 0.16 | -    | 36,36,36,36                | 0     |
| 56  | MG   | 1A    | 8052 | 1/1   | 0.94 | 0.17 | -    | 12,12,12,12                | 0     |
| 56  | MG   | 1A    | 8605 | 1/1   | 0.85 | 0.22 | -    | 41,41,41,41                | 0     |
| 56  | MG   | 2A    | 3830 | 1/1   | 0.89 | 0.13 | -    | 42,42,42,42                | 0     |
| 56  | MG   | 1A    | 8587 | 1/1   | 0.91 | 0.23 | -    | 21,21,21,21                | 0     |
| 56  | MG   | 1A    | 8289 | 1/1   | 0.91 | 0.17 | -    | 8,8,8,8                    | 0     |
| 56  | MG   | 2A    | 3257 | 1/1   | 0.83 | 0.24 | -    | 44,44,44,44                | 0     |
| 56  | MG   | 1A    | 8595 | 1/1   | 0.94 | 0.14 | -    | 35,35,35,35                | 0     |
| 56  | MG   | 2A    | 3688 | 1/1   | 0.72 | 0.13 | -    | 47,47,47,47                | 0     |
| 56  | MG   | 1A    | 8378 | 1/1   | 0.96 | 0.14 | -    | 24,24,24,24                | 0     |
| 56  | MG   | 1a    | 1723 | 1/1   | 0.86 | 0.09 | -    | 40,40,40,40                | 0     |
| 56  | MG   | 1A    | 8506 | 1/1   | 0.98 | 0.13 | -    | 30,30,30,30                | 0     |
| 56  | MG   | 1D    | 313  | 1/1   | 0.96 | 0.18 | -    | 33,33,33,33                | 0     |
| 56  | MG   | 1a    | 1742 | 1/1   | 0.88 | 0.14 | -    | 32,32,32,32                | 0     |
| 56  | MG   | 2A    | 3081 | 1/1   | 0.95 | 0.17 | -    | 27,27,27,27                | 0     |
| 56  | MG   | 13    | 101  | 1/1   | 0.99 | 0.11 | -    | 17,17,17,17                | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56  | MG   | 2A    | 3105 | 1/1   | 0.80 | 0.40 | -    | 46,46,46,46                 | 0     |
| 56  | MG   | 1A    | 8199 | 1/1   | 0.92 | 0.17 | -    | 14,14,14,14                 | 0     |
| 56  | MG   | 2A    | 3136 | 1/1   | 0.96 | 0.16 | -    | 34,34,34,34                 | 0     |
| 56  | MG   | 1A    | 8048 | 1/1   | 0.88 | 0.18 | -    | 22,22,22,22                 | 0     |
| 56  | MG   | 1a    | 1722 | 1/1   | 0.92 | 0.08 | -    | 32,32,32,32                 | 0     |
| 56  | MG   | 1a    | 1754 | 1/1   | 0.66 | 0.21 | -    | 59,59,59,59                 | 0     |
| 56  | MG   | 2A    | 3064 | 1/1   | 0.92 | 0.15 | -    | 34,34,34,34                 | 0     |
| 56  | MG   | 1a    | 1608 | 1/1   | 0.91 | 0.22 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | 1A    | 8790 | 1/1   | 0.91 | 0.11 | -    | 20,20,20,20                 | 0     |
| 56  | MG   | 1a    | 1798 | 1/1   | 0.94 | 0.13 | -    | 48,48,48,48                 | 0     |
| 56  | MG   | 1A    | 8076 | 1/1   | 0.83 | 0.44 | -    | 22,22,22,22                 | 0     |
| 56  | MG   | 2x    | 106  | 1/1   | 0.94 | 0.15 | -    | 52,52,52,52                 | 0     |
| 56  | MG   | 2A    | 3738 | 1/1   | 0.95 | 0.09 | -    | 43,43,43,43                 | 0     |
| 56  | MG   | 1a    | 1806 | 1/1   | 0.96 | 0.10 | -    | 49,49,49,49                 | 0     |
| 56  | MG   | 2A    | 3581 | 1/1   | 0.92 | 0.14 | -    | 31,31,31,31                 | 0     |
| 56  | MG   | 1A    | 8763 | 1/1   | 0.92 | 0.35 | -    | 28,28,28,28                 | 0     |
| 56  | MG   | 1a    | 1648 | 1/1   | 0.93 | 0.20 | -    | 38,38,38,38                 | 0     |
| 56  | MG   | 1A    | 8407 | 1/1   | 0.96 | 0.10 | -    | 20,20,20,20                 | 0     |
| 56  | MG   | 2A    | 3684 | 1/1   | 0.51 | 0.33 | -    | 68,68,68,68                 | 0     |
| 56  | MG   | 2a    | 1759 | 1/1   | 0.70 | 0.35 | -    | 76,76,76,76                 | 0     |
| 56  | MG   | 2a    | 1775 | 1/1   | 0.82 | 0.48 | -    | 68,68,68,68                 | 0     |
| 56  | MG   | 1a    | 1697 | 1/1   | 0.88 | 0.08 | -    | 38,38,38,38                 | 0     |
| 56  | MG   | 1a    | 1773 | 1/1   | 0.72 | 0.13 | -    | 44,44,44,44                 | 0     |
| 56  | MG   | 2A    | 3277 | 1/1   | 0.94 | 0.43 | -    | 59,59,59,59                 | 0     |
| 56  | MG   | 2A    | 3329 | 1/1   | 0.96 | 0.12 | -    | 30,30,30,30                 | 0     |
| 56  | MG   | 2a    | 1677 | 1/1   | 0.72 | 0.12 | -    | 62,62,62,62                 | 0     |
| 56  | MG   | 2a    | 1636 | 1/1   | 0.93 | 0.26 | -    | 33,33,33,33                 | 0     |
| 56  | MG   | 1a    | 1817 | 1/1   | 0.95 | 0.37 | -    | 52,52,52,52                 | 0     |
| 56  | MG   | 1A    | 8442 | 1/1   | 0.88 | 0.15 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | 1A    | 8762 | 1/1   | 0.94 | 0.07 | -    | 34,34,34,34                 | 0     |
| 56  | MG   | 1A    | 8871 | 1/1   | 0.84 | 0.39 | -    | 38,38,38,38                 | 0     |
| 56  | MG   | 2A    | 3592 | 1/1   | 0.97 | 0.19 | -    | 42,42,42,42                 | 0     |
| 56  | MG   | 2a    | 1640 | 1/1   | 0.65 | 0.21 | -    | 64,64,64,64                 | 0     |
| 56  | MG   | 2A    | 3395 | 1/1   | 0.97 | 0.07 | -    | 38,38,38,38                 | 0     |
| 56  | MG   | 2A    | 3130 | 1/1   | 0.96 | 0.12 | -    | 27,27,27,27                 | 0     |
| 56  | MG   | 2A    | 3693 | 1/1   | 0.95 | 0.20 | -    | 34,34,34,34                 | 0     |
| 56  | MG   | 2A    | 3172 | 1/1   | 0.94 | 0.25 | -    | 25,25,25,25                 | 0     |
| 56  | MG   | 20    | 103  | 1/1   | 0.93 | 0.10 | -    | 62,62,62,62                 | 0     |
| 56  | MG   | 1A    | 8351 | 1/1   | 0.97 | 0.10 | -    | 16,16,16,16                 | 0     |
| 56  | MG   | 1A    | 8796 | 1/1   | 0.97 | 0.04 | -    | 35,35,35,35                 | 0     |
| 56  | MG   | 1A    | 8079 | 1/1   | 0.95 | 0.28 | -    | 16,16,16,16                 | 0     |
| 56  | MG   | 2a    | 1760 | 1/1   | 0.88 | 0.13 | -    | 56,56,56,56                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|----------------------------|-------|
| 56  | MG   | 2A    | 3457 | 1/1   | 0.93 | 0.13 | -    | 50,50,50,50                | 0     |
| 56  | MG   | 2F    | 301  | 1/1   | 0.91 | 0.17 | -    | 43,43,43,43                | 0     |
| 56  | MG   | 2A    | 3079 | 1/1   | 0.52 | 1.09 | -    | 61,61,61,61                | 0     |
| 56  | MG   | 1A    | 8269 | 1/1   | 0.91 | 0.11 | -    | 23,23,23,23                | 0     |
| 56  | MG   | 1A    | 8260 | 1/1   | 0.82 | 0.30 | -    | 28,28,28,28                | 0     |
| 56  | MG   | 2A    | 3649 | 1/1   | 0.97 | 0.05 | -    | 42,42,42,42                | 0     |
| 56  | MG   | 2a    | 1639 | 1/1   | 0.97 | 0.09 | -    | 27,27,27,27                | 0     |
| 56  | MG   | 2A    | 3573 | 1/1   | 0.96 | 0.11 | -    | 41,41,41,41                | 0     |
| 56  | MG   | 1x    | 3007 | 1/1   | 0.92 | 0.13 | -    | 37,37,37,37                | 0     |
| 56  | MG   | 2A    | 3677 | 1/1   | 0.80 | 0.19 | -    | 60,60,60,60                | 0     |
| 56  | MG   | 2A    | 3222 | 1/1   | 0.94 | 0.05 | -    | 48,48,48,48                | 0     |
| 56  | MG   | 2A    | 3217 | 1/1   | 0.85 | 0.52 | -    | 30,30,30,30                | 0     |
| 56  | MG   | 2d    | 504  | 1/1   | 0.60 | 0.35 | -    | 64,64,64,64                | 0     |
| 56  | MG   | 2A    | 3591 | 1/1   | 0.80 | 0.21 | -    | 51,51,51,51                | 0     |
| 56  | MG   | 1a    | 1694 | 1/1   | 0.72 | 0.12 | -    | 27,27,27,27                | 0     |
| 56  | MG   | 2A    | 3193 | 1/1   | 0.97 | 0.12 | -    | 27,27,27,27                | 0     |
| 56  | MG   | 2A    | 3205 | 1/1   | 0.88 | 1.05 | -    | 44,44,44,44                | 0     |
| 56  | MG   | 1a    | 1739 | 1/1   | 0.86 | 0.15 | -    | 50,50,50,50                | 0     |
| 56  | MG   | 1a    | 1760 | 1/1   | 0.94 | 0.17 | -    | 56,56,56,56                | 0     |
| 56  | MG   | 2a    | 1789 | 1/1   | 0.90 | 0.05 | -    | 63,63,63,63                | 0     |
| 56  | MG   | 2A    | 3265 | 1/1   | 0.84 | 0.41 | -    | 56,56,56,56                | 0     |
| 56  | MG   | 2A    | 3580 | 1/1   | 0.95 | 0.11 | -    | 49,49,49,49                | 0     |
| 56  | MG   | 2A    | 3940 | 1/1   | 0.95 | 0.33 | -    | 8,8,8,8                    | 0     |
| 56  | MG   | 1A    | 8780 | 1/1   | 0.92 | 0.24 | -    | 10,10,10,10                | 0     |
| 56  | MG   | 2A    | 3065 | 1/1   | 0.95 | 0.46 | -    | 43,43,43,43                | 0     |
| 56  | MG   | 1A    | 8116 | 1/1   | 0.93 | 0.19 | -    | 25,25,25,25                | 0     |
| 56  | MG   | 2x    | 107  | 1/1   | 0.94 | 0.14 | -    | 52,52,52,52                | 0     |
| 56  | MG   | 2A    | 3626 | 1/1   | 0.94 | 0.16 | -    | 60,60,60,60                | 0     |
| 56  | MG   | 2A    | 3386 | 1/1   | 0.94 | 0.19 | -    | 29,29,29,29                | 0     |
| 56  | MG   | 2a    | 1771 | 1/1   | 0.85 | 0.11 | -    | 55,55,55,55                | 0     |
| 56  | MG   | 2A    | 3335 | 1/1   | 0.95 | 0.15 | -    | 37,37,37,37                | 0     |
| 56  | MG   | 2A    | 3248 | 1/1   | 0.85 | 0.32 | -    | 34,34,34,34                | 0     |
| 56  | MG   | 2A    | 3409 | 1/1   | 0.95 | 0.22 | -    | 31,31,31,31                | 0     |
| 56  | MG   | 2A    | 3753 | 1/1   | 0.94 | 0.28 | -    | 27,27,27,27                | 0     |
| 56  | MG   | 2A    | 3014 | 1/1   | 0.91 | 0.22 | -    | 39,39,39,39                | 0     |
| 56  | MG   | 2a    | 1637 | 1/1   | 0.84 | 0.15 | -    | 36,36,36,36                | 0     |
| 56  | MG   | 1A    | 8675 | 1/1   | 0.96 | 0.17 | -    | 17,17,17,17                | 0     |
| 56  | MG   | 1T    | 201  | 1/1   | 0.95 | 0.08 | -    | 37,37,37,37                | 0     |
| 56  | MG   | 2A    | 3198 | 1/1   | 0.95 | 0.06 | -    | 36,36,36,36                | 0     |
| 56  | MG   | 2A    | 3290 | 1/1   | 0.86 | 0.15 | -    | 31,31,31,31                | 0     |
| 56  | MG   | 1a    | 1826 | 1/1   | 0.94 | 0.14 | -    | 65,65,65,65                | 0     |
| 56  | MG   | 1a    | 1623 | 1/1   | 0.77 | 0.32 | -    | 47,47,47,47                | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56  | MG   | 1A    | 8795 | 1/1   | 0.86 | 0.36 | -    | 21,21,21,21                 | 0     |
| 56  | MG   | 1A    | 8460 | 1/1   | 0.97 | 0.14 | -    | 33,33,33,33                 | 0     |
| 56  | MG   | 2A    | 3420 | 1/1   | 0.89 | 0.17 | -    | 54,54,54,54                 | 0     |
| 56  | MG   | 2A    | 3322 | 1/1   | 0.94 | 0.09 | -    | 37,37,37,37                 | 0     |
| 56  | MG   | 2A    | 3057 | 1/1   | 0.78 | 0.27 | -    | 42,42,42,42                 | 0     |
| 56  | MG   | 2A    | 3241 | 1/1   | 0.94 | 0.22 | -    | 49,49,49,49                 | 0     |
| 56  | MG   | 1A    | 8417 | 1/1   | 0.78 | 0.11 | -    | 37,37,37,37                 | 0     |
| 56  | MG   | 1A    | 8852 | 1/1   | 0.89 | 0.11 | -    | 27,27,27,27                 | 0     |
| 56  | MG   | 2A    | 3225 | 1/1   | 0.90 | 0.35 | -    | 42,42,42,42                 | 0     |
| 56  | MG   | 2A    | 3220 | 1/1   | 0.97 | 0.33 | -    | 29,29,29,29                 | 0     |
| 56  | MG   | 1a    | 1769 | 1/1   | 0.91 | 0.20 | -    | 46,46,46,46                 | 0     |
| 56  | MG   | 1A    | 8607 | 1/1   | 0.95 | 0.12 | -    | 18,18,18,18                 | 0     |
| 56  | MG   | 2a    | 1716 | 1/1   | 0.55 | 0.33 | -    | 65,65,65,65                 | 0     |
| 56  | MG   | 1A    | 8524 | 1/1   | 0.93 | 0.20 | -    | 31,31,31,31                 | 0     |
| 56  | MG   | 2A    | 3033 | 1/1   | 0.96 | 0.27 | -    | 28,28,28,28                 | 0     |
| 56  | MG   | 2A    | 3783 | 1/1   | 0.96 | 0.13 | -    | 55,55,55,55                 | 0     |
| 56  | MG   | 2A    | 3231 | 1/1   | 0.94 | 0.41 | -    | 32,32,32,32                 | 0     |
| 56  | MG   | 2A    | 3160 | 1/1   | 0.92 | 0.16 | -    | 28,28,28,28                 | 0     |
| 56  | MG   | 1A    | 8051 | 1/1   | 0.89 | 0.20 | -    | 10,10,10,10                 | 0     |
| 56  | MG   | 1x    | 3009 | 1/1   | 0.95 | 0.23 | -    | 41,41,41,41                 | 0     |
| 56  | MG   | 2A    | 3156 | 1/1   | 0.93 | 0.17 | -    | 33,33,33,33                 | 0     |
| 56  | MG   | 1A    | 8356 | 1/1   | 0.76 | 0.12 | -    | 9,9,9,9                     | 0     |
| 56  | MG   | 2a    | 1655 | 1/1   | 0.90 | 0.19 | -    | 48,48,48,48                 | 0     |
| 56  | MG   | 1A    | 8772 | 1/1   | 0.93 | 0.06 | -    | 27,27,27,27                 | 0     |
| 56  | MG   | 1F    | 308  | 1/1   | 0.94 | 0.17 | -    | 18,18,18,18                 | 0     |
| 56  | MG   | 2a    | 1647 | 1/1   | 0.85 | 0.16 | -    | 48,48,48,48                 | 0     |
| 56  | MG   | 1A    | 8137 | 1/1   | 0.86 | 0.40 | -    | 11,11,11,11                 | 0     |
| 56  | MG   | 2A    | 3631 | 1/1   | 0.94 | 0.11 | -    | 48,48,48,48                 | 0     |
| 56  | MG   | 2A    | 3045 | 1/1   | 0.97 | 0.32 | -    | 20,20,20,20                 | 0     |
| 56  | MG   | 2A    | 3085 | 1/1   | 0.96 | 0.35 | -    | 28,28,28,28                 | 0     |
| 56  | MG   | 1A    | 8620 | 1/1   | 0.95 | 0.16 | -    | 25,25,25,25                 | 0     |
| 56  | MG   | 1A    | 8701 | 1/1   | 0.63 | 0.38 | -    | 49,49,49,49                 | 0     |
| 56  | MG   | 2E    | 305  | 1/1   | 0.93 | 0.30 | -    | 60,60,60,60                 | 0     |
| 56  | MG   | 2A    | 3902 | 1/1   | 0.83 | 0.12 | -    | 39,39,39,39                 | 0     |
| 56  | MG   | 1a    | 1729 | 1/1   | 0.67 | 0.18 | -    | 52,52,52,52                 | 0     |
| 56  | MG   | 1A    | 8221 | 1/1   | 0.80 | 0.10 | -    | 43,43,43,43                 | 0     |
| 56  | MG   | 1V    | 202  | 1/1   | 0.93 | 0.17 | -    | 26,26,26,26                 | 0     |
| 56  | MG   | 1A    | 8711 | 1/1   | 0.81 | 0.12 | -    | 27,27,27,27                 | 0     |
| 56  | MG   | 1a    | 1747 | 1/1   | 0.88 | 0.13 | -    | 65,65,65,65                 | 0     |
| 56  | MG   | 1A    | 8303 | 1/1   | 0.93 | 0.07 | -    | 11,11,11,11                 | 0     |
| 56  | MG   | 2A    | 3464 | 1/1   | 0.98 | 0.28 | -    | 40,40,40,40                 | 0     |
| 56  | MG   | 2A    | 3723 | 1/1   | 0.97 | 0.09 | -    | 45,45,45,45                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|----------------------------|-------|
| 56  | MG   | 1A    | 8690 | 1/1   | 0.95 | 0.12 | -    | 20,20,20,20                | 0     |
| 56  | MG   | 2a    | 1679 | 1/1   | 0.84 | 0.15 | -    | 51,51,51,51                | 0     |
| 56  | MG   | 2A    | 3582 | 1/1   | 0.91 | 0.27 | -    | 27,27,27,27                | 0     |
| 56  | MG   | 2a    | 1779 | 1/1   | 0.89 | 0.17 | -    | 48,48,48,48                | 0     |
| 56  | MG   | 2a    | 1769 | 1/1   | 0.71 | 0.30 | -    | 59,59,59,59                | 0     |
| 56  | MG   | 1a    | 1840 | 1/1   | 0.91 | 0.22 | -    | 55,55,55,55                | 0     |
| 56  | MG   | 1A    | 8406 | 1/1   | 0.97 | 0.17 | -    | 42,42,42,42                | 0     |
| 56  | MG   | 1a    | 1807 | 1/1   | 0.85 | 0.18 | -    | 51,51,51,51                | 0     |
| 56  | MG   | 1A    | 8514 | 1/1   | 0.52 | 0.35 | -    | 48,48,48,48                | 0     |
| 56  | MG   | 2a    | 1795 | 1/1   | 0.92 | 0.23 | -    | 65,65,65,65                | 0     |
| 56  | MG   | 1A    | 8228 | 1/1   | 0.93 | 0.37 | -    | 13,13,13,13                | 0     |
| 56  | MG   | 2A    | 3411 | 1/1   | 0.92 | 0.16 | -    | 36,36,36,36                | 0     |
| 56  | MG   | 2A    | 3408 | 1/1   | 0.94 | 0.10 | -    | 38,38,38,38                | 0     |
| 56  | MG   | 2A    | 3850 | 1/1   | 0.92 | 0.17 | -    | 39,39,39,39                | 0     |
| 56  | MG   | 2a    | 1676 | 1/1   | 0.69 | 0.17 | -    | 65,65,65,65                | 0     |
| 56  | MG   | 2A    | 3287 | 1/1   | 0.90 | 0.19 | -    | 53,53,53,53                | 0     |
| 56  | MG   | 2A    | 3175 | 1/1   | 0.95 | 0.16 | -    | 35,35,35,35                | 0     |
| 56  | MG   | 1A    | 8334 | 1/1   | 0.99 | 0.10 | -    | 13,13,13,13                | 0     |
| 56  | MG   | 1A    | 8304 | 1/1   | 0.97 | 0.09 | -    | 17,17,17,17                | 0     |
| 56  | MG   | 2A    | 3663 | 1/1   | 0.90 | 0.20 | -    | 61,61,61,61                | 0     |
| 56  | MG   | 2a    | 1744 | 1/1   | 0.85 | 0.36 | -    | 43,43,43,43                | 0     |
| 56  | MG   | 1A    | 8292 | 1/1   | 0.97 | 0.09 | -    | 26,26,26,26                | 0     |
| 56  | MG   | 2A    | 3710 | 1/1   | 0.92 | 0.16 | -    | 39,39,39,39                | 0     |
| 56  | MG   | 1A    | 8344 | 1/1   | 0.87 | 0.10 | -    | 26,26,26,26                | 0     |
| 56  | MG   | 1A    | 8773 | 1/1   | 0.84 | 0.14 | -    | 29,29,29,29                | 0     |
| 56  | MG   | 1A    | 8838 | 1/1   | 0.98 | 0.13 | -    | 7,7,7,7                    | 0     |
| 56  | MG   | 1A    | 8493 | 1/1   | 0.91 | 0.13 | -    | 16,16,16,16                | 0     |
| 56  | MG   | 1A    | 8044 | 1/1   | 0.91 | 0.23 | -    | 7,7,7,7                    | 0     |
| 56  | MG   | 2a    | 1625 | 1/1   | 0.65 | 0.23 | -    | 63,63,63,63                | 0     |
| 56  | MG   | 2A    | 3619 | 1/1   | 0.96 | 0.23 | -    | 36,36,36,36                | 0     |
| 56  | MG   | 1A    | 8038 | 1/1   | 0.93 | 0.08 | -    | 40,40,40,40                | 0     |
| 56  | MG   | 2A    | 3306 | 1/1   | 0.95 | 0.10 | -    | 29,29,29,29                | 0     |
| 56  | MG   | 2A    | 3770 | 1/1   | 0.90 | 0.08 | -    | 40,40,40,40                | 0     |
| 56  | MG   | 1A    | 8371 | 1/1   | 0.83 | 0.12 | -    | 11,11,11,11                | 0     |
| 56  | MG   | 2A    | 3124 | 1/1   | 0.86 | 0.16 | -    | 46,46,46,46                | 0     |
| 56  | MG   | 1A    | 8874 | 1/1   | 0.91 | 0.10 | -    | 9,9,9,9                    | 0     |
| 56  | MG   | 2A    | 3615 | 1/1   | 0.95 | 0.35 | -    | 36,36,36,36                | 0     |
| 56  | MG   | 2A    | 3334 | 1/1   | 0.96 | 0.13 | -    | 23,23,23,23                | 0     |
| 56  | MG   | 1A    | 8227 | 1/1   | 0.92 | 0.25 | -    | 14,14,14,14                | 0     |
| 56  | MG   | 1A    | 8329 | 1/1   | 0.97 | 0.08 | -    | 24,24,24,24                | 0     |
| 56  | MG   | 1a    | 1823 | 1/1   | 0.91 | 0.11 | -    | 42,42,42,42                | 0     |
| 56  | MG   | 1A    | 8655 | 1/1   | 0.91 | 0.17 | -    | 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   | 1a    | 1730 | 1/1   | 0.88 | 0.24 | -    | 43,43,43,43                 | 0     |
| 56  | MG   | 1A    | 8155 | 1/1   | 0.92 | 0.23 | -    | 24,24,24,24                 | 0     |
| 56  | MG   | 2a    | 1746 | 1/1   | 0.92 | 0.20 | -    | 59,59,59,59                 | 0     |
| 56  | MG   | 1A    | 8895 | 1/1   | 0.93 | 0.09 | -    | 12,12,12,12                 | 0     |
| 56  | MG   | 1a    | 1640 | 1/1   | 0.97 | 0.14 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | 2A    | 3206 | 1/1   | 0.95 | 0.20 | -    | 48,48,48,48                 | 0     |
| 56  | MG   | 1a    | 1703 | 1/1   | 0.94 | 0.12 | -    | 48,48,48,48                 | 0     |
| 56  | MG   | 1A    | 8170 | 1/1   | 0.97 | 0.27 | -    | 23,23,23,23                 | 0     |
| 56  | MG   | 2A    | 3603 | 1/1   | 0.76 | 0.51 | -    | 53,53,53,53                 | 0     |
| 56  | MG   | 2x    | 108  | 1/1   | 0.56 | 0.17 | -    | 53,53,53,53                 | 0     |
| 56  | MG   | 1A    | 8277 | 1/1   | 0.85 | 0.30 | -    | 50,50,50,50                 | 0     |
| 56  | MG   | 2A    | 3316 | 1/1   | 0.90 | 0.32 | -    | 34,34,34,34                 | 0     |
| 56  | MG   | 1A    | 8720 | 1/1   | 0.98 | 0.14 | -    | 27,27,27,27                 | 0     |
| 56  | MG   | 1A    | 8197 | 1/1   | 0.82 | 0.29 | -    | 42,42,42,42                 | 0     |
| 56  | MG   | 1A    | 8555 | 1/1   | 0.94 | 0.10 | -    | 37,37,37,37                 | 0     |
| 56  | MG   | 2B    | 3010 | 1/1   | 0.84 | 0.18 | -    | 38,38,38,38                 | 0     |
| 56  | MG   | 2A    | 3813 | 1/1   | 0.82 | 0.19 | -    | 64,64,64,64                 | 0     |
| 56  | MG   | 1A    | 8831 | 1/1   | 0.92 | 0.14 | -    | 41,41,41,41                 | 0     |
| 56  | MG   | 1A    | 8154 | 1/1   | 0.91 | 0.23 | -    | 22,22,22,22                 | 0     |
| 56  | MG   | 2A    | 3358 | 1/1   | 0.89 | 0.08 | -    | 27,27,27,27                 | 0     |
| 56  | MG   | 2a    | 1794 | 1/1   | 0.75 | 0.31 | -    | 71,71,71,71                 | 0     |
| 56  | MG   | 1a    | 1610 | 1/1   | 0.91 | 0.34 | -    | 36,36,36,36                 | 0     |
| 56  | MG   | 2A    | 3734 | 1/1   | 0.86 | 0.08 | -    | 33,33,33,33                 | 0     |
| 56  | MG   | 1A    | 8651 | 1/1   | 0.92 | 0.17 | -    | 23,23,23,23                 | 0     |
| 56  | MG   | 1A    | 8666 | 1/1   | 0.91 | 0.10 | -    | 18,18,18,18                 | 0     |
| 56  | MG   | 2A    | 3612 | 1/1   | 0.91 | 0.15 | -    | 40,40,40,40                 | 0     |
| 56  | MG   | 1A    | 8704 | 1/1   | 0.87 | 0.20 | -    | 34,34,34,34                 | 0     |
| 56  | MG   | 2a    | 1649 | 1/1   | 0.82 | 0.71 | -    | 48,48,48,48                 | 0     |
| 56  | MG   | 1a    | 1746 | 1/1   | 0.93 | 0.31 | -    | 44,44,44,44                 | 0     |
| 56  | MG   | 2A    | 3787 | 1/1   | 0.92 | 0.27 | -    | 41,41,41,41                 | 0     |
| 56  | MG   | 1A    | 8190 | 1/1   | 0.94 | 0.07 | -    | 15,15,15,15                 | 0     |
| 56  | MG   | 15    | 107  | 1/1   | 0.90 | 0.19 | -    | 17,17,17,17                 | 0     |
| 56  | MG   | 1A    | 8527 | 1/1   | 0.78 | 0.15 | -    | 11,11,11,11                 | 0     |
| 56  | MG   | 2A    | 3388 | 1/1   | 0.95 | 0.15 | -    | 23,23,23,23                 | 0     |
| 56  | MG   | 2A    | 3422 | 1/1   | 0.97 | 0.09 | -    | 45,45,45,45                 | 0     |
| 56  | MG   | 2A    | 3215 | 1/1   | 0.99 | 0.11 | -    | 26,26,26,26                 | 0     |
| 56  | MG   | 2A    | 3317 | 1/1   | 0.60 | 0.18 | -    | 68,68,68,68                 | 0     |
| 56  | MG   | 2A    | 3266 | 1/1   | 0.95 | 0.14 | -    | 25,25,25,25                 | 0     |
| 56  | MG   | 2A    | 3858 | 1/1   | 0.87 | 0.15 | -    | 46,46,46,46                 | 0     |
| 56  | MG   | 2A    | 3115 | 1/1   | 0.88 | 0.21 | -    | 41,41,41,41                 | 0     |
| 56  | MG   | 1A    | 8409 | 1/1   | 0.96 | 0.10 | -    | 35,35,35,35                 | 0     |
| 56  | MG   | 2A    | 3011 | 1/1   | 0.95 | 0.16 | -    | 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    | 8132 | 1/1   | 0.97 | 0.22 | -    | 19,19,19,19                 | 0     |
| 56  | MG   | 1A    | 8361 | 1/1   | 0.96 | 0.09 | -    | 26,26,26,26                 | 0     |
| 56  | MG   | 1A    | 8165 | 1/1   | 0.98 | 0.11 | -    | 10,10,10,10                 | 0     |
| 56  | MG   | 1A    | 8387 | 1/1   | 0.92 | 0.20 | -    | 28,28,28,28                 | 0     |
| 56  | MG   | 2A    | 3680 | 1/1   | 0.92 | 0.38 | -    | 38,38,38,38                 | 0     |
| 56  | MG   | 1a    | 1677 | 1/1   | 0.89 | 0.15 | -    | 49,49,49,49                 | 0     |
| 56  | MG   | 2A    | 3763 | 1/1   | 0.72 | 0.71 | -    | 51,51,51,51                 | 0     |
| 56  | MG   | 1A    | 8571 | 1/1   | 0.90 | 0.08 | -    | 34,34,34,34                 | 0     |
| 56  | MG   | 1A    | 8682 | 1/1   | 0.98 | 0.07 | -    | 23,23,23,23                 | 0     |
| 56  | MG   | 1A    | 8578 | 1/1   | 0.84 | 0.17 | -    | 10,10,10,10                 | 0     |
| 56  | MG   | 1A    | 8224 | 1/1   | 0.91 | 0.26 | -    | 15,15,15,15                 | 0     |
| 56  | MG   | 2A    | 3327 | 1/1   | 0.75 | 0.33 | -    | 61,61,61,61                 | 0     |
| 56  | MG   | 1A    | 8218 | 1/1   | 0.93 | 0.12 | -    | 11,11,11,11                 | 0     |
| 56  | MG   | 1A    | 8788 | 1/1   | 0.95 | 0.17 | -    | 34,34,34,34                 | 0     |
| 56  | MG   | 1B    | 3003 | 1/1   | 0.86 | 0.14 | -    | 43,43,43,43                 | 0     |
| 56  | MG   | 1R    | 203  | 1/1   | 0.98 | 0.24 | -    | 16,16,16,16                 | 0     |
| 56  | MG   | 1A    | 8706 | 1/1   | 0.97 | 0.06 | -    | 39,39,39,39                 | 0     |
| 56  | MG   | 1A    | 8615 | 1/1   | 0.85 | 0.21 | -    | 13,13,13,13                 | 0     |
| 56  | MG   | 2A    | 3299 | 1/1   | 0.96 | 0.04 | -    | 41,41,41,41                 | 0     |
| 56  | MG   | 2A    | 3896 | 1/1   | 0.95 | 0.04 | -    | 28,28,28,28                 | 0     |
| 56  | MG   | 2A    | 3149 | 1/1   | 0.89 | 0.21 | -    | 32,32,32,32                 | 0     |
| 56  | MG   | 1A    | 8905 | 1/1   | 0.84 | 0.08 | -    | 42,42,42,42                 | 0     |
| 56  | MG   | 1a    | 1770 | 1/1   | 0.97 | 0.19 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | 2A    | 3625 | 1/1   | 0.93 | 0.14 | -    | 51,51,51,51                 | 0     |
| 56  | MG   | 2A    | 3120 | 1/1   | 0.95 | 0.15 | -    | 28,28,28,28                 | 0     |
| 56  | MG   | 1A    | 8764 | 1/1   | 0.93 | 0.12 | -    | 27,27,27,27                 | 0     |
| 56  | MG   | 2A    | 3167 | 1/1   | 0.90 | 0.16 | -    | 26,26,26,26                 | 0     |
| 56  | MG   | 1A    | 8913 | 1/1   | 0.95 | 0.14 | -    | 48,48,48,48                 | 0     |
| 56  | MG   | 2A    | 3094 | 1/1   | 0.97 | 0.12 | -    | 38,38,38,38                 | 0     |
| 56  | MG   | 1A    | 8767 | 1/1   | 0.88 | 0.10 | -    | 33,33,33,33                 | 0     |
| 56  | MG   | 2A    | 3333 | 1/1   | 0.97 | 0.14 | -    | 39,39,39,39                 | 0     |
| 56  | MG   | 2A    | 3546 | 1/1   | 0.90 | 0.21 | -    | 54,54,54,54                 | 0     |
| 56  | MG   | 2A    | 3035 | 1/1   | 0.90 | 0.15 | -    | 37,37,37,37                 | 0     |
| 56  | MG   | 2A    | 3697 | 1/1   | 0.94 | 0.37 | -    | 35,35,35,35                 | 0     |
| 56  | MG   | 1A    | 8047 | 1/1   | 0.97 | 0.30 | -    | 6,6,6,6                     | 0     |
| 56  | MG   | 1A    | 8306 | 1/1   | 0.94 | 0.14 | -    | 14,14,14,14                 | 0     |
| 56  | MG   | 2A    | 3701 | 1/1   | 0.94 | 0.22 | -    | 42,42,42,42                 | 0     |
| 56  | MG   | 1A    | 8535 | 1/1   | 0.99 | 0.07 | -    | 31,31,31,31                 | 0     |
| 56  | MG   | 2A    | 3273 | 1/1   | 0.86 | 0.27 | -    | 44,44,44,44                 | 0     |
| 56  | MG   | 2H    | 8001 | 1/1   | 0.64 | 0.56 | -    | 71,71,71,71                 | 0     |
| 56  | MG   | 2A    | 3201 | 1/1   | 0.62 | 0.29 | -    | 51,51,51,51                 | 0     |
| 56  | MG   | 2Q    | 202  | 1/1   | 0.98 | 0.15 | -    | 23,23,23,23                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56  | MG   | 2A    | 3730 | 1/1   | 0.91 | 0.23 | -    | 50,50,50,50                 | 0     |
| 56  | MG   | 2A    | 3226 | 1/1   | 0.93 | 0.22 | -    | 27,27,27,27                 | 0     |
| 56  | MG   | 1A    | 8139 | 1/1   | 0.96 | 0.19 | -    | 15,15,15,15                 | 0     |
| 56  | MG   | 2A    | 3109 | 1/1   | 0.92 | 0.21 | -    | 41,41,41,41                 | 0     |
| 56  | MG   | 1a    | 1792 | 1/1   | 0.91 | 0.10 | -    | 41,41,41,41                 | 0     |
| 56  | MG   | 2A    | 3958 | 1/1   | 0.81 | 0.26 | -    | 51,51,51,51                 | 0     |
| 56  | MG   | 2A    | 3339 | 1/1   | 0.85 | 0.12 | -    | 35,35,35,35                 | 0     |
| 56  | MG   | 1A    | 8252 | 1/1   | 0.83 | 0.23 | -    | 24,24,24,24                 | 0     |
| 56  | MG   | 2A    | 3153 | 1/1   | 0.94 | 0.19 | -    | 39,39,39,39                 | 0     |
| 56  | MG   | 1A    | 8454 | 1/1   | 0.98 | 0.09 | -    | 16,16,16,16                 | 0     |
| 56  | MG   | 1A    | 8325 | 1/1   | 0.94 | 0.19 | -    | 21,21,21,21                 | 0     |
| 56  | MG   | 2A    | 3481 | 1/1   | 0.94 | 0.14 | -    | 39,39,39,39                 | 0     |
| 56  | MG   | 13    | 102  | 1/1   | 0.96 | 0.21 | -    | 20,20,20,20                 | 0     |
| 56  | MG   | 1A    | 8078 | 1/1   | 0.98 | 0.15 | -    | 9,9,9,9                     | 0     |
| 56  | MG   | 2A    | 3628 | 1/1   | 0.88 | 0.16 | -    | 59,59,59,59                 | 0     |
| 56  | MG   | 1A    | 8681 | 1/1   | 0.96 | 0.15 | -    | 32,32,32,32                 | 0     |
| 56  | MG   | 2A    | 3728 | 1/1   | 0.89 | 0.12 | -    | 56,56,56,56                 | 0     |
| 56  | MG   | 1A    | 8414 | 1/1   | 0.95 | 0.06 | -    | 35,35,35,35                 | 0     |
| 56  | MG   | 1A    | 8322 | 1/1   | 0.94 | 0.16 | -    | 45,45,45,45                 | 0     |
| 56  | MG   | 2A    | 3537 | 1/1   | 0.93 | 0.15 | -    | 33,33,33,33                 | 0     |
| 56  | MG   | 2A    | 3616 | 1/1   | 0.96 | 0.15 | -    | 39,39,39,39                 | 0     |
| 56  | MG   | 2A    | 3562 | 1/1   | 0.94 | 0.20 | -    | 33,33,33,33                 | 0     |
| 56  | MG   | 1a    | 1719 | 1/1   | 0.97 | 0.20 | -    | 35,35,35,35                 | 0     |
| 56  | MG   | 10    | 102  | 1/1   | 0.98 | 0.11 | -    | 19,19,19,19                 | 0     |
| 56  | MG   | 1a    | 1741 | 1/1   | 0.92 | 0.17 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | 1A    | 8963 | 1/1   | 0.95 | 0.36 | -    | 14,14,14,14                 | 0     |
| 56  | MG   | 1A    | 8206 | 1/1   | 0.88 | 0.31 | -    | 18,18,18,18                 | 0     |
| 56  | MG   | 1A    | 8168 | 1/1   | 0.90 | 0.14 | -    | 23,23,23,23                 | 0     |
| 56  | MG   | 2A    | 3022 | 1/1   | 0.95 | 0.30 | -    | 29,29,29,29                 | 0     |
| 56  | MG   | 2a    | 1755 | 1/1   | 0.79 | 0.15 | -    | 52,52,52,52                 | 0     |
| 56  | MG   | 1A    | 8265 | 1/1   | 0.95 | 0.16 | -    | 18,18,18,18                 | 0     |
| 56  | MG   | 1A    | 8656 | 1/1   | 0.94 | 0.08 | -    | 22,22,22,22                 | 0     |
| 56  | MG   | 2A    | 3486 | 1/1   | 0.82 | 0.22 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | 2a    | 1622 | 1/1   | 0.83 | 0.25 | -    | 59,59,59,59                 | 0     |
| 56  | MG   | 1A    | 8423 | 1/1   | 0.81 | 0.11 | -    | 28,28,28,28                 | 0     |
| 56  | MG   | 1W    | 3003 | 1/1   | 0.96 | 0.12 | -    | 12,12,12,12                 | 0     |
| 56  | MG   | 2A    | 3018 | 1/1   | 0.89 | 0.25 | -    | 55,55,55,55                 | 0     |
| 56  | MG   | 1A    | 8394 | 1/1   | 0.95 | 0.09 | -    | 37,37,37,37                 | 0     |
| 56  | MG   | 1A    | 8819 | 1/1   | 0.95 | 0.22 | -    | 20,20,20,20                 | 0     |
| 56  | MG   | 2A    | 3059 | 1/1   | 0.95 | 0.12 | -    | 21,21,21,21                 | 0     |
| 56  | MG   | 1a    | 1738 | 1/1   | 0.97 | 0.12 | -    | 43,43,43,43                 | 0     |
| 56  | MG   | 15    | 108  | 1/1   | 0.95 | 0.16 | -    | 28,28,28,28                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56  | MG   | 2A    | 3660 | 1/1   | 0.76 | 0.27 | -    | 51,51,51,51                 | 0     |
| 56  | MG   | 2B    | 3015 | 1/1   | 0.66 | 0.25 | -    | 59,59,59,59                 | 0     |
| 56  | MG   | 2a    | 1671 | 1/1   | 0.96 | 0.11 | -    | 34,34,34,34                 | 0     |
| 56  | MG   | 2a    | 1704 | 1/1   | 0.94 | 0.45 | -    | 38,38,38,38                 | 0     |
| 56  | MG   | 2A    | 3645 | 1/1   | 0.95 | 0.31 | -    | 29,29,29,29                 | 0     |
| 56  | MG   | 2A    | 3810 | 1/1   | 0.73 | 0.11 | -    | 53,53,53,53                 | 0     |
| 56  | MG   | 2A    | 3542 | 1/1   | 0.94 | 0.15 | -    | 23,23,23,23                 | 0     |
| 56  | MG   | 2a    | 1681 | 1/1   | 0.88 | 0.18 | -    | 45,45,45,45                 | 0     |
| 56  | MG   | 1A    | 8123 | 1/1   | 0.81 | 0.67 | -    | 22,22,22,22                 | 0     |
| 56  | MG   | 2A    | 3798 | 1/1   | 0.73 | 0.20 | -    | 59,59,59,59                 | 0     |
| 56  | MG   | 1a    | 1762 | 1/1   | 0.81 | 0.07 | -    | 54,54,54,54                 | 0     |
| 56  | MG   | 1A    | 8053 | 1/1   | 0.97 | 0.07 | -    | 11,11,11,11                 | 0     |
| 56  | MG   | 2A    | 3720 | 1/1   | 0.60 | 0.32 | -    | 60,60,60,60                 | 0     |
| 56  | MG   | 2A    | 3705 | 1/1   | 0.86 | 0.18 | -    | 48,48,48,48                 | 0     |
| 56  | MG   | 1A    | 8362 | 1/1   | 0.96 | 0.06 | -    | 52,52,52,52                 | 0     |
| 56  | MG   | 1A    | 8343 | 1/1   | 0.95 | 0.12 | -    | 12,12,12,12                 | 0     |
| 56  | MG   | 1e    | 201  | 1/1   | 0.96 | 0.10 | -    | 28,28,28,28                 | 0     |
| 56  | MG   | 2A    | 3766 | 1/1   | 0.89 | 0.12 | -    | 41,41,41,41                 | 0     |
| 56  | MG   | 2A    | 3691 | 1/1   | 0.97 | 0.15 | -    | 29,29,29,29                 | 0     |
| 56  | MG   | 1A    | 8857 | 1/1   | 0.86 | 0.18 | -    | 44,44,44,44                 | 0     |
| 56  | MG   | 2a    | 1644 | 1/1   | 0.92 | 0.17 | -    | 46,46,46,46                 | 0     |
| 56  | MG   | 2A    | 3508 | 1/1   | 0.94 | 0.12 | -    | 44,44,44,44                 | 0     |
| 56  | MG   | 2A    | 3885 | 1/1   | 0.68 | 0.17 | -    | 55,55,55,55                 | 0     |
| 56  | MG   | 2x    | 111  | 1/1   | 0.78 | 0.15 | -    | 67,67,67,67                 | 0     |
| 56  | MG   | 2A    | 3511 | 1/1   | 0.98 | 0.13 | -    | 39,39,39,39                 | 0     |
| 56  | MG   | 1A    | 8067 | 1/1   | 0.96 | 0.18 | -    | 10,10,10,10                 | 0     |
| 56  | MG   | 2A    | 3609 | 1/1   | 0.91 | 0.12 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | 27    | 101  | 1/1   | 0.96 | 0.35 | -    | 39,39,39,39                 | 0     |
| 56  | MG   | 1A    | 8376 | 1/1   | 0.96 | 0.07 | -    | 14,14,14,14                 | 0     |
| 56  | MG   | 2A    | 3556 | 1/1   | 0.91 | 0.15 | -    | 49,49,49,49                 | 0     |
| 56  | MG   | 2A    | 3383 | 1/1   | 0.93 | 0.17 | -    | 27,27,27,27                 | 0     |
| 56  | MG   | 2A    | 3644 | 1/1   | 0.89 | 0.07 | -    | 40,40,40,40                 | 0     |
| 56  | MG   | 2a    | 1782 | 1/1   | 0.92 | 0.48 | -    | 61,61,61,61                 | 0     |
| 56  | MG   | 2a    | 1753 | 1/1   | 0.79 | 0.20 | -    | 57,57,57,57                 | 0     |
| 56  | MG   | 2A    | 3793 | 1/1   | 0.89 | 0.16 | -    | 34,34,34,34                 | 0     |
| 56  | MG   | 1A    | 8618 | 1/1   | 0.90 | 0.29 | -    | 41,41,41,41                 | 0     |
| 56  | MG   | 1A    | 8719 | 1/1   | 0.91 | 0.14 | -    | 9,9,9,9                     | 0     |
| 56  | MG   | 1a    | 1704 | 1/1   | 0.88 | 0.17 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | 1A    | 8850 | 1/1   | 0.94 | 0.33 | -    | 34,34,34,34                 | 0     |
| 56  | MG   | 1A    | 8084 | 1/1   | 0.95 | 0.20 | -    | 23,23,23,23                 | 0     |
| 56  | MG   | 2a    | 1757 | 1/1   | 0.92 | 0.26 | -    | 55,55,55,55                 | 0     |
| 56  | MG   | 2A    | 3478 | 1/1   | 0.93 | 0.15 | -    | 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    | 3125 | 1/1   | 0.79 | 0.87 | -    | 39,39,39,39                 | 0     |
| 56  | MG   | 1A    | 8829 | 1/1   | 0.90 | 0.34 | -    | 42,42,42,42                 | 0     |
| 56  | MG   | 1B    | 3024 | 1/1   | 0.97 | 0.13 | -    | 18,18,18,18                 | 0     |
| 56  | MG   | 1Q    | 204  | 1/1   | 0.97 | 0.07 | -    | 20,20,20,20                 | 0     |
| 56  | MG   | 1B    | 3011 | 1/1   | 0.90 | 0.08 | -    | 39,39,39,39                 | 0     |
| 56  | MG   | 1A    | 8463 | 1/1   | 0.94 | 0.18 | -    | 7,7,7,7                     | 0     |
| 56  | MG   | 2a    | 1610 | 1/1   | 0.52 | 0.81 | -    | 63,63,63,63                 | 0     |
| 56  | MG   | 1A    | 8261 | 1/1   | 0.87 | 0.16 | -    | 55,55,55,55                 | 0     |
| 56  | MG   | 2A    | 3066 | 1/1   | 0.92 | 0.17 | -    | 26,26,26,26                 | 0     |
| 56  | MG   | 2B    | 3002 | 1/1   | 0.50 | 0.20 | -    | 60,60,60,60                 | 0     |
| 56  | MG   | 2A    | 3769 | 1/1   | 0.92 | 0.07 | -    | 31,31,31,31                 | 0     |
| 56  | MG   | 2B    | 3012 | 1/1   | 0.94 | 0.14 | -    | 52,52,52,52                 | 0     |
| 56  | MG   | 1A    | 8219 | 1/1   | 0.97 | 0.38 | -    | 12,12,12,12                 | 0     |
| 56  | MG   | 1a    | 1663 | 1/1   | 0.94 | 0.14 | -    | 51,51,51,51                 | 0     |
| 56  | MG   | 2A    | 3818 | 1/1   | 0.97 | 0.25 | -    | 44,44,44,44                 | 0     |
| 56  | MG   | 1A    | 8503 | 1/1   | 0.97 | 0.04 | -    | 23,23,23,23                 | 0     |
| 56  | MG   | 2A    | 3627 | 1/1   | 0.95 | 0.19 | -    | 55,55,55,55                 | 0     |
| 56  | MG   | 1a    | 1693 | 1/1   | 0.97 | 0.10 | -    | 29,29,29,29                 | 0     |
| 56  | MG   | 1x    | 3004 | 1/1   | 0.93 | 0.09 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | 2A    | 3452 | 1/1   | 0.85 | 0.09 | -    | 34,34,34,34                 | 0     |
| 56  | MG   | 2A    | 3471 | 1/1   | 0.98 | 0.12 | -    | 35,35,35,35                 | 0     |
| 56  | MG   | 1A    | 8240 | 1/1   | 0.85 | 0.20 | -    | 13,13,13,13                 | 0     |
| 56  | MG   | 2A    | 3531 | 1/1   | 0.96 | 0.17 | -    | 36,36,36,36                 | 0     |
| 56  | MG   | 1A    | 8400 | 1/1   | 0.97 | 0.25 | -    | 42,42,42,42                 | 0     |
| 56  | MG   | 10    | 108  | 1/1   | 0.96 | 0.13 | -    | 35,35,35,35                 | 0     |
| 56  | MG   | 10    | 107  | 1/1   | 0.88 | 0.10 | -    | 36,36,36,36                 | 0     |
| 56  | MG   | 1a    | 1790 | 1/1   | 0.93 | 0.13 | -    | 46,46,46,46                 | 0     |
| 56  | MG   | 2A    | 3539 | 1/1   | 0.84 | 0.19 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | 15    | 106  | 1/1   | 0.89 | 0.34 | -    | 20,20,20,20                 | 0     |
| 56  | MG   | 2A    | 3236 | 1/1   | 0.94 | 0.39 | -    | 46,46,46,46                 | 0     |
| 56  | MG   | 2A    | 3569 | 1/1   | 0.93 | 0.08 | -    | 43,43,43,43                 | 0     |
| 56  | MG   | 2A    | 3737 | 1/1   | 0.89 | 0.19 | -    | 44,44,44,44                 | 0     |
| 56  | MG   | 2A    | 3303 | 1/1   | 0.89 | 0.11 | -    | 30,30,30,30                 | 0     |
| 56  | MG   | 2A    | 3762 | 1/1   | 0.94 | 0.17 | -    | 44,44,44,44                 | 0     |
| 56  | MG   | 2A    | 3473 | 1/1   | 0.96 | 0.27 | -    | 51,51,51,51                 | 0     |
| 56  | MG   | 1A    | 8205 | 1/1   | 0.78 | 0.21 | -    | 25,25,25,25                 | 0     |
| 56  | MG   | 10    | 103  | 1/1   | 0.94 | 0.22 | -    | 21,21,21,21                 | 0     |
| 56  | MG   | 2a    | 1783 | 1/1   | 0.69 | 0.11 | -    | 59,59,59,59                 | 0     |
| 56  | MG   | 2A    | 3519 | 1/1   | 0.87 | 0.20 | -    | 31,31,31,31                 | 0     |
| 56  | MG   | 1A    | 8896 | 1/1   | 0.92 | 0.10 | -    | 35,35,35,35                 | 0     |
| 56  | MG   | 2A    | 3165 | 1/1   | 0.82 | 0.28 | -    | 42,42,42,42                 | 0     |
| 56  | MG   | 1A    | 8867 | 1/1   | 0.95 | 0.12 | -    | 55,55,55,55                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|----------------------------|-------|
| 56  | MG   | 1a    | 1714 | 1/1   | 0.85 | 0.09 | -    | 42,42,42,42                | 0     |
| 56  | MG   | 2B    | 3009 | 1/1   | 0.86 | 0.21 | -    | 67,67,67,67                | 0     |
| 56  | MG   | 2a    | 1670 | 1/1   | 0.90 | 0.23 | -    | 53,53,53,53                | 0     |
| 56  | MG   | 1a    | 1674 | 1/1   | 0.98 | 0.15 | -    | 40,40,40,40                | 0     |
| 56  | MG   | 1A    | 8441 | 1/1   | 0.99 | 0.05 | -    | 16,16,16,16                | 0     |
| 56  | MG   | 2a    | 1673 | 1/1   | 0.97 | 0.05 | -    | 33,33,33,33                | 0     |
| 56  | MG   | 2A    | 3224 | 1/1   | 0.77 | 0.29 | -    | 48,48,48,48                | 0     |
| 56  | MG   | 2A    | 3433 | 1/1   | 0.65 | 0.14 | -    | 43,43,43,43                | 0     |
| 56  | MG   | 1A    | 8273 | 1/1   | 0.94 | 0.10 | -    | 32,32,32,32                | 0     |
| 56  | MG   | 1A    | 8734 | 1/1   | 0.82 | 0.14 | -    | 22,22,22,22                | 0     |
| 56  | MG   | 1A    | 8160 | 1/1   | 0.94 | 0.10 | -    | 20,20,20,20                | 0     |
| 56  | MG   | 2A    | 3635 | 1/1   | 0.95 | 0.10 | -    | 36,36,36,36                | 0     |
| 56  | MG   | 2A    | 3258 | 1/1   | 0.93 | 0.17 | -    | 36,36,36,36                | 0     |
| 56  | MG   | 1A    | 8263 | 1/1   | 0.85 | 0.14 | -    | 26,26,26,26                | 0     |
| 56  | MG   | 2a    | 1624 | 1/1   | 0.88 | 0.50 | -    | 48,48,48,48                | 0     |
| 56  | MG   | 2a    | 1664 | 1/1   | 0.73 | 0.13 | -    | 44,44,44,44                | 0     |
| 56  | MG   | 1A    | 8211 | 1/1   | 0.95 | 0.38 | -    | 15,15,15,15                | 0     |
| 56  | MG   | 2A    | 3747 | 1/1   | 0.86 | 0.29 | -    | 39,39,39,39                | 0     |
| 56  | MG   | 1A    | 8040 | 1/1   | 0.91 | 0.32 | -    | 32,32,32,32                | 0     |
| 56  | MG   | 1B    | 3001 | 1/1   | 0.83 | 0.15 | -    | 37,37,37,37                | 0     |
| 56  | MG   | 2a    | 1698 | 1/1   | 0.96 | 0.27 | -    | 40,40,40,40                | 0     |
| 56  | MG   | 2a    | 1790 | 1/1   | 0.91 | 0.15 | -    | 51,51,51,51                | 0     |
| 56  | MG   | 1A    | 8237 | 1/1   | 0.83 | 0.22 | -    | 41,41,41,41                | 0     |
| 56  | MG   | 1a    | 1709 | 1/1   | 0.99 | 0.08 | -    | 30,30,30,30                | 0     |
| 56  | MG   | 2a    | 1666 | 1/1   | 0.90 | 0.16 | -    | 55,55,55,55                | 0     |
| 56  | MG   | 2A    | 3754 | 1/1   | 0.93 | 0.28 | -    | 36,36,36,36                | 0     |
| 56  | MG   | 2A    | 3098 | 1/1   | 0.73 | 1.60 | -    | 62,62,62,62                | 0     |
| 56  | MG   | 2A    | 3126 | 1/1   | 0.94 | 0.15 | -    | 32,32,32,32                | 0     |
| 56  | MG   | 2a    | 1707 | 1/1   | 0.85 | 0.22 | -    | 61,61,61,61                | 0     |
| 56  | MG   | 1A    | 8545 | 1/1   | 0.96 | 0.11 | -    | 33,33,33,33                | 0     |
| 56  | MG   | 2A    | 3031 | 1/1   | 0.92 | 0.49 | -    | 27,27,27,27                | 0     |
| 56  | MG   | 2A    | 3817 | 1/1   | 0.83 | 0.56 | -    | 52,52,52,52                | 0     |
| 56  | MG   | 2A    | 3093 | 1/1   | 0.72 | 0.42 | -    | 61,61,61,61                | 0     |
| 56  | MG   | 2a    | 1726 | 1/1   | 0.83 | 0.09 | -    | 51,51,51,51                | 0     |
| 56  | MG   | 1A    | 8500 | 1/1   | 0.94 | 0.18 | -    | 45,45,45,45                | 0     |
| 56  | MG   | 1a    | 1743 | 1/1   | 0.91 | 0.15 | -    | 41,41,41,41                | 0     |
| 56  | MG   | 1A    | 8229 | 1/1   | 0.98 | 0.13 | -    | 21,21,21,21                | 0     |
| 56  | MG   | 1A    | 8090 | 1/1   | 0.96 | 0.09 | -    | 36,36,36,36                | 0     |
| 56  | MG   | 2A    | 3876 | 1/1   | 0.95 | 0.53 | -    | 30,30,30,30                | 0     |
| 56  | MG   | 2A    | 3103 | 1/1   | 0.93 | 0.22 | -    | 30,30,30,30                | 0     |
| 56  | MG   | 2A    | 3454 | 1/1   | 0.97 | 0.09 | -    | 28,28,28,28                | 0     |
| 56  | MG   | 1A    | 8177 | 1/1   | 0.90 | 0.55 | -    | 55,55,55,55                | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56  | MG   | 1A    | 8327 | 1/1   | 0.94 | 0.17 | -    | 32,32,32,32                 | 0     |
| 56  | MG   | 1A    | 8062 | 1/1   | 0.97 | 0.18 | -    | 13,13,13,13                 | 0     |
| 56  | MG   | 1a    | 1781 | 1/1   | 0.42 | 0.24 | -    | 68,68,68,68                 | 0     |
| 56  | MG   | 2a    | 1756 | 1/1   | 0.94 | 0.13 | -    | 38,38,38,38                 | 0     |
| 56  | MG   | 2A    | 3722 | 1/1   | 0.89 | 0.12 | -    | 42,42,42,42                 | 0     |
| 56  | MG   | 2a    | 1739 | 1/1   | 0.94 | 0.14 | -    | 48,48,48,48                 | 0     |
| 56  | MG   | 2A    | 3401 | 1/1   | 0.92 | 0.15 | -    | 38,38,38,38                 | 0     |
| 56  | MG   | 2a    | 1689 | 1/1   | 0.90 | 0.16 | -    | 41,41,41,41                 | 0     |
| 56  | MG   | 1A    | 8251 | 1/1   | 0.86 | 0.19 | -    | 33,33,33,33                 | 0     |
| 56  | MG   | 1a    | 1783 | 1/1   | 0.80 | 0.39 | -    | 60,60,60,60                 | 0     |
| 56  | MG   | 2A    | 3415 | 1/1   | 0.91 | 0.31 | -    | 34,34,34,34                 | 0     |
| 56  | MG   | 2A    | 3751 | 1/1   | 0.94 | 0.21 | -    | 32,32,32,32                 | 0     |
| 56  | MG   | 2A    | 3521 | 1/1   | 0.92 | 0.19 | -    | 34,34,34,34                 | 0     |
| 56  | MG   | 2A    | 3434 | 1/1   | 0.70 | 0.13 | -    | 34,34,34,34                 | 0     |
| 56  | MG   | 1A    | 8243 | 1/1   | 0.97 | 0.17 | -    | 17,17,17,17                 | 0     |
| 56  | MG   | 2D    | 303  | 1/1   | 0.97 | 0.17 | -    | 25,25,25,25                 | 0     |
| 56  | MG   | 2A    | 3449 | 1/1   | 0.98 | 0.20 | -    | 25,25,25,25                 | 0     |
| 56  | MG   | 1A    | 8906 | 1/1   | 0.93 | 0.13 | -    | 13,13,13,13                 | 0     |
| 56  | MG   | 1A    | 8715 | 1/1   | 0.94 | 0.11 | -    | 17,17,17,17                 | 0     |
| 56  | MG   | 2A    | 3200 | 1/1   | 0.88 | 0.22 | -    | 21,21,21,21                 | 0     |
| 59  | K    | 2A    | 3001 | 1/1   | 0.93 | 0.17 | -    | 65,65,65,65                 | 0     |
| 56  | MG   | 1A    | 8152 | 1/1   | 0.91 | 0.09 | -    | 28,28,28,28                 | 0     |
| 56  | MG   | 2A    | 3865 | 1/1   | 0.93 | 0.16 | -    | 48,48,48,48                 | 0     |
| 56  | MG   | 2A    | 3379 | 1/1   | 0.91 | 0.11 | -    | 36,36,36,36                 | 0     |
| 56  | MG   | 2A    | 3500 | 1/1   | 0.86 | 0.33 | -    | 45,45,45,45                 | 0     |
| 56  | MG   | 1A    | 8250 | 1/1   | 0.85 | 0.51 | -    | 50,50,50,50                 | 0     |
| 56  | MG   | 1A    | 8054 | 1/1   | 0.92 | 0.16 | -    | 9,9,9,9                     | 0     |
| 56  | MG   | 1a    | 1728 | 1/1   | 0.93 | 0.10 | -    | 38,38,38,38                 | 0     |
| 56  | MG   | 2A    | 3037 | 1/1   | 0.90 | 0.17 | -    | 50,50,50,50                 | 0     |
| 56  | MG   | 2A    | 3904 | 1/1   | 0.96 | 0.29 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | 2a    | 1804 | 1/1   | 0.87 | 0.23 | -    | 65,65,65,65                 | 0     |
| 56  | MG   | 1A    | 8599 | 1/1   | 0.93 | 0.15 | -    | 24,24,24,24                 | 0     |
| 56  | MG   | 2a    | 1696 | 1/1   | 0.87 | 0.19 | -    | 36,36,36,36                 | 0     |
| 56  | MG   | 2A    | 3051 | 1/1   | 0.89 | 0.23 | -    | 29,29,29,29                 | 0     |
| 56  | MG   | 1a    | 1795 | 1/1   | 0.82 | 0.10 | -    | 52,52,52,52                 | 0     |
| 56  | MG   | 1a    | 1706 | 1/1   | 0.95 | 0.08 | -    | 27,27,27,27                 | 0     |
| 56  | MG   | 1a    | 1758 | 1/1   | 0.83 | 0.14 | -    | 38,38,38,38                 | 0     |
| 56  | MG   | 2A    | 3223 | 1/1   | 0.82 | 0.19 | -    | 52,52,52,52                 | 0     |
| 59  | K    | 1x    | 3001 | 1/1   | 0.94 | 0.16 | -    | 46,46,46,46                 | 0     |
| 56  | MG   | 1A    | 8447 | 1/1   | 0.89 | 0.21 | -    | 13,13,13,13                 | 0     |
| 56  | MG   | 2A    | 3936 | 1/1   | 0.94 | 0.12 | -    | 20,20,20,20                 | 0     |
| 56  | MG   | 2a    | 1741 | 1/1   | 0.84 | 0.09 | -    | 61,61,61,61                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56  | MG   | 1A    | 8372 | 1/1   | 0.94 | 0.08 | -    | 51,51,51,51                 | 0     |
| 56  | MG   | 1A    | 8174 | 1/1   | 0.93 | 0.13 | -    | 28,28,28,28                 | 0     |
| 56  | MG   | 2A    | 3235 | 1/1   | 0.89 | 0.32 | -    | 43,43,43,43                 | 0     |
| 56  | MG   | 1A    | 8012 | 1/1   | 0.90 | 0.12 | -    | 18,18,18,18                 | 0     |
| 56  | MG   | 1A    | 8630 | 1/1   | 0.78 | 0.19 | -    | 36,36,36,36                 | 0     |
| 56  | MG   | 2A    | 3234 | 1/1   | 0.81 | 0.20 | -    | 42,42,42,42                 | 0     |
| 56  | MG   | 1A    | 8616 | 1/1   | 0.90 | 0.27 | -    | 61,61,61,61                 | 0     |
| 56  | MG   | 2X    | 101  | 1/1   | 0.96 | 0.12 | -    | 33,33,33,33                 | 0     |
| 56  | MG   | 2A    | 3102 | 1/1   | 0.95 | 0.22 | -    | 29,29,29,29                 | 0     |
| 56  | MG   | 2A    | 3046 | 1/1   | 0.96 | 0.24 | -    | 26,26,26,26                 | 0     |
| 56  | MG   | 2B    | 3001 | 1/1   | 0.91 | 0.12 | -    | 59,59,59,59                 | 0     |
| 56  | MG   | 1A    | 8884 | 1/1   | 0.81 | 0.19 | -    | 65,65,65,65                 | 0     |
| 56  | MG   | 1A    | 8735 | 1/1   | 0.82 | 0.16 | -    | 15,15,15,15                 | 0     |
| 56  | MG   | 2A    | 3392 | 1/1   | 0.97 | 0.07 | -    | 35,35,35,35                 | 0     |
| 56  | MG   | 1A    | 8410 | 1/1   | 0.92 | 0.07 | -    | 35,35,35,35                 | 0     |
| 56  | MG   | 1A    | 8231 | 1/1   | 0.94 | 0.12 | -    | 25,25,25,25                 | 0     |
| 56  | MG   | 2g    | 3001 | 1/1   | 0.97 | 0.12 | -    | 52,52,52,52                 | 0     |
| 56  | MG   | 2a    | 1618 | 1/1   | 0.95 | 0.14 | -    | 38,38,38,38                 | 0     |
| 56  | MG   | 1a    | 1629 | 1/1   | 0.87 | 0.29 | -    | 36,36,36,36                 | 0     |
| 56  | MG   | 2A    | 3978 | 1/1   | 0.91 | 0.16 | -    | 41,41,41,41                 | 0     |
| 56  | MG   | 1A    | 8882 | 1/1   | 0.92 | 0.15 | -    | 38,38,38,38                 | 0     |
| 56  | MG   | 2a    | 1743 | 1/1   | 0.82 | 0.41 | -    | 41,41,41,41                 | 0     |
| 56  | MG   | 1a    | 1771 | 1/1   | 0.97 | 0.11 | -    | 46,46,46,46                 | 0     |
| 56  | MG   | 1A    | 8238 | 1/1   | 0.96 | 0.15 | -    | 19,19,19,19                 | 0     |
| 56  | MG   | 2A    | 3835 | 1/1   | 0.57 | 0.19 | -    | 40,40,40,40                 | 0     |
| 56  | MG   | 2A    | 3468 | 1/1   | 0.90 | 0.18 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | 2A    | 3210 | 1/1   | 0.93 | 0.15 | -    | 34,34,34,34                 | 0     |
| 56  | MG   | 1A    | 8195 | 1/1   | 0.95 | 0.23 | -    | 8,8,8,8                     | 0     |
| 56  | MG   | 1A    | 8865 | 1/1   | 0.89 | 0.20 | -    | 28,28,28,28                 | 0     |
| 56  | MG   | 1A    | 8419 | 1/1   | 0.86 | 0.20 | -    | 31,31,31,31                 | 0     |
| 56  | MG   | 1a    | 1688 | 1/1   | 0.99 | 0.12 | -    | 43,43,43,43                 | 0     |
| 56  | MG   | 2A    | 3184 | 1/1   | 0.97 | 0.20 | -    | 25,25,25,25                 | 0     |
| 56  | MG   | 2A    | 3050 | 1/1   | 0.89 | 0.21 | -    | 39,39,39,39                 | 0     |
| 56  | MG   | 2A    | 3576 | 1/1   | 0.75 | 0.27 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | 2a    | 1634 | 1/1   | 0.95 | 0.40 | -    | 54,54,54,54                 | 0     |
| 56  | MG   | 2A    | 3736 | 1/1   | 0.87 | 0.29 | -    | 51,51,51,51                 | 0     |
| 56  | MG   | 1A    | 8816 | 1/1   | 0.94 | 0.10 | -    | 12,12,12,12                 | 0     |
| 56  | MG   | 2U    | 202  | 1/1   | 0.94 | 0.37 | -    | 50,50,50,50                 | 0     |
| 56  | MG   | 1A    | 8333 | 1/1   | 0.94 | 0.16 | -    | 39,39,39,39                 | 0     |
| 56  | MG   | 1a    | 1664 | 1/1   | 0.94 | 0.17 | -    | 38,38,38,38                 | 0     |
| 56  | MG   | 2A    | 3970 | 1/1   | 0.97 | 0.42 | -    | 53,53,53,53                 | 0     |
| 56  | MG   | 2A    | 3567 | 1/1   | 0.91 | 0.11 | -    | 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    | 8907 | 1/1   | 0.90 | 0.35 | -    | 26,26,26,26                 | 0     |
| 56  | MG   | 1a    | 1815 | 1/1   | 0.81 | 0.17 | -    | 57,57,57,57                 | 0     |
| 56  | MG   | 2A    | 3772 | 1/1   | 0.82 | 0.25 | -    | 43,43,43,43                 | 0     |
| 56  | MG   | 2A    | 3598 | 1/1   | 0.94 | 0.09 | -    | 50,50,50,50                 | 0     |
| 56  | MG   | 1a    | 1750 | 1/1   | 0.91 | 0.20 | -    | 56,56,56,56                 | 0     |
| 56  | MG   | 1A    | 8262 | 1/1   | 0.96 | 0.28 | -    | 58,58,58,58                 | 0     |
| 56  | MG   | 1l    | 203  | 1/1   | 0.90 | 0.15 | -    | 56,56,56,56                 | 0     |
| 56  | MG   | 2A    | 3589 | 1/1   | 0.97 | 0.40 | -    | 30,30,30,30                 | 0     |
| 56  | MG   | 2A    | 3190 | 1/1   | 0.94 | 0.35 | -    | 32,32,32,32                 | 0     |
| 56  | MG   | 1A    | 8901 | 1/1   | 0.94 | 0.17 | -    | 34,34,34,34                 | 0     |
| 56  | MG   | 2A    | 3312 | 1/1   | 0.85 | 0.14 | -    | 25,25,25,25                 | 0     |
| 56  | MG   | 2a    | 1702 | 1/1   | 0.73 | 0.25 | -    | 54,54,54,54                 | 0     |
| 56  | MG   | 1a    | 1812 | 1/1   | 0.86 | 0.08 | -    | 35,35,35,35                 | 0     |
| 56  | MG   | 1A    | 8862 | 1/1   | 0.95 | 0.07 | -    | 42,42,42,42                 | 0     |
| 56  | MG   | 2A    | 3842 | 1/1   | 0.97 | 0.09 | -    | 48,48,48,48                 | 0     |
| 56  | MG   | 2A    | 3372 | 1/1   | 0.94 | 0.13 | -    | 48,48,48,48                 | 0     |
| 56  | MG   | 2A    | 3652 | 1/1   | 0.94 | 0.06 | -    | 43,43,43,43                 | 0     |
| 56  | MG   | 1A    | 8235 | 1/1   | 0.97 | 0.19 | -    | 9,9,9,9                     | 0     |
| 56  | MG   | 1A    | 8754 | 1/1   | 0.96 | 0.21 | -    | 18,18,18,18                 | 0     |
| 56  | MG   | 1A    | 8731 | 1/1   | 0.91 | 0.41 | -    | 40,40,40,40                 | 0     |
| 56  | MG   | 2a    | 1606 | 1/1   | 0.86 | 0.17 | -    | 35,35,35,35                 | 0     |
| 56  | MG   | 1A    | 8283 | 1/1   | 0.91 | 0.22 | -    | 13,13,13,13                 | 0     |
| 56  | MG   | 2A    | 3749 | 1/1   | 0.89 | 0.28 | -    | 50,50,50,50                 | 0     |
| 56  | MG   | 2A    | 3685 | 1/1   | 0.70 | 0.16 | -    | 50,50,50,50                 | 0     |
| 56  | MG   | 1A    | 8523 | 1/1   | 0.91 | 0.14 | -    | 23,23,23,23                 | 0     |
| 56  | MG   | 2A    | 3216 | 1/1   | 0.97 | 0.26 | -    | 28,28,28,28                 | 0     |
| 56  | MG   | 2a    | 1692 | 1/1   | 0.95 | 0.24 | -    | 44,44,44,44                 | 0     |
| 56  | MG   | 2a    | 1648 | 1/1   | 0.94 | 0.26 | -    | 33,33,33,33                 | 0     |
| 56  | MG   | 1A    | 8902 | 1/1   | 0.87 | 0.46 | -    | 51,51,51,51                 | 0     |
| 56  | MG   | 2A    | 3672 | 1/1   | 0.81 | 0.17 | -    | 46,46,46,46                 | 0     |
| 56  | MG   | 2A    | 3301 | 1/1   | 0.98 | 0.12 | -    | 52,52,52,52                 | 0     |
| 56  | MG   | 2A    | 3674 | 1/1   | 0.96 | 0.06 | -    | 32,32,32,32                 | 0     |
| 56  | MG   | 2A    | 3270 | 1/1   | 0.95 | 0.11 | -    | 20,20,20,20                 | 0     |
| 56  | MG   | 2a    | 1792 | 1/1   | 0.92 | 0.19 | -    | 55,55,55,55                 | 0     |
| 56  | MG   | 1A    | 8932 | 1/1   | 0.96 | 0.20 | -    | 21,21,21,21                 | 0     |
| 56  | MG   | 2B    | 3006 | 1/1   | 0.79 | 0.42 | -    | 48,48,48,48                 | 0     |
| 56  | MG   | 1A    | 8692 | 1/1   | 0.94 | 0.14 | -    | 19,19,19,19                 | 0     |
| 56  | MG   | 2A    | 3188 | 1/1   | 0.91 | 0.33 | -    | 33,33,33,33                 | 0     |
| 56  | MG   | 1A    | 8433 | 1/1   | 0.93 | 0.12 | -    | 14,14,14,14                 | 0     |
| 56  | MG   | 1B    | 3007 | 1/1   | 0.89 | 0.11 | -    | 37,37,37,37                 | 0     |
| 56  | MG   | 1x    | 3012 | 1/1   | 0.95 | 0.13 | -    | 38,38,38,38                 | 0     |
| 56  | MG   | 2A    | 3158 | 1/1   | 0.77 | 0.40 | -    | 40,40,40,40                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|----------------------------|-------|
| 56  | MG   | 2A    | 3072 | 1/1   | 0.75 | 0.23 | -    | 36,36,36,36                | 0     |
| 56  | MG   | 2A    | 3777 | 1/1   | 0.91 | 0.43 | -    | 61,61,61,61                | 0     |
| 56  | MG   | 2t    | 201  | 1/1   | 0.85 | 0.22 | -    | 46,46,46,46                | 0     |
| 56  | MG   | 2A    | 3238 | 1/1   | 0.95 | 0.12 | -    | 24,24,24,24                | 0     |
| 56  | MG   | 1A    | 8072 | 1/1   | 0.99 | 0.17 | -    | 11,11,11,11                | 0     |
| 56  | MG   | 1A    | 8515 | 1/1   | 0.95 | 0.10 | -    | 28,28,28,28                | 0     |
| 56  | MG   | 2A    | 3534 | 1/1   | 0.98 | 0.10 | -    | 35,35,35,35                | 0     |
| 56  | MG   | 2B    | 3003 | 1/1   | 0.95 | 0.08 | -    | 37,37,37,37                | 0     |
| 56  | MG   | 2A    | 3056 | 1/1   | 0.97 | 0.09 | -    | 29,29,29,29                | 0     |
| 56  | MG   | 1A    | 8600 | 1/1   | 0.91 | 0.33 | -    | 26,26,26,26                | 0     |
| 56  | MG   | 2A    | 3980 | 1/1   | 0.92 | 0.15 | -    | 51,51,51,51                | 0     |
| 56  | MG   | 2A    | 3413 | 1/1   | 0.85 | 0.19 | -    | 44,44,44,44                | 0     |
| 56  | MG   | 2A    | 3606 | 1/1   | 0.81 | 0.17 | -    | 42,42,42,42                | 0     |
| 56  | MG   | 1A    | 8694 | 1/1   | 0.97 | 0.06 | -    | 30,30,30,30                | 0     |
| 56  | MG   | 1A    | 8888 | 1/1   | 0.75 | 0.48 | -    | 62,62,62,62                | 0     |
| 56  | MG   | 1A    | 8814 | 1/1   | 0.85 | 0.07 | -    | 62,62,62,62                | 0     |
| 56  | MG   | 2S    | 201  | 1/1   | 0.95 | 0.14 | -    | 27,27,27,27                | 0     |
| 56  | MG   | 2a    | 1656 | 1/1   | 0.81 | 0.32 | -    | 65,65,65,65                | 0     |
| 56  | MG   | 2a    | 1803 | 1/1   | 0.88 | 0.10 | -    | 41,41,41,41                | 0     |
| 56  | MG   | 2A    | 3416 | 1/1   | 0.91 | 0.10 | -    | 28,28,28,28                | 0     |
| 56  | MG   | 1a    | 1804 | 1/1   | 0.82 | 0.14 | -    | 46,46,46,46                | 0     |

## 6.5 Other polymers

There are no such residues in this entry.